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

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ABSTRACT. In this paper we describe the propagation of singularities of tempered distributional solutions $u \in \mathcal{S}'$ of $(H-\lambda)u = 0$, 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' refers to a microlocal description of the lack of decay at infinity. Thus, we prove 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 $H - \lambda$, 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. We also analyze Lagrangian properties of this relation, which shows that the relation is not 'too large' in terms of its dimension.

1. INTRODUCTION

In this paper 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 prove 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 [19] for the wave equation in domains with corners. Indeed, in this case the propagation result itself, which was proved in [37], 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

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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 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. Note that these results only provide the answer as to where in phase space the singularities of generalized eigenfunctions may be located; they leave open the question of what these singularities are like, i.e. we do not have FIO-type results. Such results exist at least in certain 3-body settings [33, 9], see the remarks in the next section. In addition, we show that in our setting, if there are no bound states in any subsystems, then the broken bicharacteristic relation has the correct Lagrangian geometry to give rise to such FIO results. We also obtain a similar result on a certain natural part of the broken bicharacteristic relation under the assumption that the set of thresholds is discrete.

We also prove 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, [25]. In the Euclidean many-body setting this construction has been done by Skibsted [32] 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 [17], 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 [33, 9, 36], or indeed in many-body scattering under the additional assumption that there are no bound states in any subsystem [37]. 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 [32] 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 [14]. 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-matrices are (non-classical, if the potentials are long-range) pseudo-differential operators, which differ from the identity operator by operators of order -1 if the potentials are short range. 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).

It may seem that the (generalized) broken bicharacteristic relation is rather large since a single bicharacteristic can be continued in many ways after it hits a collision plane. In fact, this is not the case, since many bicharacteristics do not hit these collision planes at all. A more precise statement would be the that the wave front relation of the S-matrices is given by a union of Lagrangian submanifolds, so at least it has the same structure as if the S-matrices were (sums of) Fourier integral operators. Indeed, we prove that if there are no bound states in any subsystems, then the wave front relations of the S-matrices are given by *finite* unions of smooth Lagrangian relations, and we obtain a similar result on a part of the wave front relation under the assumption that the set of thresholds is discrete.

We remark that the results of this paper 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. [37]; instead, one needs to use the constructions of Isozaki-Kitada [17] (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 [12, 24] 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 [23]. 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.

Indeed, there is some freedom in the precise definition of the wave front set; see the remarks preceeding the statement of Theorem 2.2. The alternative definitions differ slightly, but agree for generalized eigenfunctions, and the corresponding propagation results are based on the same positive commutator estimates. Thus, the reader may find the explicit microlocal estimates of Section 7 particularly clear. However, piecing together these estimates to describe propagation is more cumbersome than making simple geometric statements based on wave front sets; for this reason we emphasize the latter.

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 [18], Gérard, Isozaki and Skibsted [6, 7] and Wang [38]. 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 [15, 16, 35] 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 [28, 29, 31, 30, 8, 2, 39]. In particular, Yafaev's paper [39] 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 [36, 37] and the present paper, and which is then used to prove asymptotic completeness.

We briefly outline of the positive commutator proofs. They consist of two parts: first, the construction of a symbol (and an associated pseudo-differential operator) that we claim has a microlocally positive commutator with H, when localized in energy, and second, the proof that the commutator is indeed positive in the appropriate part of the phase space. The first part has much in common with the analysis of generalized broken bicharacteristics, since both are intimately connected to various Hamilton vector fields associated to the subsystems. The second part is essentially a microlocal version of the proof of the Mourre estimate that was obtained by Froese and Herbst [5]. Indeed, we could follow the full indicial operator version of this proof, as was done in [36] and [37]. However, in the presence of bound states in the proper subsystems we would have to rely more heavily on the approximate product structure of the Hamiltonian at each cluster. Indeed, in the full geometric problem considered in [37], the L^2 eigenvalues and eigenfunctions of the indicial operator of H can vary as one moves along the collision planes, which makes even the description of the bicharacteristics more complicated. However, it turns out that in the Euclidean many-body setting, after an explicit calculation of the indicial operators, we can use the Mourre estimate explicitly in the normal (non-commutative) variables at each cluster, and use the standard Poisson bracket formula for the commutator in the tangential (commutative) variables. Since it eliminates the need to present arguments that are essentially simple (microlocal) modifications of the Froese-Herbst proof of the Mourre estimate, we adopt the second approach.

The structure of the paper is the following. In the next section we set up the framework of many-body scattering, mostly following the book of Dereziński and Gérard, [3], and we state the precise results on the propagation of singularities. In Section 3 we relate this to the Melrose's approach to scattering via compactification [23]. We also include in this section the outline of the resolved space construction and the definition of the algebra of many-body scattering differential operators from [37]. As we indicate in this section, from an algebraic point of view, it is the lack of commutativity of this algebra to 'top weight' (at infinity) that gives rise to the breaks in the generalized broken bicharacteristics along which singularities propagate. In Section 4 we recall the definition and basic properties of many-body scattering pseudo-differential operators as well as the definition of the corresponding wave front set from [37], and we analyze the characteristic variety of many-body Hamiltonians. Microlocal elliptic regularity is stated here in Corollary 4.3. In Section 5 we describe generalized broken bicharacteristics, and in Section 6 we explain the positive commutator argument that is the key to our propagation results. Propagation of singularities itself, stated in Theorem 2.2, is proved in Section 7. Sections 8-10 turn this result into theorems on the resolvent and the scattering matrices, stated in Theorems 2.4-2.10. Finally, in Appendix A we show that if the set of thresholds of H is discrete, or if H is a four-body Hamiltonian, generalized broken bicharacteristics are piecewise integral curves of the Hamilton vector fields, with only a finite number of breaks, and then in Appendix B we analyze the Lagrangian structure of the broken bicharacteristic relation.

Most results of this paper were announced in [34]; this paper contains the detailed proofs.

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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:

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

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 [23]. Thus, we let

$$\bar{X} = \bar{X}_0 = \mathbb{S}^n_+ \tag{2.3}$$

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 [23] that $\mathrm{RC} : \mathbb{R}^n \to \mathbb{S}^n_+$ is given by

$$\mathrm{RC}(w) = (1/(1+|w|^2)^{1/2}, w/(1+|w|^2)^{1/2}) \in \mathbb{S}^n_+ \subset \mathbb{R}^{n+1}, \quad w \in \mathbb{R}^n. \tag{2.4}$$

Here we use the notation RC instead of SP, used in [23], 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

$$\bar{X}_a = \mathrm{cl}(\mathrm{RC}(X_a)), \quad C_a = \bar{X}_a \cap \partial\mathbb{S}^n_+. \tag{2.5}$$

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

$$\mathcal{C} = \{C_a : \ a \in I\}. \tag{2.6}$$

Thus, $C_0 = \partial\mathbb{S}^n_+ = \mathbb{S}^{n-1}$, and $a \leq b$ if and only if $C_b \subset C_a$. Since throughout this paper we work in the Euclidean setting, where the notation X, X_a, etc., has been used for the (non-compact) vector spaces, we always use a bar, as in $\bar{X}$, $\bar{X}_a$, etc., to denote the corresponding compact spaces. In particular, even when talking about general compact manifolds with boundary in the following sections, recalling the results of [37], we will write them as $\bar{X}$.

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

$$C_{a,\mathrm{sing}} = \cup_{b \not\leq a}(C_b \cap C_a), \tag{2.7}$$

and its 'regular part' as the set

$$C'_a = C_a \setminus \cup_{b \not\leq a} C_b = C_a \setminus C_{a,\mathrm{sing}}. \tag{2.8}$$

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

$$S^m_{\mathrm{phg}}(\mathbb{S}^n_+) = x^{-m}\mathcal{C}^\infty(\mathbb{S}^n_+). \tag{2.9}$$

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

$$H^{k,l}_{\mathrm{sc}}(\mathbb{S}^n_+) = H^{k,l} = H^{k,l}(\mathbb{R}^n) = \langle w \rangle^{-l} H^k(\mathbb{R}^n) \tag{2.10}$$

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

$$H^a = \Delta + \sum_{b \leq a} V_b, \tag{2.11}$$

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

$$\Lambda_a = \cup_{b<a} \operatorname{spec}_{pp}(H^b) \tag{2.12}$$

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

$$\Lambda'_a = \Lambda_a \cup \operatorname{spec}_{pp}(H^a) = \cup_{b\leq a} \operatorname{spec}_{pp}(H^b). \tag{2.13}$$

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 $\operatorname{spec}_{pp}(H^a)$ can only accumulate at Λ_a. Moreover, $R(\lambda)$, considered as an operator on weighted Sobolev spaces, has a limit

$$R(\lambda \pm i0) : H^{k,l}_{\mathrm{sc}}(\mathbb{S}^n_+) \to H^{k+2,l'}_{\mathrm{sc}}(\mathbb{S}^n_+) \tag{2.14}$$

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

$$\Lambda = \Lambda_1 \cup \operatorname{spec}_{pp}(H). \tag{2.15}$$

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

$$\sum_{j=1}^n a_j \, dw_j \tag{2.16}$$

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 [23], 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 [23], 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

$${}^{\mathrm{sc}}\dot{T}^*\mathbb{S}^n_+ = \cup_a {}^{\mathrm{sc}}T^*_{C'_a}\bar{X}_a. \tag{2.17}$$

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 [24] and Lebeau [19] on the wave equation in domains with smooth boundaries or corners, respectively.

We also recall from [23] 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

$$\Sigma_b(\lambda) = \{\xi_b \in {}^{\mathrm{sc}}T^*_{C_b}\bar{X}_b : \ \lambda - |\xi_b|^2 \in \mathrm{spec}_{pp} H^b\} \subset {}^{\mathrm{sc}}T^*_{C_b}\bar{X}_b; \tag{2.18}$$

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

$$\dot{\Sigma}(\lambda) = \cup_a \dot{\Sigma}_a(\lambda), \qquad \dot{\Sigma}_a(\lambda) = \cup_{C_b \supset C_a} \pi_{ba}(\Sigma_b(\lambda)) \cap {}^{\mathrm{sc}}T^*_{C'_a}\bar{X}_a, \tag{2.19}$$

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 [37] 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.

$$2\langle w\rangle \xi \cdot \partial_w \in \mathcal{V}(T^*\mathbb{R}^n) = \mathcal{V}(\mathbb{R}^n \times \mathbb{R}^n) \tag{2.20}$$

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 [37], 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 ${}^{\mathrm{sc}}H_g^b$ of the metric g_b in the subsystem b. Thus, under the inclusion map

$$\imath_b : {}^{\mathrm{sc}}T^*_{C_b}\bar X_b \hookrightarrow {}^{\mathrm{sc}}T^*_{C_b}\mathbb{S}^n_+ \tag{2.21}$$

induced by the inclusion $X_b \hookrightarrow \mathbb{R}^n$ in the fibers, $(\imath_b)_*{}^{\mathrm{sc}}H_g^b = {}^{\mathrm{sc}}H_g$ (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 ${}^{\mathrm{sc}}H_g^b$ 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 $f \in \mathcal{C}^\infty({}^{\mathrm{sc}}T^*_{\mathbb{S}^{n-1}}\mathbb{S}^n_+)$,

$$D_\pm(f_\pi \circ \gamma)(t_0) \geq \inf\{{}^{\mathrm{sc}}H_g^b f(\tilde\xi_0) :\ \tilde\xi_0 \in \hat\pi_b^{-1}(\xi_0),\ C_a \subset C_b\}. \tag{2.22}$$

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, in Theorem 5.10 we prove the following. 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 [37], 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 [37]. There are several possible definitions of $\mathrm{WF}_{\mathrm{Sc}}$, all of which agree for generalized eigenfunctions of H, but the one given in [37] that is modelled on the fibred-cusp wave front set of Mazzeo and Melrose [20] enjoys many properties of the usual wave front set. A slightly different definition, for which the crucial property in the last line of (4.35) still holds, was discussed in [36]; this is the only essential property for the positive commutator estimates in this paper. Also, the discussion after (9.13) indicates why 'finite order' versions of the wave front set, i.e. versions in which we only require a fixed (though possibly high) number of the symbol estimates for ps.d.o.'s, somewhat akin to the constructions of [6], would be helpful; nonetheless, the Mazzeo-Melrose definition appears to be the most natural one from the point of view of general microlocal analysis.

We recall the precise definitions in Section 4; here we also translate our results into statements on the S-matrices where the usual wave front set can be used. We remark that 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, [23], 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. The definition of $\mathrm{WF}_{\mathrm{Sc}}(u)$ is more complicated, but if $u = \psi(H)v$ for some $\psi\in\mathcal{C}^\infty_c(\mathbb{R})$ (any other operator in $\Psi^{-\infty,0}_{\mathrm{Sc}}(\bar{X},\mathcal{C})$ would do instead of $\psi(H)$), then the following is a sufficient condition for $(\omega,\xi_a)\in {}^{\mathrm{sc}}T^*_{C'_a}\bar{X}_a$, considered as $C'_a\times X_a$, not to be in $\mathrm{WF}_{\mathrm{Sc}}(u)$. Suppose that there exists $\phi\in\mathcal{C}^\infty(\mathbb{S}^n_+)$, $\phi(\omega)\neq 0$, and $\rho\in\mathcal{C}^\infty_c(X_a)$, $\rho(\xi_a)\neq 0$, and $((\pi^a)^*\rho)\mathcal{F}(\phi u)\in\mathcal{S}(\mathbb{R}^n) = \mathcal{S}(X_0)$. Then $(\omega,\xi_a)\notin\mathrm{WF}_{\mathrm{Sc}}(u)$. 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, $(H-\lambda)u = 0$. Note that if $(H-\lambda)u=0$, then $u=\psi(H)u$ for $\psi\in\mathcal{C}^\infty_c(\mathbb{R})$, $\psi\equiv 1$ near λ, so the above description of $\mathrm{WF}_{\mathrm{Sc}}(u)$ is applicable.

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

$$\mathrm{WF}_{Sc}(u)\setminus\mathrm{WF}_{Sc}((H-\lambda)u) \tag{2.23}$$

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 ${}^{\mathrm{sc}}H^b_g(\tilde\xi_0) = 0$ 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

$$R_\pm(\lambda) = \{\xi = (\omega,\xi_a)\in {}^{\mathrm{sc}}T^*_{C'_a}\bar{X}_a :\ \exists b,\ C_a\subset C_b,\ \lambda-\tau(\xi)^2\in\mathrm{spec}_{pp}(H^b),\ \pm\tau(\xi) = |\xi_a|\} \tag{2.24}$$

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

$$\tau = -\frac{w\cdot\xi}{|w|}; \tag{2.25}$$

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, 33], see the remarks about this in [37]; 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

(2.26)
$$\begin{aligned}\Phi_+(K) =\{&\xi_0 \in \dot{\Sigma}(\lambda) :\ \exists \text{ a generalized broken bicharacteristic } \gamma : (-\infty, t_0] \to \dot{\Sigma}(\lambda) \\ &\text{s.t. } \gamma(t_0) = \xi_0,\ \overline{\gamma((-\infty, t_0])} \cap K \neq \emptyset\}.\end{aligned}$$

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,*

$$\mathrm{WF}_{Sc}(R(\lambda + i0)v) \subset \Phi_+(\mathrm{WF}_{Sc}(v)) \cup \Phi_+(R_-(\lambda)). \tag{2.27}$$

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 [35] 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 $g \in \mathcal{C}_c^\infty(C_a')$, there is a unique $u \in \mathcal{S}'(\mathbb{R}^n)$ such that $(H - \lambda)u = 0$, and u has the form

$$u = e^{-i\sqrt{\lambda - \epsilon_\alpha} r} r^{-\dim C_a/2} ((\pi^a)^* \psi_\alpha) v_- + R(\lambda + i0)f, \tag{2.28}$$

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

$$P_{\alpha,+}(\lambda) : \mathcal{C}_c^\infty(C_a') \to \mathcal{S}'(\mathbb{R}^n) \text{ defined by } P_{\alpha,+}(\lambda)g = u. \tag{2.29}$$

The term $R(\lambda + i0)f$ 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 [35] for the precise definitions.

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

$$I_a = \sum_{b \not\leq a} V_b,\ \tilde{I}_a = (r_a I_a)|_{C_a} \in \mathcal{C}^\infty(C_a), \tag{2.30}$$

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 (2.28) must be replaced by

$$e^{-i\sqrt{\lambda-\epsilon_\beta}r} r^{-\dim C_a/2} r^{i\tilde{I}_a/2\sqrt{\lambda-\epsilon_\alpha}}((\pi^a)^*\psi_\alpha)v_- \tag{2.31}$$

plus lower order terms; see Section 9 for details.

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

$$S_{\beta\alpha}(\lambda) = \frac{1}{2i\sqrt{\lambda-\epsilon_\beta}}((H-\lambda)\tilde{P}_{\beta,-}(\lambda))^* P_{\alpha,+}(\lambda), \tag{2.32}$$

$\lambda > \max(\epsilon_\alpha, \epsilon_\beta)$, $\lambda \notin \Lambda$. 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 [35]. 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 [17].

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 [32] 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 (2.32) and

$$P_{\alpha,+}(\lambda) = \tilde{P}_{\alpha,+}(\lambda) - R(\lambda + i0)(H-\lambda)\tilde{P}_{\alpha,+}(\lambda). \tag{2.33}$$

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 this paper we make the following assumption:

$$\text{either } \epsilon_\alpha \in \mathrm{spec}_d(H^a) \text{ and } \epsilon_\beta \in \mathrm{spec}_d(H^b), \text{ or } V_c \in \mathcal{S}(X^c) \text{ for all } c. \tag{2.34}$$

It is easy to describe the wave front set of $\tilde{P}_{\alpha,+}(\lambda)g$, $g \in \mathcal{C}_c^{-\infty}(C'_a)$, near its 'beginning point', i.e. near the $(\alpha,+)$-incoming set. Namely, it is the union of integral curves of ${}^{\mathrm{sc}}H_g^a$ (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

$$\tau_a = \sqrt{\lambda-\epsilon_\alpha}\cos(s-s_0),\ (y_a,\mu_a) = \sqrt{\lambda-\epsilon_\alpha}\sin(s-s_0)\exp((s-s_0){}^{\mathrm{sc}}H_g^a)(\zeta) \tag{2.35}$$

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 (2.33), 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 $\mathcal{R}_{\alpha,+} \subset \dot{\Sigma}(\lambda) \times S^*C'_a$ given by

$$\mathcal{R}_{\alpha,+} = \{(\zeta, \xi) \in \dot{\Sigma}(\lambda) \times S^*C'_a : \ \Phi_-(\{\xi\}) \cap \gamma_{\alpha,-}(\zeta) \neq \emptyset\}. \tag{2.36}$$

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, $\mathcal{R}_{\beta\alpha} \subset S^*C'_b \times S^*C'_a$ is defined as the composite relation of $\mathcal{R}_{\alpha,+}$ and $\mathcal{R}^{-1}_{\beta,-}$:

$$\mathcal{R}_{\beta\alpha} = \{(\zeta, \zeta') \in S^*C'_b \times S^*C'_a : \ \exists \xi \in \dot{\Sigma}(\lambda), (\zeta, \xi) \in \mathcal{R}_{\alpha,+}, \ (\zeta', \xi) \in \mathcal{R}_{\beta,-}\}. \tag{2.37}$$

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 $\mathcal{R} \subset B \times A$ is a relation, $K \subset A$, by $\mathcal{R}(K)$ we mean $\{\xi \in B : \ \exists \zeta \in K, \ (\xi, \zeta) \in \mathcal{R}\}$. Similarly, if $U \subset B$, by $\mathcal{R}^{-1}(U)$ we mean $\{\zeta \in A : \ \exists \xi \in U, \ (\xi, \zeta) \in \mathcal{R}\}$. 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

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

This definition, (2.33) and Theorem 2.4 immediately prove the following proposition.

Proposition 2.6. *Suppose that H is a many-body Hamiltonian, $\lambda \notin \Lambda$, and* (2.34) *holds. Suppose also that $g \in \mathcal{C}^\infty_c(C'_a)$. Then*

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

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

$$\mathrm{WF}_{Sc}(P_{\alpha,+}(\lambda)g) \setminus R_+(\lambda) \subset \Phi_+(R_-(\lambda)) \cup \mathcal{R}_{\alpha,+}(\mathrm{WF}(g)). \tag{2.39}$$

One of the main features of (2.38) 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, (2.32) 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* (2.34) *holds. Suppose $g \in \mathcal{C}^\infty_c(C'_a)$. Then $\mathrm{WF}(S_{\beta\alpha}(\lambda)g) \subset \mathcal{R}^{-1}_{\beta,-}(R_-(\lambda))$. 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 (2.34) holds. Then $S_{\beta\alpha}(\lambda)$ 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*

$$\mathrm{WF}(S_{\beta\alpha}(\lambda)g) \subset \mathcal{R}_{\beta,-}^{-1}(R_-(\lambda)) \cup \mathcal{R}_{\beta\alpha}(\mathrm{WF}(g)). \tag{2.40}$$

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 [37].

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.*

It may seem that our results are too weak in the sense that some broken bicharacteristics can be continued in many ways when they hit a collision plane. However, it should be noted that not every broken bicharacteristic hits a collision plane; indeed, if the dimension of a collision plane increases, more broken bicharacteristics will hit it, but each will generate a lower dimensional family of continuations. We can make this precise in terms of a Lagrangian characterization of the wave front relation of the S-matrices. To do so, recall first that the wave front relation of operators mapping $\mathcal{C}_c^\infty(C'_a)$ to $\mathcal{C}^{-\infty}(C'_b)$ is often understood as a subset of $T^*C'_b \times T^*C'_a \setminus 0$ corresponding to the wave front set of its Schwartz kernel, with the sign of the second component, the one in $T^*C'_a$, switched. For example, in this sense, the wave front relation of an FIO, say P, is given by a homogeneous canonical relation, i.e. by a Lagrangian submanifold $\tilde{\Lambda}$ of $T^*C'_b \times T^*C'_a$, Lagrangian with respect to the usual twisted symplectic form $\omega_b - \omega_a$, that is conic with respect to the diagonal $\mathbb{R}^+$ action in $T^*C'_b \times T^*C'_a$. Here ω_a denotes the canonical symplectic form on T^*C_a, etc. The wave front set mapping properties of such an operator are that Pu is defined if $(0 \times \mathrm{WF}(u)) \cap \tilde{\Lambda} = \emptyset$, and if Pu is thus defined,

$$\begin{aligned}\mathrm{WF}(Pu) \subset &\tilde{\Lambda}(\mathrm{WF}(u)) \cup \{\xi \in T^*C'_b \setminus 0 :\ (\xi, 0) \in \tilde{\Lambda}\}\\ &= \{\xi \in T^*C'_b \setminus 0 :\ (\xi, 0) \in \tilde{\Lambda} \text{ or } \exists \xi' \in \mathrm{WF}(u),\ (\xi, \xi') \in \tilde{\Lambda}\}.\end{aligned} \tag{2.41}$$

Note that $\mathrm{WF}(u)$ is a conic subset of $T^*C'_a$, so it is better to regard it as a subset of $S^*C'_a$ (quotient out by the $\mathbb{R}^+$ action on $T^*C'_a \setminus 0$); indeed, this is what we have done. But every element ζ of $S^*C'_a$ (thought of as the quotient bundle) has several representatives ξ in $T^*C'_a$. Correspondingly, the wave front relation, understood as a relation connecting $S^*C'_a$ and $S^*C'_b$, i.e. as a subset of $S^*C'_b \times S^*C'_a$, only determines the corresponding conic relation on $(T^*C'_b \setminus 0) \times (T^*C'_a \setminus 0)$ up to the rescaling of one factor with respect to the other. Thus, our results by themselves cannot pinpoint the wave front set of the Schwartz kernel of $S_{\beta\alpha}(\lambda)$ itself, only its image under the quotient map with respect to the $\mathbb{R}^+ \times \mathbb{R}^+$ action. Note, however, that $\tilde{\Lambda} \cap (T^*C'_b \times 0)$ and $\tilde{\Lambda} \cap (0 \times T^*C'_a)$ show up in the mapping properties of P, namely whether it can be applied to all distributions, and whether it maps smooth functions to smooth functions. Thus, by Theorem 2.8 we would expect, if $S_{\beta\alpha}(\lambda)$ were an FIO, that the (twisted) wave front set of its kernel lies in

$$(\mathcal{R}_{\beta,-}^{-1}(R_-(\lambda)) \times 0) \cup (0 \times \mathcal{R}_{\alpha,+}^{-1}(R_+(\lambda)) \cup \tilde{\Lambda}_0, \tag{2.42}$$

where $\tilde{\Lambda}_0 \subset (T^*C'_b \setminus 0) \times (T^*C'_a \setminus 0)$ is conic Lagrangian and projects to $\mathcal{R}_{\beta\alpha}$ under the quotient map in both factors. While, as explained, our results as stated do not prove that the wave front set of the kernel of $S_{\beta\alpha}(\lambda)$ lies in (2.42), we can prove its 'quotiented' version, at least if 0 is the only threshold of H, and obtain partial results if the set of thresholds is discrete.

To see what the expected result is, recall that if the set of thresholds is discrete, the generalized broken bicharacteristics are actually broken bicharacteristics with a finite number of breaks (and a uniform bound on this finite number). Correspondingly, we can associate to each generalized broken bicharacteristic one of a finite number of collision patterns which describe from which clusters in which sequence the bicharacteristics reflect, and along which collision plane at which kinetic energy they travel meanwhile. Each of these collision patterns can be described as a composition of smooth Lagrangian relations. If all the compositions are transversal, it follows automatically that the composite relation is also smooth and Lagrangian. (The other criteria for such a conclusion are automatically satisfied in our setting.) In Appendix B we show transversality if 0 is the only threshold, and discuss other cases when it holds. We briefly outline these below. First, however, we mention that even if the intersection fails to be transversal, and presumably fails to be clean as well, the composite relation can probably be described as a stratified space, since each of the elementary Lagrangians is algebraic. Such a treatment would, however, go beyond the scope of this paper, where the Lagrangian property is only used to illustrate the size of the broken bicharacteristic relation and to connect it to FIOs.

An important property of broken bicharacteristics is whether, upon breaking at C'_c, they become tangential to C'_c. We will say that a broken bicharacteristic has the *non-tangential breaking property* if it never becomes tangential to C'_c upon hitting it. Thus, a broken bicharacteristic γ having this property means that for all $t_0 \in \mathbb{R}$, $\gamma(t_0) \in {}^{\mathrm{sc}}T^*_{C'_c}\bar{X}_c$ implies that there exists a (small) $\epsilon > 0$, such that the inverse image of ${}^{\mathrm{sc}}T^*_{C'_c}\bar{X}_c$ under $\gamma|_{(t_0-\epsilon,t_0+\epsilon)}$ is either a single point, t_0, or it is the whole interval $(t_0-\epsilon, t_0+\epsilon)$ (hence $\gamma|_{(t_0-\epsilon,t_0+\epsilon)}$ maps into ${}^{\mathrm{sc}}T^*_{C'_c}\bar{X}_c$, is an integral curve of ${}^{\mathrm{sc}}H^c_g$, and in particular does not break). In the former case the broken bicharacteristic is said to be normal to C'_c, in the latter case it is said to be tangential. Note that if we replaced $(t_0-\epsilon, t_0+\epsilon)$ by $(t_0-\epsilon, t_0]$ or $[t_0, t_0+\epsilon)$, the conclusion would follow automatically since broken bicharacteristics are piecewise (projections of) integral curves of ${}^{\mathrm{sc}}H_g$. Thus, the non-tangential breaking property amounts to stating that broken bicharacteristics are normal both immediately prior to and immediately following a collision. Below, when we refer to the *non-tangential part of the broken bicharacteristic relation*, we mean the subset of $\mathcal{R}_{\beta\alpha}$, etc., which replaces 'generalized broken bicharacteristic' by 'non-tangentially breaking broken bicharacteristics' in Definition 2.3.

If there are no bound states in the proper subsystems, or indeed if $\Lambda_1 = \{0\}$, then by the conservation of kinetic energy, any broken bicharacteristic that has a break point ξ at C'_c, must either have been tangential both before and after the collision, and hence had actually no break at ξ, or both the incoming and the outgoing bicharacteristic segments are normal to C'_c. Thus, $\Lambda_1 = \{0\}$ implies that every broken bicharacteristic has the non-tangential breaking property. We prove in Appendix B that for each of the collision patterns, the non-tangentially breaking part of the corresponding relation, the composition of the smooth Lagrangian relations is indeed transversal, hence the composite gives a (typically not closed) conic

Lagrangian submanifold of $T^*(C'_b \times C'_a) \setminus 0$. We remark that under the absence of bound states assumption, the proof of the result is essentially the same as in the three-body setting [33, 9]; Hassell's proof employing Jacobi vector fields on the sphere is particularly easy (and transparent!) to adapt.

We thus prove the following theorem.

Theorem 2.10. *Suppose that H is a many-body Hamiltonian, $\lambda \notin \Lambda$, and (2.34) holds. Suppose also that Λ_1 is discrete. The part of the wave front relation of $S_{\beta\alpha}(\lambda)$ induced by non-tangential breaking broken bicharacteristics is a subset of the projection of a finite union of conic Lagrangian submanifolds of $T^*(C'_a \times C'_b) \setminus 0$, given by the broken bicharacteristic relation of H. Some of the Lagrangians may lie in $T^*C'_a \times 0$ or $0 \times T^*C'_b$ where 0 denotes the zero section.*

Corollary 2.11. *If $\Lambda_1 = \{0\}$, $\lambda > 0$, then the whole wave front relation of $S_{00}(\lambda)$ is a subset of the projection of a finite union of conic Lagrangian submanifolds of $T^*(C'_0 \times C'_0) \setminus 0$ as above.*

The statements of this theorem and corollary show that, e.g. if $\Lambda_1 = \{0\}$, the wave front relation of the S-matrix has the correct structure to be the wave front relation of a Fourier integral operator (FIO). However, the construction of such an FIO would require a much better understanding of the symplectic geometry of, and related analysis on, manifolds with corners that are equipped with certain boundary fibrations (corresponding to the resolved space $[\bar{X}; \mathcal{C}]$ and the fibration given by the blow-down map which are discussed in the next section). In relatively simple settings this has been discussed in [20, 10], but much progress is needed for dealing with the general case.

3. Scattering geometry and analysis

Next, we recall from [23] Melrose's definition of the Lie algebra of 'scattering vector fields' $\mathcal{V}_{\mathrm{sc}}(\bar{X})$, defined for every manifold with boundary $\bar{X}$. Thus,

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

where $\mathcal{V}_{\mathrm{b}}(\bar{X})$ is the set of smooth vector fields on $\bar{X}$ which are tangent to $\partial\bar{X}$. If $(x, y_1, \ldots, y_{n-1})$ are coordinates on $\bar{X}$ where x is a boundary defining function, then locally a basis of $\mathcal{V}_{\mathrm{sc}}(\bar{X})$ 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 ${}^{\mathrm{sc}}T\bar{X}$ over $\bar{X}$, called the scattering tangent bundle of $\bar{X}$, such that $\mathcal{V}_{\mathrm{sc}}(\bar{X})$ is the set of all smooth sections of ${}^{\mathrm{sc}}T\bar{X}$:

$$\mathcal{V}_{\mathrm{sc}}(\bar{X}) = \{v \in \mathcal{C}^\infty(\bar{X}; {}^{\mathrm{sc}}T\bar{X}) :\ \forall p \in \bar{X},\ v_p \in {}^{\mathrm{sc}}T_p\bar{X}\}. \tag{3.3}$$

The dual bundle of ${}^{\mathrm{sc}}T\bar{X}$ (called the scattering cotangent bundle) is denoted by ${}^{\mathrm{sc}}T^*\bar{X}$. Thus, covectors $v \in {}^{\mathrm{sc}}T^*_p\bar{X}$, p near $\partial\bar{X}$, 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 ${}^{\mathrm{sc}}T^*\bar{X}$ near $\partial\bar{X}$. The scattering density bundle ${}^{\mathrm{sc}}\Omega\bar{X}$ is the density bundle associated to ${}^{\mathrm{sc}}T^*\bar{X}$, so locally near $\partial\bar{X}$ it is spanned by $x^{-n-1}\,dx\,dy$ over $\mathcal{C}^\infty(\bar{X})$. Finally, $\mathrm{Diff}_{\mathrm{sc}}(\bar{X})$ is the algebra of differential operators generated by the vector fields in $\mathcal{V}_{\mathrm{sc}}(\bar{X})$; $\mathrm{Diff}^m_{\mathrm{sc}}(\bar{X})$ stands for scattering differential operators of order (at most) m.

An example is provided by the radial compactification of Euclidean space, $\bar{X} = \mathbb{S}^n_+$. 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 introduce local coordinates on $\bar{X}$ near $p \in \partial\bar{X}$ as above, and use these to identify the coordinate neighborhood U of p with a coordinate patch U' on the closed upper hemisphere $\mathbb{S}^n_+$ (which is just a closed ball) near its boundary. Such an identification preserves the scattering structure since this structure is completely natural. We further identify $\mathbb{S}^n_+$ with $\mathbb{R}^n$ via the radial compactification RC as in (2.4). 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, $V \in \mathcal{V}_{\mathrm{sc}}(\mathbb{S}^n_+)$ can be expressed as (ignoring the lifting in the notation)

$$V = \sum_{j=1}^{n} a_j \partial_{w_j}, \quad a_j \in \mathcal{C}^\infty(\mathbb{S}^n_+). \tag{3.5}$$

As mentioned above, $a_j \in \mathcal{C}^\infty(\mathbb{S}^n_+)$ is equivalent to requiring that $\mathrm{RC}^*\, a_j$ 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 $\mathrm{Diff}^2_{\mathrm{sc}}(\mathbb{S}^n_+)$, and that ${}^{\mathrm{sc}}\Omega\mathbb{S}^n_+$ is spanned by the pull-back of the standard Euclidean density $|dw|$. In terms of the 'inverted' polar coordinates on $\mathbb{R}^n$, covectors $\xi \cdot dw = \sum_j \xi_j\, dw_j$ 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 orthogonal 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.

We next show 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 blow-up process is simply an invariant way of introducing polar coordinates about a submanifold. A full description appears in [21] and a more concise one in [23, Appendix A], but we give a brief summary here. Near C_a, $\mathbb{S}^n_+$ can be identified with the inward-pointing normal bundle N^+C_a of C_a. Here N^+C_a is the image of the inward-pointing tangent bundle, $T^+\mathbb{S}^n_+$, in the quotient bundle $NC_a = T_{C_a}\mathbb{S}^n_+/TC_a$; $W \in T_q\mathbb{S}^n_+$ is inward pointing if $Wx(q) \geq 0$. The blow up $[\mathbb{S}^n_+; C_a]$ of C_a in $\mathbb{S}^n_+$ is then locally given by the blow up of N^+C_a at the zero section, which amounts to introducing polar coordinates in its fibers. The front face of the blow up (the lift of C_a) is then identified with the inward pointing sphere bundle, S^+NC_a, which is the quotient of $N^+C_a \setminus 0$ by the natural $\mathbb{R}^+$ action in its fibers (0 denotes the zero section). We denote the blow-down map (which is $\mathcal{C}^\infty$) by $\beta[\mathbb{S}^n_+; C_a] : [\mathbb{S}^n_+; C_a] \to \mathbb{S}^n_+$. Now S^+NC_a is a hemisphere bundle over C_a, which can be identified with the radial compactification of the normal bundle of C_a in $\mathbb{S}^{n-1}$ whose fibers can in turn be identified with X^a.

To see this in more concrete terms, we proceed by finding local coordinates on $[\bar{X}; C_a]$ explicitly. Near C_a in $\mathbb{S}^n_+$ we have $|w_a| > c|w^a|$ for some $c > 0$. Hence, near any point $p \in C_a$ one of the coordinate functions $(w_a)_j$ which we take to be $(w_a)_m$ for the sake of definiteness, satisfies $|(w_a)_m| > c'|(w_a)_j|$, $|(w_a)_m| > c'|w^a|$ for some $c' > 0$. Taking into account the coordinate form of RC we see that

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

give coordinates on $\mathbb{S}^n_+$ near p where we think of the y_j as coordinates on the unit sphere C_a. In these coordinates C_a is defined by $x = 0$, $z = 0$. Sometimes we write these coordinates as x_a, y_a, z_a to emphasize the collision plane. *Note that here the notation regarding y and z is reversed as compared to* [37]. We call these the standard coordinates around C_a; we will always use these in this paper. Correspondingly, we have coordinates

$$x,\ y_j\ (j = 1, \dots, m-1),\ Z_j = z_j/x\ (j = 1, \dots, n-m), \tag{3.8}$$

i.e.

$$x = |w_a|^{-1},\ y_j = \frac{(w_a)_j}{|w_a|}\ (j = 1, \dots, m-1),\ Z_j = (w^a)_j\ (j = 1, \dots, n-m) \tag{3.9}$$

near the interior of the front face ff of the blow-up $[\bar{X}; C_a]$, i.e. near the interior of ff $= \beta[\bar{X}; C_a]^* C_a$. Similarly, one can easily write down local coordinates near the corner ff $\cap \beta[\bar{X}; C_a]^* \partial\bar{X}$, see [37, Section 2]. As a result of such calculations, we deduce the following lemma and its corollary.

Lemma 3.1. *(*[37, Lemma 2.5]*) Suppose that $\bar{X} = \mathbb{S}^n_+$ and let $\beta = \beta[\bar{X}; C_a]$ be the blow-down map. Then the pull-back $\beta^*(\mathrm{RC}^{-1})^*\pi^a$ of $\pi^a : \mathbb{R}^n \to X^a$ extends to a $\mathcal{C}^\infty$ map, which we also denote by π^a,*

$$\pi^a : [\bar{X}; C_a] \to \bar{X}^a. \tag{3.10}$$

Moreover, if x^a is a boundary defining function on $\bar{X}^a$ (e.g. $x^a = |w^a|^{-1}$ for $|w^a| > 1$), then $\rho_{\partial\bar{X}} = (\pi^a)^* x^a$ is a defining function for the lift of $\partial\bar{X}$ to $[\bar{X}; C_a]$, i.e. for $\beta^*\partial\bar{X}$.

Corollary 3.2. *(*[37, Corollary 2.6]*) Suppose that $\bar{X} = \mathbb{S}^n_+$, $f \in S^r_{phg}(X^a)$. Then*

$$(\pi^a)^* f \in \rho_{\partial\bar{X}}^{-r} \mathcal{C}^\infty([\bar{X}; C_a]). \tag{3.11}$$

Here, following the previous lemma, we regard π^a as the map in (3.10)*, and $\rho_{\partial\bar{X}}$ is the defining function of $\beta[\bar{X}; C_a]^*\partial\bar{X}$, i.e. of the lift of $\partial\bar{X}$, and the subscript phg refers to classical (one-step polyhomogeneous) symbols.*

This corollary shows that for a Euclidean many-body Hamiltonian, $H = \Delta + \sum_a V_a$, V_a becomes a smooth function on the compact resolved space $[\mathbb{S}^n_+; C_a]$. Thus, to understand H, we need to blow up *all* the C_a. The iterative construction was carried out in detail in [37, 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 $[\mathbb{S}^n_+;\mathcal{C}]$, and the blow-down map (which is $\mathcal{C}^\infty$) is written as

$$\beta_{\mathrm{Sc}} = \beta[\mathbb{S}^n_+;\mathcal{C}] : [\mathbb{S}^n_+;\mathcal{C}] \to \mathbb{S}^n_+. \tag{3.12}$$

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

$$\mathrm{Diff}_{\mathrm{Sc}}(\mathbb{S}^n_+,\mathcal{C}) = \mathcal{C}^\infty([\mathbb{S}^n_+;\mathcal{C}]) \otimes_{\mathcal{C}^\infty(\mathbb{S}^n_+)} \mathrm{Diff}_{\mathrm{sc}}(\mathbb{S}^n_+). \tag{3.13}$$

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

$$P = \sum_{|\alpha|\leq m} a_\alpha D_w^\alpha, \quad a_\alpha \in \mathcal{C}^\infty([\mathbb{S}^n_+;\mathcal{C}]) \tag{3.14}$$

where we again ignored the pull-back by RC in the notation.

The coordinates on ${}^{\mathrm{sc}}T^*\bar{X}$ induced by the standard coordinates around C_a are

$$\tau_a \frac{dx_a}{x_a^2} + \mu_a \cdot \frac{dy_a}{x_a} + \nu_a \cdot \frac{dz_a}{x_a}; \tag{3.15}$$

we included the subscript a to emphasize the element $C = C_a$ of $\mathcal{C}$ around which the local coordinates are centered. *Again, the roles of μ and ν have been switched from* [37]. In terms of the splitting $\mathbb{R}^n = X_0 = X_a \oplus X^a$, and the corresponding splitting $\xi = (\xi_a, \xi^a)$ of the dual coordinates, this gives

$$\xi^a = \nu_a, \text{ and, at } C_a,\ \tau_a = \tau,\ \mu_a \text{ the orthogonal projection of } \xi_a \text{ to } T_yC_a. \tag{3.16}$$

One of the main differences between $\mathrm{Diff}_{\mathrm{Sc}}(\mathbb{S}^n_+,\mathcal{C})$ and $\mathrm{Diff}_{\mathrm{sc}}(\mathbb{S}^n_+)$ is that the former is not commutative to 'top weight'. That is, while for $P \in \mathrm{Diff}^m_{\mathrm{sc}}(\mathbb{S}^n_+)$, $Q \in \mathrm{Diff}^{m'}_{\mathrm{sc}}(\mathbb{S}^n_+)$, we have $[P,Q] \in x\,\mathrm{Diff}^{m+m'-1}_{\mathrm{sc}}(\mathbb{S}^n_+)$, this is replaced by $[P,Q] \in \rho_{C_0}\,\mathrm{Diff}^{m+m'-1}_{\mathrm{Sc}}(\mathbb{S}^n_+,\mathcal{C})$ for $P \in \mathrm{Diff}^m_{\mathrm{Sc}}(\mathbb{S}^n_+,\mathcal{C})$, $Q \in \mathrm{Diff}^{m'}_{\mathrm{Sc}}(\mathbb{S}^n_+,\mathcal{C})$ 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. From an algebraic point of view, it is this non-commutativity that causes the breaks in the propagation of singularities by necessitating the use of the compressed bundle for wave front sets; one can only microlocalize in the commutative (tangential) variables, i.e. at C_a (where $z_a = 0$) only in x_a, y_a (i.e. w_a), and τ_a, μ_a (i.e. ξ_a).

For a closed embedded submanifold C of $\partial\bar{X}$, the relative scattering tangent bundle ${}^{\mathrm{sc}}T(C;\bar{X})$ of C in $\bar{X}$ is the subbundle of ${}^{\mathrm{sc}}T_C\bar{X}$ consisting of $v \in {}^{\mathrm{sc}}T_p\bar{X}$, $p \in C$, for which there exists

$$V \in \mathcal{V}_{\mathrm{sc}}(\bar{X};C) \subset \mathcal{V}_{\mathrm{sc}}(\bar{X}) \tag{3.17}$$

with $V_p = v$ (equality understood in ${}^{\mathrm{sc}}T_p\bar{X}$). Here

$$\mathcal{V}_{\mathrm{sc}}(\bar{X};C) = x\mathcal{V}_{\mathrm{b}}(\bar{X};C) = x\{V \in \mathcal{V}_{\mathrm{b}}(\bar{X}) :\ V \text{ is tangent to } C\} \tag{3.18}$$

and tangency is defined using the (non-injective) inclusion map ${}^{\mathrm{b}}TX \to T\bar{X}$.

Thus, in local coordinates (x,y,z) near $p \in C$ such that C is defined by $x = 0$, $z = 0$, ${}^{\mathrm{sc}}T(C;\bar{X})$ is spanned by $x^2\partial_x$ and $x\partial_{y_j}$, $j = 1,\ldots,m-1$ where $n-m$ is the codimension on C in $\partial\bar{X}$. Thus, in our Euclidean setting, $\bar{X} = \mathbb{S}^n_+$, $C = C_a = \partial\bar{X}_a$, g the Euclidean metric, ${}^{\mathrm{sc}}T(C;\bar{X})$ is naturally isomorphic to ${}^{\mathrm{sc}}T_C\bar{X}_a$, i.e. it should be regarded as the bundle of scattering tangent vectors of the collision plane at infinity, spanned by $\partial_{(w_a)_j}$, $j = 1,\ldots,m$, $m = \dim X_a$.

For $C = C_a \in \mathcal{C}$, the metric g defines the orthocomplement $({}^{\mathrm{sc}}T(C;\bar{X}))^{\perp}$ of ${}^{\mathrm{sc}}T(C;\bar{X})$ in ${}^{\mathrm{sc}}T_C\bar{X}$. The subbundle of ${}^{\mathrm{sc}}T^*_C\bar{X}$ consisting of covectors that annihilate $({}^{\mathrm{sc}}T(C;\bar{X}))^{\perp}$ is denoted by ${}^{\mathrm{sc}}T^*(C;\bar{X})$; it is called the relative scattering cotangent bundle of C in $\bar{X}$. In our Euclidean setting, ${}^{\mathrm{sc}}T^*(C_a;\bar{X})$ is naturally isomorphic to ${}^{\mathrm{sc}}T^*_{C_a}\bar{X}_a$ and is spanned by $d(w_a)_j$, $j = 1, \dots, m$; so we simply write

$$ {}^{\mathrm{sc}}T^*(C_a;\bar{X}) = {}^{\mathrm{sc}}T^*_{C_a}\bar{X}_a. \tag{3.19}$$

In our standard local coordinates (x, y, z) near $p \in C$, $C = C_a$, C defined by $x = 0$, $z = 0$, and $x\partial_{z_j}$ give an orthonormal basis of $({}^{\mathrm{sc}}T(C;\bar{X}))^{\perp}$. Note that a basis of ${}^{\mathrm{sc}}T(C;\bar{X})$ is given by $x^2\partial_x$ and $x\partial_{y_j}$, while a basis of ${}^{\mathrm{sc}}T^*(C;\bar{X})$ is given by $x^{-2}\,dx$, $x^{-1}\,dy_j$. A covector in ${}^{\mathrm{sc}}T^*\bar{X}$ can be written in these local coordinates as

$$ \tau_a \frac{dx_a}{x_a^2} + \mu_a \cdot \frac{dy_a}{x_a} + \nu_a \cdot \frac{dz_a}{x_a}. \tag{3.20}$$

Thus, local coordinates on ${}^{\mathrm{sc}}T^*_{\partial\bar{X}}\bar{X}$ are given by (y, z, τ, μ, ν), while on ${}^{\mathrm{sc}}T^*(C_a;\bar{X})$ by $(y, \tau, \nu) = (y_a, \tau_a, \mu_a)$.

Now if $C = C_a$, $C_b \in \mathcal{C}$ with $C_a \subset C_b$, we can further adjust our coordinates so that C_b is defined by $x = 0$, $z'' = 0$, for some splitting $z = (z', z'')$. In fact, we can use the decomposition

$$ \mathbb{R}^n = X_a \oplus X_b^a \oplus X^{ab}, \quad X_b^a = X^a \cap X_b,\ X^{ab} = X^a \cap X^b; \tag{3.21}$$

the sum is of course still orthogonal with respect to g. Then the splitting $z = (z', z'')$ corresponds to the splitting $X^a = X_b^a \oplus X^{ab}$ in terms of the coordinates (3.7). Following (3.21), we write these coordinates as $z_a = (z_{ab}, z_a^b)$

With the corresponding splitting of the dual variable, $\nu = (\nu', \nu'') = (\nu_{ab}, \nu_a^b)$, we obtain a well-defined projection

$$ \pi_{ba} : {}^{\mathrm{sc}}T^*_{C_a}(C_b;\bar{X}) \to {}^{\mathrm{sc}}T^*(C_a;\bar{X}), \tag{3.22}$$

$$ \pi_{ba}(0, y_a, \tau_a, \mu_a, \nu_{ab}) = (y_a, \tau_a, \mu_a). \tag{3.23}$$

In our Euclidean setting this is just the obvious projection

$$ \pi_{ba} : {}^{\mathrm{sc}}T^*_{\partial\bar{X}_a}\bar{X}_b \to {}^{\mathrm{sc}}T^*_{\partial\bar{X}_a}\bar{X}_a \tag{3.24}$$

under the inclusion $\bar{X}_a \subset \bar{X}_b$. We write π for the collection of these maps.

4. Indicial operators and the characteristic set

We start by recalling from [37] the definition of the many-body pseudo-differential calculus via the quantization of symbols. Thus, the non-polyhomogeneous space $\Psi^{m,l}_{\mathrm{Scc}}(\mathbb{S}^n_+, \mathcal{C})$ is the following. Suppose that, with the notation of [22],

$$ a \in \mathcal{A}^{-m,l}([\mathbb{S}^n_+;\mathcal{C}] \times \mathbb{S}^n_+). \tag{4.1}$$

That is, identifying $\mathrm{int}(\mathbb{S}^n_+)$ and $\mathrm{int}([\mathbb{S}^n_+;\mathcal{C}])$ with $\mathbb{R}^n$ as usual (via RC^{-1}), suppose that $a \in \mathcal{C}^\infty(\mathbb{R}^n_w \times \mathbb{R}^n_\xi)$ has the following property. For every $P \in \mathrm{Diff}^k_{\mathrm{b}}(\mathbb{S}^n_+)$, acting on the second factor of $\mathbb{S}^n_+$ (i.e. in the ξ variable), and $Q \in \mathrm{Diff}^{k'}_{\mathrm{b}}([\mathbb{S}^n_+;\mathcal{C}])$, acting on the first factor of $\mathbb{S}^n_+$ (i.e. in the w variable), $k, k' \in \mathbb{N}$,

$$ PQa \in \rho_\infty^{-m}\rho_\partial^l L^\infty(\mathbb{S}^n_+ \times \mathbb{S}^n_+) \tag{4.2}$$

where ρ_∞ and ρ_∂ are defining functions of the first and second factors of $\mathbb{S}^n_+$ respectively. Let $A = q_L(a)$ denote the left quantization of a:

$$Au(w) = (2\pi)^{-n} \int e^{i(w-w')\cdot\xi} a(w,\xi) u(w')\, dw'\, d\xi, \tag{4.3}$$

understood as an oscillatory integral. Then $A \in \Psi^{m,l}_{\mathrm{Scc}}(\mathbb{S}^n_+, \mathcal{C})$. We could have equally well used other (right, Weyl, etc.) quantizations as well.

In addition, the polyhomogeneous class $\Psi^{m,l}_{\mathrm{Sc}}(\mathbb{S}^n_+, \mathcal{C})$ is given by the quantization of symbols

$$a \in \rho_\infty^{-m} \rho_\partial^l \mathcal{C}^\infty([\mathbb{S}^n_+; \mathcal{C}] \times \mathbb{S}^n_+). \tag{4.4}$$

Since differential operators $\sum a_\alpha(w) D^\alpha$ are just the left quantization of the symbols $a(w,\xi) = \sum a_\alpha(w)\xi^\alpha$, it follows immediately that

$$\mathrm{Diff}^m_{\mathrm{Sc}}(\mathbb{S}^n_+, \mathcal{C}) \subset \Psi^m_{\mathrm{Sc}}(\mathbb{S}^n_+, \mathcal{C}). \tag{4.5}$$

It was shown in [37] that $\Psi_{\mathrm{Scc}}(\mathbb{S}^n_+, \mathcal{C})$ and $\Psi_{\mathrm{sc}}(\mathbb{S}^n_+, \mathcal{C})$ are $*$-algebras with respect to composition and taking adjoints. Moreover, $\Psi^{m,l}_{\mathrm{Scc}}(\mathbb{S}^n_+, \mathcal{C})$ is bounded from $H^{r,s}_{\mathrm{sc}}(\mathbb{S}^n_+)$ to $H^{r-m,s+l}_{\mathrm{sc}}(\mathbb{S}^n_+)$; this follows from the inclusion $\Psi^{m,0}_{\mathrm{Scc}}(\mathbb{S}^n_+, \mathcal{C}) \subset \Psi^m_\infty(\mathbb{R}^n)$ where the latter is Hörmander's 'uniform' calculus in $\mathbb{R}^n$, see [12, Section 18.1].

In the standard pseudo-differential calculus on compacts manifolds without boundary Fredholm properties are captured by the principal symbol. In our setting, Hörmander's principal symbol map on $\Psi^m_\infty(\mathbb{R}^n)$ restricts to a principal symbol map

$$\sigma_{\mathrm{Sc},m} : \Psi^{m,0}_{\mathrm{Sc}}(\mathbb{S}^n_+, \mathcal{C}) \to S^m_h({}^{\mathrm{Sc}}T^*[\mathbb{S}^n_+; \mathcal{C}]), \tag{4.6}$$

$S_h({}^{\mathrm{Sc}}T^*[\mathbb{S}^n_+; \mathcal{C}])$ denoting the space of smooth symbols which are homogeneous of degree m on ${}^{\mathrm{Sc}}T^*[\mathbb{S}^n_+; \mathcal{C}]$, the pull-back of ${}^{\mathrm{sc}}T^*\mathbb{S}^n_+$ by the blow-down map. However, the invertibility of the principal symbol is not sufficient for an operator to be Fredholm, since the behavior near infinity must be taken into account as well. The additional piece of information that is necessary is the invertibility of the indicial operators whose definition we briefly recall below. First, however, we remind the reader what the structure of the lift of C_a to $[\bar{X}; \mathcal{C}]$ is.

For $C_a \in \mathcal{C}$ let

$$\mathcal{C}_a = \{C_b \in \mathcal{C} : \ C_b \subsetneq C_a\}, \tag{4.7}$$

$$\mathcal{C}^a = \{C_b \in \mathcal{C} : \ C_a \subsetneq C_b\}. \tag{4.8}$$

We carry out the blow-up $[\mathbb{S}^n_+; \mathcal{C}]$ by first blowing up $\mathcal{C}_a$. Since all elements of $\mathcal{C}_a$ are p-submanifolds (i.e. product submanifolds) of C_a, the lift $\beta[\mathbb{S}^n_+; \mathcal{C}_a]^* C_a$ of C_a to $[\mathbb{S}^n_+; \mathcal{C}_a]$ is naturally diffeomorphic to

$$\tilde{C}_a = [C_a; \mathcal{C}_a]. \tag{4.9}$$

Thus, over C'_a, the regular part of C_a, $\tilde{C}_a$ can be identified with C_a. The front face of the new blow-up, i.e. of the blow up of $\beta[\mathbb{S}^n_+; \mathcal{C}_a]^* C_a$ in $[\mathbb{S}^n_+; \mathcal{C}_a]$ is thus a hemisphere (i.e. ball) bundle over $\tilde{C}_a$, namely $S^+ N\tilde{C}_a$. We write the bundle projection, which is just the restriction of the new blow-down map to the front face, $S^+ N\tilde{C}_a$ as

$$\rho_a : S^+ N\tilde{C}_a \to \tilde{C}_a. \tag{4.10}$$

In our Euclidean setting, these fibers can be naturally identified with $\bar{X}^a$ via the projection π^a (extended as in Lemma 3.1).

Every remaining blow up in $[\mathbb{S}^n_+;\mathcal{C}]$ concerns submanifolds that are either disjoint from this new front face or are the lift of elements of $\mathcal{C}^a$. The former do not affect the structure near the new front face, $S^+N\tilde{C}_a = \beta[\mathbb{S}^n_+;\mathcal{C}_a;C_a]^*C_a$, while the latter, which are given by the lifts of elements of $\mathcal{C}^a$, correspond to blow ups that can be performed in the fibers of $S^+N\tilde{C}_a$. Note that the lift of $C_b \in \mathcal{C}^a$, meets the new front face only at its boundary since all C_b are subsets of $\mathbb{S}^{n-1} = \partial\mathbb{S}^n_+$. In particular, the lift $\beta^*_{\mathrm{Sc}}C_a$ of C_a to $[\mathbb{S}^n_+;\mathcal{C}]$ fibers over $\tilde{C}_a$ and the fibers are diffeomorphic to a hemisphere (i.e. ball) with certain boundary submanifolds blown up. More specifically, the intersection of $\beta[\mathbb{S}^n_+;\mathcal{C}_a;C_a]^*C_b$, $C_b \in \mathcal{C}^a$, with the front face $S^+N\tilde{C}_a$ is the image of $T\beta[\mathbb{S}^n_+;\mathcal{C}_a]^*C_b$ under the quotients defining the spherical normal bundle; $\beta^*_{\mathrm{Sc}}C_a$ is obtained by blowing these up in $S^+N\tilde{C}_a$. Hence, the fiber of $\beta^*_{\mathrm{Sc}}C_a$ over $p \in \tilde{C}_a$ is given by $[S^+N_qC_a;T_q\mathcal{C}^a]$ where $q = \beta[\mathbb{S}^n_+;\mathcal{C}_a](p) \in C_a$. In particular, in our Euclidean setting, the fibers of $\beta^*_{\mathrm{Sc}}C_a$ over $\tilde{C}_a$ can be naturally identified with $[\bar{X}^a;\mathcal{C}^a]$ via π^a.

We now define ${}^{\mathrm{sc}}T^*(\tilde{C}_a;\mathbb{S}^n_+)$ denote the pull-back of ${}^{\mathrm{sc}}T^*(C_a;\mathbb{S}^n_+)$ by the blow-down map $\beta[C_a;\mathcal{C}_a]$:

$$ {}^{\mathrm{sc}}T^*(\tilde{C}_a;\mathbb{S}^n_+) = \beta[C_a;\mathcal{C}_a]^{*\mathrm{sc}}T^*(C_a;\mathbb{S}^n_+). \tag{4.11}$$

Thus, ${}^{\mathrm{sc}}T^*(\tilde{C}_a;\mathbb{S}^n_+)$ is, via the metric g, naturally diffeomorphic to $\tilde{C}_a \times X_a$, where the metric is used to identify X_a with its dual. If $C_a \subset C_b$ then π_{ba} lifts to a map

$$ \tilde{\pi}_{ba} : {}^{\mathrm{sc}}T^*_{\beta[C_b;\mathcal{C}_b]^*C_a}(\tilde{C}_b;\bar{X}) \to {}^{\mathrm{sc}}T^*(\tilde{C}_a;\bar{X}). \tag{4.12}$$

For each operator $A \in \Psi^{m,l}_{\mathrm{Sc}}(\bar{X},\mathcal{C})$, the C_a-indicial operator of A, denoted by $\hat{A}_{a,l}$, will be a collection of operators, one for each $\zeta \in {}^{\mathrm{sc}}T^*_p(\tilde{C}_a;\bar{X})$, acting on functions on the fiber $\rho_a^{-1}(p)$ of ρ_a. Recall that the interior of these fibers can be naturally identified with X^a. So suppose that $u \in \dot{\mathcal{C}}^\infty(\rho_a^{-1}(p))$, i.e. u is a Schwartz function on the the fiber above p which is a compactification of X^a; we need to define $\hat{A}_a(\zeta)u$. For this purpose choose $\tilde{f} \in \mathcal{C}^\infty(\mathbb{S}^n_+;\mathbb{R})$ such that $d(\tilde{f}/x)$, evaluated at $\beta[C_a;\mathcal{C}_a](p)$, is equal to ζ. Then let $\tilde{A} = e^{-i\tilde{f}/x}x^{-l}Ae^{i\tilde{f}/x} \in \Psi^{m,0}_{\mathrm{Sc}}(\bar{X},\mathcal{C})$, and choose $u' \in \mathcal{C}^\infty([\bar{X};\mathcal{C}])$ such that $u'|_{\rho_a^{-1}(p)} = u$. Then

$$ \hat{A}_{a,l}(\zeta)u = (\tilde{A}u')|_{\rho_a^{-1}(p)}, \tag{4.13}$$

which is independent of all the choices we made.

In our Euclidean setting we can simply take f to be the pull-back of a function in $\mathcal{C}^\infty(\bar{X}_a)$ (which we write, abusing the notation, as $f \in \mathcal{C}^\infty(\bar{X}_a)$). Thus, at least in the regular part C'_a of $\tilde{C}_a$, the a-indicial operator of A arises by thinking of A as a scattering pseudo-differential operator on $\bar{X}_a$ with values in operators on X^a, and finding its scattering symbol at $C'_a \subset C_a = \partial\bar{X}_a$. In fact, $\hat{A}_{a,l}(\xi)$ is a smooth function of $\xi \in {}^{\mathrm{sc}}T^*(\tilde{C}_a;\bar{X})$, so the above description also determines $\hat{A}_{a,l}$ at $\partial\tilde{C}_a$. We often simplify (and thereby abuse) the notation and drop the index l, i.e. we write $\hat{A}_a = \hat{A}_{a,l}$, when the value of l is understood.

In the case of Euclidean many-body scattering, $\hat{A}_{a,l}$ is a function on $\beta_a^{*\mathrm{sc}}T^*_{C_a}\bar{X}_a$ with values in operators on $\mathcal{S}(X^a)$; here

$$ \beta_a = \beta[C_a;\mathcal{C}_a] : \tilde{C}_a = [C_a;\mathcal{C}_a] \to C_a \tag{4.14}$$

is the blow-down map. Thus, β_a is simply the restriction of $\beta[\bar{X}_a; \mathcal{C}_a]$ to the lift $\tilde{C}_a = \beta[\bar{X}_a; \mathcal{C}_a]^* C_a$. Then

$$\hat{A}_{a,l} \in \mathcal{C}^\infty(\beta_a^{*\mathrm{sc}} T^*_{\partial \bar{X}_a} \bar{X}_a, \Psi_{\mathrm{Sc}}^{m,0}(\bar{X}^a, \mathcal{C}^a)). \tag{4.15}$$

We write the space on the right as

$$\hat{A}_{a,l} \in \Psi^{r,0}_{\mathrm{Sc},\rho_a^\sharp}(\beta_a^{*\mathrm{sc}} T^*(\tilde{C}_a; \bar{X}), \tilde{\mathcal{C}}_a). \tag{4.16}$$

An explicit formula for the indicial operator of A, given by (4.3), at $\tilde{C}_a$ is

(4.17)

$$\hat{A}_a(y_a, \xi_a) u(Z_a) = (2\pi)^{-\dim X^a} \int e^{i(Z_a - w^a)\cdot \xi^a} a(0, y_a, Z_a, \xi_a, \xi^a) u(w^a)\, d\xi^a\, dw^a.$$

Note that the oscillatory testing definition that we adopted automatically shows that the indicial operator map is multiplicative.

The principal symbol and the indicial operators together indeed describe compactness properties of ps.d.o's. In particular, if $A \in \Psi^{m,l}_{\mathrm{Sc}}(\mathbb{S}^n_+, \mathcal{C})$, $\sigma_{\mathrm{Sc},m}(A)$ never vanishes, and for every a, $\hat{A}_{a,l}$ is invertible in $\Psi^{r,0}_{\mathrm{Sc},\rho_a^\sharp}(\beta_a^{*\mathrm{sc}} T^*(\tilde{C}_a; \bar{X}), \tilde{\mathcal{C}}_a)$, then there is a two-sided parametrix P for A such that $PA - \mathrm{Id}, AP - \mathrm{Id} \in \Psi^{-\infty,\infty}_{\mathrm{Sc}}(\mathbb{S}^n_+, \mathcal{C})$. For $A \in \Psi^{m,0}_{\mathrm{Sc}}(\mathbb{S}^n_+, \mathcal{C})$ self-adjoint, $m > 0$, such that $\sigma_{\mathrm{Sc},m}(A)$ never vanishes (but no assumptions made on the indicial operators of A), $\lambda \in \mathbb{C} \setminus \mathbb{R}$, we conclude that $(A - \lambda)^{-1} \in \Psi^{-m,0}_{\mathrm{Sc}}(\mathbb{S}^n_+, \mathcal{C})$. The invertibility of the indicial operators of $A - \lambda$ is automatic since $\widehat{(A - \lambda)}_{a,0} = \hat{A}_{a,0} - \lambda$, and then an iterative argument, starting at $a = 0$, using the self-adjointness of A, shows the required invertibility. In addition, an argument using almost analytic extensions and the Cauchy representation also shows that certain functions of self-adjoint ps.d.o's are ps.d.o's themselves. In particular, for $A \in \Psi^{m,0}_{\mathrm{Sc}}(\mathbb{S}^n_+, \mathcal{C})$ self-adjoint, $m > 0$, such that $\sigma_{\mathrm{Sc},m}(A)$ never vanishes, $\phi \in \mathcal{C}^\infty_c(\mathbb{R})$, we conclude that $\phi(A) \in \Psi^{-\infty,0}_{\mathrm{Sc}}(\mathbb{S}^n_+, \mathcal{C})$ (see [37, Propositions 4.7-4.8], and see [3] and [11] for a general discussion of functions of ps.d.o.'s).

Now it is particularly easy to identify the indicial operators: for each $\xi = (y, \tau, \mu) \in {}^{\mathrm{sc}}T^*_p(\tilde{C}_a; \bar{X})$, they are operators on X^a, identified as the fiber of the front face $\rho_a^{-1}(p)$ over p. A simple calculation, see [36, Sections 4 and 11] for more details, shows that the indicial operators of H are given by

$$\hat{H}_{a,0}(\xi) = \hat{H}_{a,0}((p, 0)) + |\xi|^2,\ \xi = (y, \tau, \mu) \in {}^{\mathrm{sc}}T^*(\tilde{C}_a; \bar{X}), \tag{4.18}$$

$$\hat{H}_{a,0}(p, 0) = \Delta_Z + V(p, Z) = H^a \tag{4.19}$$

where Z are Euclidean coordinates on the interior of $\rho_a^{-1}(p)$, i.e. on X^a, and Δ_Z is the Euclidean Laplacian. Note that under these natural identifications (that $\rho_a^{-1}(p)$ is regarded as X^a for all p) the a-indicial operators of H only depend on $|\xi|^2$, i.e. on the metric function of g_a.

Equations (4.18)-(4.19) show that $\hat{H}_{a,0}(p, 0)$ is uniformly bounded below, so for any $\psi \in \mathcal{C}^\infty_c(\mathbb{R})$ the set

$$\cup_a \operatorname{cl}(\{\xi \in {}^{\mathrm{sc}}T^*(\tilde{C}_a; \bar{X}) :\ \psi(\hat{H}_a(\xi)) \neq 0\}) \tag{4.20}$$

is compact.

Note that $\hat{H}_{a,0}(\xi) - \lambda$ is invertible in $\Psi_{\mathrm{Sc}}(\bar{X}^a, \mathcal{C}^a)$ if and only if $\lambda - |\xi_a|^2$ is not in the spectrum of H^a. Indeed, by the HVZ theorem, this means that $\lambda - |\xi_a|^2$ is not an L^2 eigenvalue of H^a, and it is smaller than all of its thresholds, $\lambda - |\xi_a|^2 < \inf \Lambda_a$, i.e. smaller than the eigenvalues of subsystems of H^a. By an iterative argument corresponding to $C_a \subsetneq C_b$, $\lambda - |\xi_a|^2 < \inf \Lambda_a$ guarantees the invertibility of the indicial operators of $\hat{H}_{a,0}(\xi) - \lambda$, so $\hat{H}_{a,0}(\xi) - \lambda$ is Fredholm, and hence invertible if and only if it has no L^2 eigenfunctions. Thus, we define the characteristic variety $\dot{\Sigma}(\lambda) \subset {}^{\mathrm{sc}}\dot{T}^*\bar{X}$ of $H - \lambda$ to be the union image of these sets under π:

$$\dot{\Sigma}(\lambda) = \cup_a \dot{\Sigma}_a(\lambda) \subset {}^{\mathrm{sc}}\dot{T}^*\bar{X}, \tag{4.21}$$

(4.22)
$$\begin{aligned}\dot{\Sigma}_a(\lambda) = &\{\xi_a \in {}^{\mathrm{sc}}T^*_{C'_a}(C_a;\bar{X}) : \ \lambda - |\xi_a|^2 \geq \sigma \text{ for some } \sigma \in \operatorname{spec}_{pp} H^b, \ C_a \subsetneq C_b\} \\ &\cup \{\xi_a \in {}^{\mathrm{sc}}T^*_{C'_a}(C_a;\bar{X}) : \ \lambda - |\xi_a|^2 \in \operatorname{spec}_{pp} H^a\}.\end{aligned}$$

If there are no bound states in the subsystems, a compactness argument as in [37] allows one to show that the free Laplacian governs the propagation of singularities except that breaks occur at the collision planes C_a where the usual law of reflection is satisfied. This indicates that one should think of the characteristic variety $\dot{\Sigma}(\lambda)$ as the union of projection of the characteristic sets corresponding to the bound states of the various subsystems. Thus, let

$$\Sigma_b(\lambda) = \{\xi_b \in {}^{\mathrm{sc}}T^*_{C_b}\bar{X}_b : \ \lambda - |\xi_b|^2 \in \operatorname{spec}_{pp} H^b\}. \tag{4.23}$$

For a with $C_a \subset C_b$, the projection of $\Sigma_b(\lambda)$ under π_{ba} is

(4.24)
$$\begin{aligned}\pi_{ba}(\Sigma_b(\lambda)) &= \{\xi_a \in {}^{\mathrm{sc}}T^*_{C_a}\bar{X}_a : \ \exists \xi_b \in {}^{\mathrm{sc}}T^*_{C_b}\bar{X}_b \text{ with } \pi_{ba}(\xi_b) = \xi_a \text{ and } \lambda - |\xi_b|^2 \in \operatorname{spec}_{pp} H^b\} \\ &= \{\xi_a \in {}^{\mathrm{sc}}T^*_{C_a}\bar{X}_a : \ \lambda - |\xi_a|^2 \geq \sigma \text{ for some } \sigma \in \operatorname{spec}_{pp} H^b\}.\end{aligned}$$

Thus,

$$\dot{\Sigma}_a(\lambda) = \cup_{C_b \supset C_a} \pi_{ba}(\Sigma_b(\lambda)) \cap {}^{\mathrm{sc}}T^*_{C'_a}(C_a;\bar{X}). \tag{4.25}$$

In fact, letting $\pi_b : {}^{\mathrm{sc}}T^*_{C_b}\bar{X}_b \to {}^{\mathrm{sc}}\dot{T}^*\bar{X}$ be the projection, we thus conclude that

$$\dot{\Sigma}(\lambda) = \cup_b \pi_b(\Sigma_b(\lambda)). \tag{4.26}$$

We write $\hat{\pi}_b$ for the restriction of π_b to $\Sigma_b(\lambda)$.

We proceed to recall the basic topological properties of ${}^{\mathrm{sc}}\dot{T}^*\bar{X}$ from [37, Section 5]. We put the topology induced by $\pi : {}^{\mathrm{sc}}T^*_{\partial\bar{X}}\bar{X} \to {}^{\mathrm{sc}}\dot{T}^*\bar{X}$ on ${}^{\mathrm{sc}}\dot{T}^*\bar{X}$. Thus, $C \subset {}^{\mathrm{sc}}\dot{T}^*\bar{X}$ is closed if and only if $\pi^{-1}(C)$ is closed, so if f is continuous on ${}^{\mathrm{sc}}T^*_{\partial\bar{X}}\bar{X}$ and π-invariant, then f_π is continuous on ${}^{\mathrm{sc}}\dot{T}^*\bar{X}$. In particular, there are always continuous functions separating points on ${}^{\mathrm{sc}}\dot{T}^*\bar{X}$: if $p(\bar{\xi}) \neq p(\bar{\xi}')$ (here $p : {}^{\mathrm{sc}}\dot{T}^*\bar{X} \to \partial\bar{X}$ stands for projection to the base), one can use the pull-back of an appropriate function on $\partial\bar{X}$, and if $p(\bar{\xi}) = p(\bar{\xi}') \in C'_a$, then $\bar{\xi}, \bar{\xi}' \in {}^{\mathrm{sc}}T^*_{C'_a}\bar{X}_a$ are of the form $(\bar{y}_a, \bar{\xi}_a)$ and $(\bar{y}'_a, \bar{\xi}'_a)$, $\bar{\xi}_a \neq \bar{\xi}'_a$, and the function $\xi \mapsto \xi_a$ is well-defined and π-invariant on a neighborhood of $p(\bar{\xi})$, so multiplying it by the pull-back of a cutoff on $\partial\bar{X}$ gives a globally well-defined separating continuous function. Thus, ${}^{\mathrm{sc}}\dot{T}^*\bar{X}$ is Hausdorff.

By the continuity of π, if $K \subset {}^{\mathrm{sc}}T^*_{\partial\bar{X}}\bar{X}$ is compact, the same holds for $\pi(K)$. But by (4.26), $\dot{\Sigma}(\lambda) = \pi(\cup_b \imath_b(\overline{\Sigma_b(\lambda)}))$ (see (2.21)), and $\imath_b(\overline{\Sigma_b(\lambda)})$ is compact for each b, so $\dot{\Sigma}(\lambda)$ is compact, hence closed in ${}^{\mathrm{sc}}\dot{T}^*\bar{X}$. In particular $C \subset \dot{\Sigma}(\lambda)$ is closed in $\dot{\Sigma}(\lambda)$ if and only if it is closed in ${}^{\mathrm{sc}}\dot{T}^*\bar{X}$, i.e. if and only if $\pi^{-1}(C)$ is closed in ${}^{\mathrm{sc}}T^*_{\partial\bar{X}}\bar{X}$. Also, if $C \subset \dot{\Sigma}(\lambda)$ is closed, then $\hat{\pi}_0^{-1}(C)$ is compact.

Note that for all $C \subset \dot{\Sigma}(\lambda)$ and for any $R > 0$ with $R > \lambda - \inf \Lambda_1$,

$$\pi(\pi^{-1}(C)) = \pi(\pi^{-1}(C) \cap \{\xi \in {}^{\mathrm{sc}}T^*_{\partial \bar{X}}\bar{X} : \ |\xi|^2 \leq R\}). \tag{4.27}$$

Indeed, if $\xi \in \pi^{-1}(C)$, $\pi(\xi) \in {}^{\mathrm{sc}}T^*_{C'_a}\bar{X}_a$, then by $C \subset \dot{\Sigma}(\lambda)$, $|\imath_a(\pi(\xi))|^2 < R$, $\pi(\imath_a(\pi(\xi))) = \pi(\xi)$, so $\pi(\imath_a(\pi(\xi)))$ is in the right hand side, showing one inclusion, and the other is clear. For any b then

$$\hat{\pi}_b^{-1}(C) = \pi_{0b}(\pi^{-1}(C) \cap \{\xi : \ |\xi|^2 \leq R\} \cap {}^{\mathrm{sc}}T^*_{C_b}\bar{X}) \cap \Sigma_b(\lambda), \tag{4.28}$$

and π_{0b} is continuous, so $\hat{\pi}_b^{-1}(C)$ is also compact (and similarly $\pi_b^{-1}(C)$ is closed). Thus, all the maps π_b, $\hat{\pi}_b$, are continuous.

Also, fix $\bar{\xi} \in {}^{\mathrm{sc}}T^*_{C'_a}\bar{X}_a$, write $\bar{\xi} = (\bar{y}_a, \bar{\xi}_a)$, and choose a neighborhood U_0 of $\bar{y}_a = p(\bar{\xi})$ in $\partial\bar{X}$ such that $\overline{U_0} \cap C_b = \emptyset$ unless $C_a \subset C_b$. Let $\omega_{\bar{\xi}} = \omega : {}^{\mathrm{sc}}\dot{T}^*_{\overline{U_0}}\bar{X} \to \mathbb{R}$ be given by the following π-invariant function on ${}^{\mathrm{sc}}T^*_{\overline{U_0}}\bar{X}$ (also denoted by ω):

$$\omega(\xi) = (y_a - \bar{y}_a)^2 + |z_a|^2 + (\xi_a - \bar{\xi}_a)^2 \geq 0 \tag{4.29}$$

in the coordinates (y_a, z_a, ξ_a, ξ^a). Suppose that U is open in $\dot{\Sigma}(\lambda)$, $\bar{\xi} \in U$. Thus, $K = (\dot{\Sigma}(\lambda) \cap {}^{\mathrm{sc}}\dot{T}^*_{\overline{U_0}}\bar{X}) \setminus U$ is compact, so, unless K is empty, ω assumes a minimum on it which thus has to be non-negative. But $\omega(\xi) = 0$ implies $z_a = 0$, so $p(\xi) \in C_a$, and then $y_a = \bar{y}_a$, $\xi_a = \bar{\xi}_a$ show that $\xi = \bar{\xi}$. Since $\bar{\xi} \in U$, this shows that there exists $\delta > 0$ such that $\omega \geq \delta$ on K. Replacing $\delta > 0$ by possibly a smaller number, we can also assume that $\omega(\xi) < \delta$ implies $p(\xi) \in U_0$. We thus conclude that if U is a neighborhood of $\bar{\xi}$, then there exists $\delta > 0$ such that

$$\{\xi \in \dot{\Sigma}(\lambda) : \ \omega(\xi) < \delta\} \subset U. \tag{4.30}$$

Of course, we could have equally well used (τ_a, μ_a) in place of ξ_a. These sets are open since ω is continuous, hence they form a basis for the topology as $\bar{\xi}$ and δ vary; it is easy to see that if one restricts both of these to suitable countable sets, one still has a basis. Note that, separating the complement of U from $\bar{\xi}$ by a level set of ω shows explicitly that $\dot{\Sigma}(\lambda)$ is regular, and a simple compactness argument using these $\omega_{\bar{\xi}}$ (composed with cut-off functions on the reals as in the next paragraph) shows that $\dot{\Sigma}(\lambda)$ is normal, hence it is a compact metrizable space.

Composing ω with a $\mathcal{C}^\infty$ function on $\mathbb{R}$ supported near 0 also shows that given any $\bar{\xi} \in \dot{\Sigma}(\lambda)$ and any neighborhood U of $\bar{\xi}$ in $\dot{\Sigma}(\lambda)$, one can construct a π-invariant $\mathcal{C}^\infty$ function f on ${}^{\mathrm{sc}}T^*_{\partial\bar{X}}\bar{X}$ for which $f_\pi(\bar{\xi}) \neq 0$ and $\operatorname{supp} f_\pi \subset U$. This also shows the existence of smooth partitions of unity on $\dot{\Sigma}(\lambda)$, smoothness understood as smoothness for the pull-back to ${}^{\mathrm{sc}}T^*\bar{X}$.

If we define

$$\dot{\Sigma}(I) = \cup_{\lambda \in I} \dot{\Sigma}(\lambda) \tag{4.31}$$

for $I \subset \mathbb{R}$ compact, all the previous statements remain valid with trivial modifications with $\dot{\Sigma}(I)$ in place of $\dot{\Sigma}(\lambda)$. We write

$$\Sigma_b(I) = \cup_{\lambda \in I} \Sigma_b(\lambda), \ \hat{\pi}_{b,I} = \pi_b|_{\Sigma_b(I)}. \tag{4.32}$$

Thus, $\dot{\Sigma}(I) = \cup_b \pi_b(\Sigma_b(I))$,

$$\tilde{\xi} \in \hat{\pi}_{b,I}^{-1}(\{\xi\}) \text{ iff } \pi_b(\tilde{\xi}) = \xi \text{ and } \exists \sigma \in \operatorname{spec}_{pp}(H^b) \text{ such that } |\tilde{\xi}|^2 + \sigma \in I. \tag{4.33}$$

We end this section by recalling from [37, Section 5] the definition of the operator wave front set and the wave front set of distributions in the many-body setting.

Both of these are closed subsets of ${}^{\mathrm{sc}}\dot T^*\mathbb{S}^n_+$ which were modelled on the fibred cusp wave front set introduced by Mazzeo and Melrose in [20]. Rather than using the invariant definition given there in terms of oscillatory testing, we recall the one given in terms of representation of ps.d.o.'s via quantization.

So suppose that $A \in \Psi^{-\infty,l}_{\mathrm{Sc}}(\mathbb{S}^n_+,\mathcal{C})$ is the left quantization of a symbol $a \in \rho^l_\partial \mathcal{C}^\infty([\mathbb{S}^n_+;\mathcal{C}]\times\mathbb{S}^n_+)$ which vanishes to infinite order at $[\mathbb{S}^n_+;\mathcal{C}]\times\partial\mathbb{S}^n_+$. Then $\xi\notin \mathrm{WF}'_{\mathrm{Sc}}(A)$, $\xi\in{}^{\mathrm{sc}}T^*_p(C_a;\bar X)$, $p\in C'_a$, if and only if there exists a neighborhood U of ξ in ${}^{\mathrm{sc}}\dot T^*\mathbb{S}^n_+$ such that a vanishes at $U'\subset(\partial[\mathbb{S}^n_+;\mathcal{C}])\times\mathbb{R}^n$ to infinite order where U' is the inverse image of U under the composite map

$$\tilde\pi : (\partial[\mathbb{S}^n_+;\mathcal{C}])\times\mathbb{R}^n \xrightarrow{\beta_{\mathrm{Sc}}\times\mathrm{id}} (\partial\mathbb{S}^n_+)\times\mathbb{R}^n = {}^{\mathrm{sc}}T^*_{\mathbb{S}^{n-1}}\mathbb{S}^n_+ \xrightarrow{\pi} {}^{\mathrm{sc}}\dot T^*\mathbb{S}^n_+. \tag{4.34}$$

It follows immediately from the usual formulae relating quantizations that this definition is independent of such choices. For example, we could have equally well written A as the right quantization of a symbol with similar properties.

The general definition for $A\in\Psi^{m,l}_{\mathrm{Sc}}(\bar X,\mathcal{C})$, again following the paper [20], in the explicit quantization form as in the previous paragraph, would also require the rapid decay of a in an open cone (conic in the cotangent variable, $\tilde\xi$, i.e. in the second factor, $\mathbb{R}^n$, in (4.34)) that includes U'. For $A\in\Psi^{-\infty,l}_{\mathrm{Sc}}(\bar X,\mathcal{C})$, a is rapidly decreasing in every direction as $|\xi|\to\infty$, so this statement is vacuous, and we recover the above definition. The main point is that if $A\in\Psi^{0,0}_{\mathrm{Sc}}(\bar X,\mathcal{C})$, $\hat A_a(\xi)$ is invertible, then there exists a microlocal parametrix for A, i.e. there exists $G\in\Psi^{0,0}_{\mathrm{Sc}}(\bar X,\mathcal{C})$ such that $\mathrm{Id}=AG+R_R$, $\mathrm{Id}=GA+R_L$, with $R_R,R_L\in\Psi^{0,0}_{\mathrm{Sc}}(\bar X,\mathcal{C})$, $\xi\notin\mathrm{WF}'_{\mathrm{Sc}}(R_R)$, $\xi\notin\mathrm{WF}'_{\mathrm{Sc}}(R_L)$; see [20, Lemmas 14-15].

We recall that the many-body wave front set $\mathrm{WF}_{\mathrm{Sc}}(u)$ of $u\in\mathcal{C}^{-\infty}(\bar X)$, defined in [37, Section 5], is a subset of ${}^{\mathrm{sc}}\dot T^*\bar X$, defined as follows. The definition is somewhat delicate due to the relation among the principal symbols $\sigma_{\mathrm{Sc},0}(\hat A_a(\xi))$ as ξ varies, see [37] for a detailed discussion, but it becomes much simpler for approximate generalized eigenfunctions of H as the proposition following the definition shows. Although the definition is complicated, it ensures that all the desired properties hold: for all $u\in\mathcal{C}^{-\infty}(X)$, $\mathrm{WF}_{\mathrm{Sc}}(u)$ is closed in ${}^{\mathrm{sc}}\dot T^*\bar X$,

(4.35)
$$\begin{aligned}
&u_1,u_2\in\mathcal{C}^{-\infty}(\bar X)\Rightarrow \mathrm{WF}_{\mathrm{Sc}}(u_1+u_2)\subset\mathrm{WF}_{\mathrm{Sc}}(u_1)\cup\mathrm{WF}_{\mathrm{Sc}}(u_2),\\
&u\in\mathcal{C}^{-\infty}(\bar X),\ A\in\Psi^{m,l}_{\mathrm{Sc}}(\bar X,\mathcal{C})\Rightarrow\mathrm{WF}_{\mathrm{Sc}}(Au)\subset\mathrm{WF}_{\mathrm{Sc}}(u),\\
&A\in\Psi^{-\infty,l}_{\mathrm{Sc}}(\bar X,\mathcal{C}),\ u\in\mathcal{C}^{-\infty}(\bar X),\ \mathrm{WF}'_{\mathrm{Sc}}(A)\text{ compact},\ \mathrm{WF}'_{\mathrm{Sc}}(A)\cap\mathrm{WF}_{\mathrm{Sc}}(u)=\emptyset\\
&\qquad\qquad\Rightarrow Au\in\dot{\mathcal{C}}^\infty(\bar X).
\end{aligned}$$

The central one of these means that '$\Psi^{*,*}_{\mathrm{Sc}}(\bar X,\mathcal{C})$ is microlocal'.

Definition 4.1. ([37, Definition 5.2]) We say that

(4.36)
$$\begin{aligned}
\xi\notin\mathrm{WF}_{\mathrm{Sc}}(u)\cap{}^{\mathrm{sc}}T^*_{C'_a}(C_a;\bar X)\ \text{iff}\ &\exists A\in\Psi^{0,0}_{\mathrm{Sc}}(\bar X,\mathcal{C}),\ \hat A_{a,0}(\xi)\text{ invertible in }\Psi^{0,0}_{\mathrm{Sc}}(\bar X^a,\mathcal{C}^a),\\
&\exists B_j\in\Psi^{-\infty,0}_{\mathrm{Sc}}(\bar X,\mathcal{C}),\ \xi\notin\mathrm{WF}'_{\mathrm{Sc}}(B_j),\\
&\exists u_j\in\mathcal{C}^{-\infty}(\bar X),\ j=1,\dots,s,\ f\in\dot{\mathcal{C}}^\infty(\bar X),\\
&Au=\sum_{j=1}^s B_ju_j+f.
\end{aligned}$$

Similarly, the filtered version of the Sc-wave front set is given by

(4.37)
$$\begin{aligned}\xi \notin \mathrm{WF}^{m,l}_{\mathrm{Sc}}(u) \cap {}^{\mathrm{sc}}T^*_{C'_a}(C_a;\bar{X}) \text{ iff } &\exists A \in \Psi^{0,0}_{\mathrm{Sc}}(\bar{X},\mathcal{C}),\ \hat{A}_{a,0}(\xi) \text{ invertible in } \Psi^{0,0}_{\mathrm{Sc}}(\bar{X}^a,\mathcal{C}^a),\\ &\exists B_j \in \Psi^{-\infty,0}_{\mathrm{Sc}}(\bar{X},\mathcal{C}),\ \xi \notin \mathrm{WF}'_{\mathrm{Sc}}(B_j),\\ &\exists u_j \in \mathcal{C}^{-\infty}(\bar{X}),\ j=1,\ldots,s,\ f \in H^{m,l}_{\mathrm{sc}}(\bar{X}),\\ &Au = \sum_{j=1}^{s} B_j u_j + f.\end{aligned}$$

The wave front set has the following property which is useful for approximate generalized eigenfunctions of H.

Proposition 4.2. *([37, Proposition 5.5]) Suppose that $u \in \mathcal{C}^{-\infty}(\bar{X})$, $\lambda \in \mathbb{R}$, and define $W \subset {}^{sc}\dot{T}^*\bar{X}$ by*

(4.38)
$$\begin{aligned}\xi \notin W \cap {}^{sc}T^*_{C'_a}(C_a;\bar{X}) \text{ iff } &\exists \psi \in \mathcal{C}^\infty_c(\mathbb{R}),\ \psi(\lambda)=1,\\ &\exists A \in \Psi^{-\infty,0}_{Sc}(\bar{X},\mathcal{C}),\ \hat{A}_a(\xi) = \widehat{\psi(H)}_a(\xi), Au \in \dot{\mathcal{C}}^\infty(\bar{X}).\end{aligned}$$

Then

$$\mathrm{WF}_{Sc}(u) \subset \mathrm{WF}_{Sc}((H-\lambda)u) \cup W. \tag{4.39}$$

The same conclusion holds with WF_{Sc} replaced by $\mathrm{WF}^{m,l}_{Sc}$ and $Au \in \dot{\mathcal{C}}^\infty(\bar{X})$ by $Au \in H^{m,l}_{sc}(\bar{X})$.

Corollary 4.3. *(Microlocal elliptic regularity.) Suppose that $u \in \mathcal{C}^{-\infty}(\bar{X})$, $\lambda \in \mathbb{R}$. Then $\mathrm{WF}_{Sc}(u) \subset \mathrm{WF}_{Sc}((H-\lambda)u) \cup \dot{\Sigma}(\lambda)$.*

Proof. If $\bar{\xi}_a \notin \dot{\Sigma}(\lambda)$, $\bar{\xi}_a \in {}^{\mathrm{sc}}T^*_{C'_a}\bar{X}_a$, one can choose $\psi \in \mathcal{C}^\infty_c(\mathbb{R})$ such that $\psi(\lambda) = 1$ and $\widehat{\psi(H)}_a(\bar{\xi}_a) = \psi(H^a + |\bar{\xi}_a|^2) = 0$ by making the support of ψ sufficiently small. Then we can take A to be the zero operator, showing that $\bar{\xi}_a \notin W$. Thus, Proposition 4.2 proves the corollary. □

5. Broken bicharacteristics

Since at C'_a a particle can be in a bound state of any of the clusters C_b with $C_a \subset C_b$, it can be expected that the Hamilton vector fields associated to the b-external kinetic energy, i.e. to Δ_{X_b}, govern the propagation of singularities. If the particle is in a b-bound state of energy ϵ_β, its b-external kinetic energy is $\lambda - \epsilon_\beta$. The symbol of $\Delta_{X_b} - (\lambda - \epsilon_\beta)$ at $C_b = \partial\bar{X}_b$ (i.e. its sc-indicial operator) is $|\xi_b|^2 + \epsilon_\beta - \lambda$. The Hamilton vector field of $g_b = |\xi_b|^2$ (or $|\xi_b|^2 + \epsilon_\beta - \lambda$) on T^*X_b is

$$H^b_g = 2\xi_b \cdot \partial_{w_b}. \tag{5.1}$$

Following the general principle that it is more convenient to do analysis on compact spaces than analyzing uniform properties in a non-compact setting, we rescale H^b_g and regard the result as a smooth vector field on ${}^{\mathrm{sc}}T^*\bar{X}_b$, i.e. as an element of $\mathcal{V}({}^{\mathrm{sc}}T^*\bar{X}_b)$. Thus, the rescaled Hamilton vector field

$${}^{\mathrm{sc}}H^b_g = x_b^{-1} H^b_g \tag{5.2}$$

of $g_b = |\xi_b|^2$, introduced in [23], is

(5.3)
$$\begin{aligned}{}^{\mathrm{sc}}H_g^b &= 2|w_b|\xi_b \cdot \partial_{w_b}\\ &= 2\tau_b(x_b\partial_{x_b} + \mu_b \cdot \partial_{\mu_b}) - 2|\mu_b|^2\partial_{\tau_b} + H_{|\mu_b|^2} + x_b W', \quad W' \in \mathcal{V}_{\mathrm{b}}({}^{\mathrm{sc}}T^*\bar{X}_b),\end{aligned}$$

so its restriction to C_b, also denoted by ${}^{\mathrm{sc}}H_g^b$, is

$$ {}^{\mathrm{sc}}H_g^b = 2\tau_b\mu_b \cdot \partial_{\mu_b} - 2|\mu_b|^2\partial_{\tau_b} + H_{|\mu_b|^2}. \tag{5.4}$$

Thus, for $C_a \subset C_b$,

$$ {}^{\mathrm{sc}}H_g^b = 2x_b^{-1}(\xi_a \cdot \partial_{w_a} + \xi_{ab} \cdot \partial_{w_{ab}}) = (x_a/x_b)({}^{\mathrm{sc}}H_g^a + 2\xi_{ab} \cdot \partial_{w_{ab}}). \tag{5.5}$$

If $b = 0$, then in agreement with [23] we write

$$ {}^{\mathrm{sc}}H_g = {}^{\mathrm{sc}}H_g^0. \tag{5.6}$$

Before defining generalized broken bicharacteristics, we discuss how the rescaled Hamilton vector fields are related for various b. First, note that ${}^{\mathrm{sc}}T^*_{C_b}\bar{X}$ is the bundle direct sum of ${}^{\mathrm{sc}}T^*_{C_b}\bar{X}_b$ and the annihilator of ${}^{\mathrm{sc}}T_{C_b}(C_b;\bar{X})$. Let

$$ \imath_b : {}^{\mathrm{sc}}T^*_{C_b}\bar{X}_b \hookrightarrow {}^{\mathrm{sc}}T^*_{C_b}\bar{X} \tag{5.7}$$

be the inclusion map as the zero section in the second summand, so

$$ \imath_b(y_b, \tau_b, \mu_b) = (y_b, 0, \tau_b, \mu_b, 0), \tag{5.8}$$

i.e. $\nu_b(\imath_b(\xi)) = 0$ for all $\xi \in {}^{\mathrm{sc}}T^*_{C_b}\bar{X}_b$. Then

$$ (\imath_b)_* {}^{\mathrm{sc}}H_g^b = {}^{\mathrm{sc}}H_g, \tag{5.9}$$

since the corresponding statement for the non-rescaled Hamilton vector fields is easy to see and x_b/x is $\mathcal{C}^\infty$ near C_b, equal to 1 at C_b.

Next, note that

$$ T^*\mathbb{R}^n = T^*X_a \times T^*X^a. \tag{5.10}$$

Thus, if f is a smooth function on ${}^{\mathrm{sc}}T^*_{C_a}\bar{X}_a$, we can extend it to a smooth function on ${}^{\mathrm{sc}}T^*\bar{X}_a$ using polar coordinates (i.e. so that it is independent of x_a, at least near C_a), and pull-back the result to $T^*\mathbb{R}^n$ using the projection to the first factor. The result is then smooth on ${}^{\mathrm{sc}}T^*\mathbb{S}^n_+$ in a neighborhood of C_a (in fact, everywhere away from the closure of X^a in $\mathbb{S}^n_+$). Thus, we have a pull-back, which we denote as $F = (\pi_a^e)^* f$. Note that $F = (\pi_a^e)^* f$ is π-invariant near C'_a. Moreover,

$$ {}^{\mathrm{sc}}H_g F = \frac{x_a}{x}\,(\pi_a^e)^{*\,\mathrm{sc}}H_g^a f. \tag{5.11}$$

One often drops the pull-back notation, and simply writes f in place of F. A similar formula also holds for ${}^{\mathrm{sc}}H_g^b f$ by (5.9).

It is worth calculating the derivatives of two functions in particular along the rescaled Hamilton vector fields. First,

$$ {}^{\mathrm{sc}}H_g \tau = -2|\mu|^2, \tag{5.12}$$

so by (5.9),

$$ {}^{\mathrm{sc}}H_g^b \tau = -2|\mu_b|^2. \tag{5.13}$$

Next, consider

$$\eta_a = z_a \cdot \nu_a = \frac{\xi^a \cdot w^a}{|w_a|}. \tag{5.14}$$

Then

$$^{\mathrm{sc}}H_g \eta_a = \frac{x_a}{x}(2\tau_a\eta_a + 2|\xi^a|^2), \tag{5.15}$$

so

$$^{\mathrm{sc}}H_g^b \eta_a = \frac{x_a}{x}(2\tau_a\eta_a + 2|\xi^a_b|^2) = \frac{x_a}{x}(2\tau_a\eta_a + 2|\nu_{ab}|^2). \tag{5.16}$$

We define generalized broken bicharacteristics of $H-\lambda$ partly following Lebeau [19], but in such a way that all the analytic properties (compactness, applicability of positive commutator estimates) will be clear. However, the geometric properties will be less apparent, and we will devote some time to clarifying these.

First, we say that a function $f \in \mathcal{C}^\infty({}^{\mathrm{sc}}T^*_{\partial\bar{X}}\bar{X})$ is π-invariant if for $\tilde{\xi}, \tilde{\xi}' \in {}^{\mathrm{sc}}T^*_{\partial\bar{X}}\bar{X}$, $\pi(\tilde{\xi}) = \pi(\tilde{\xi}')$ implies $f(\tilde{\xi}) = f(\tilde{\xi}')$. A π-invariant function f naturally defines a function f_π on ${}^{\mathrm{sc}}\dot{T}^*\bar{X}$ by $f_\pi(\xi) = f(\tilde{\xi})$ where $\tilde{\xi} \in {}^{\mathrm{sc}}T^*_{\partial\bar{X}}\bar{X}$ is chosen so that $\pi(\tilde{\xi}) = \xi$.

We also need to introduce notation for the upper and lower one-sided derivatives of functions f defined on an interval I:

$$\begin{aligned}
(D_+f)(t_0) &= \liminf_{t\to t_0+} \frac{f(t)-f(t_0)}{t-t_0},\\
(D_-f)(t_0) &= \liminf_{t\to t_0-} \frac{f(t)-f(t_0)}{t-t_0},\\
(D^+f)(t_0) &= \limsup_{t\to t_0+} \frac{f(t)-f(t_0)}{t-t_0},\\
(D^-f)(t_0) &= \limsup_{t\to t_0-} \frac{f(t)-f(t_0)}{t-t_0}.
\end{aligned} \tag{5.17}$$

A function f is thus differentiable at t_0 if and only if these four assume the same (finite) value; then we write these as $Df(t_0)$. Similarly, f is differentiable from the left at t_0 if and only if $(D_-f)(t_0) = (D^-f)(t_0)$ is finite; we write the common value as $Df(t_0-)$.

Definition. (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 $f \in \mathcal{C}^\infty({}^{\mathrm{sc}}T^*_{\partial\bar{X}}\bar{X})$,

$$D_\pm(f_\pi \circ \gamma)(t_0) \geq \inf\{{}^{\mathrm{sc}}H_g^b f(\tilde{\xi}_0) :\ \tilde{\xi}_0 \in \hat{\pi}_b^{-1}(\xi_0),\ C_a \subset C_b\}. \tag{5.18}$$

In this section we usually drop the word 'generalized' for the sake of brevity.

Remark 5.1. Considering $-f$ in place of f, the definition immediately gives a similar estimate for $D^\pm(f_\pi \circ \gamma)(t_0)$. In addition, the function f only has to be defined on ${}^{\mathrm{sc}}T^*_U\bar{X}$ where U is a neighborhood of p in $\partial\bar{X}$, $\gamma(t_0) \in {}^{\mathrm{sc}}T^*_p(C_a;\bar{X})$. Indeed, otherwise one can consider ϕf, where ϕ is (the pull-back of) a cut-off function supported in U that is identically 1 near p, without affecting any of the statements above.

Remark 5.2. The local coordinates y_a and ξ_a are actually differentiable along γ at t_0 since the Hamilton vector fields ${}^{\mathrm{sc}}H_g^b$ applied to them give π-invariant results which agree with each other by (5.9) and (5.11). In addition, over C_0', $\hat{\pi}$ is one-to-one, so if J is an interval and $\gamma|_J$ lies in ${}^{\mathrm{sc}}T^*_{C_0'}\bar{X}$ then $\gamma|_J$ is a bicharacteristic of ${}^{\mathrm{sc}}H_g$.

Moreover, since $\cup_b \hat{\pi}_b^{-1}(\dot{\Sigma}(\lambda))$ is compact, it follows that for any π-invariant function f, the derivatives $D_\pm(f_\pi \circ \gamma)$, $D^\pm(f_\pi \circ \gamma)$ are bounded (independently of t_0, and even of γ), hence $f_\pi \circ \gamma$ is Lipschitz; in fact, uniformly so (i.e. the Lipschitz constant depends on f, but not on γ). This at once implies the equicontinuity of the set of broken bicharacteristics as in [19].

Lemma 5.3. *(cf. Lebeau's proof,* [19, Proposition 6]*) For any compact interval $I = [T_1, T_2]$, the set $\mathcal{R}$ of broken bicharacteristics $\gamma : I \to \dot{\Sigma}(\lambda)$ is equicontinuous.*

Proof. Let d be a metric defining the topology on $\dot{\Sigma}(\lambda)$. Suppose $\mathcal{R}$ is not equicontinuous. That is, suppose that there exists $\epsilon_0 > 0$, sequences s_k, s_k' in I, $\gamma_k \in \mathcal{R}$, such that $|s_k - s_k'| \leq 1/k$ but $d(\gamma_k(s_k), \gamma_k(s_k')) \geq \epsilon_0$. Since $\dot{\Sigma}(\lambda)$ is compact, one can pass to subsequences (which we do not show in the notation) such that $\gamma_k(s_k)$ and $\gamma_k(s_k')$ converge to points ξ and ξ' respectively. Note that $\xi \neq \xi'$ since $d(\xi, \xi') \geq \epsilon_0$. For any π-invariant function f, $f_\pi \circ \gamma_k$ is uniformly Lipschitz (i.e. the Lipschitz constant is independent of k), so $|s_k - s_k'| \leq 1/k$ shows that $|f_\pi(\gamma_k(s_k)) - f_\pi(\gamma_k(s_k'))| \leq M/k$; M independent of k. But f_π is continuous, so $\lim_{k\to\infty} f_\pi(\gamma_k(s_k)) = f_\pi(\xi)$, $\lim_{k\to\infty} f_\pi(\gamma_k(s_k')) = f_\pi(\xi')$, so we conclude $f_\pi(\xi) = f_\pi(\xi')$. But let a be such that $\xi \in {}^{\mathrm{sc}}T_p^*\bar{X}_a$, $p \in C_a'$. All functions on $\bar{X}$, pulled back by the bundle projection to ${}^{\mathrm{sc}}T^*\bar{X}$, are π-invariant, so we see that $\xi' \in {}^{\mathrm{sc}}T_p^*\bar{X}_a$ as well. But $(\xi_a)_j$ is π-invariant near ξ for all j, so this shows $\xi = \xi'$, a contradiction. $\square$

Next, we note that the uniform limit of broken bicharacteristics is a broken bicharacteristic.

Proposition 5.4. *Suppose that I is a compact interval $I = [T_1, T_2]$, $\gamma_k : I \to \dot{\Sigma}(\lambda)$ are broken bicharacteristics, $\gamma : I \to \dot{\Sigma}(\lambda)$, and $\gamma_k \to \gamma$ uniformly on I. Then γ is a broken bicharacteristic.*

Proof. Let f be a π-invariant function, $t_0 \in I$, $\xi_0 = \gamma(t_0)$, and let

$$c_0 = \inf\{{}^{\mathrm{sc}}H_g^b f(\tilde{\xi}_0) : \ \tilde{\xi}_0 \in \hat{\pi}_b^{-1}(\xi_0) : \ C_a \subset C_b\}. \tag{5.19}$$

We need to show that $D_\pm(f_\pi \circ \gamma)(t_0) \geq c_0$. We only consider D_+ for the sake of definiteness. So let $\epsilon > 0$; we need to prove that there exists $\delta > 0$ such that for all $t \in (t_0, t_0 + \delta)$, $f_\pi \circ \gamma(t) - f_\pi \circ \gamma(t_0) \geq (c_0 - \epsilon)(t - t_0)$.

But by the continuity of ${}^{\mathrm{sc}}H_g^b f$ on ${}^{\mathrm{sc}}T^*_{C_b}\bar{X}_b$, there exists a neighborhood U of ξ_0 in $\dot{\Sigma}(\lambda)$ such that ${}^{\mathrm{sc}}H_g^b f(\tilde{\xi}) \geq c_0 - \epsilon/3$ for all b, $\tilde{\xi} \in \hat{\pi}_b^{-1}(\xi)$, $\xi \in U$. Next, by the uniform convergence of the γ_k, there exist $\delta > 0$ and $M \in \mathbb{N}$ such that for $t \in (t_0 - \delta, t_0 + \delta)$, $k \geq M$, $\gamma_k(t) \in U$. Let

$$F_k : I \to \mathbb{R}, \quad F_k(t) = f_\pi \circ \gamma_k(t) - (c_0 - \epsilon/3)t. \tag{5.20}$$

Thus, for $t \in (t_0, t_0 + \delta)$, $k \geq M$, F_k satisfies $D_+ F_k \geq 0$, hence F_k is non-decreasing, so for $t \in (t_0, t_0 + \delta)$, $k \geq M$,

$$f_\pi \circ \gamma_k(t) - f_\pi \circ \gamma_k(t_0) \geq (c_0 - \epsilon/3)(t - t_0). \tag{5.21}$$

Now given $t \in (t_0, t_0+\delta)$, simply choose $k \geq M$ such that $|f_\pi \circ \gamma_k(t) - f_\pi \circ \gamma(t)| < \epsilon(t-t_0)/3$, $|f_\pi \circ \gamma_k(t_0) - f_\pi \circ \gamma(t_0)| < \epsilon(t-t_0)/3$, which is possible since f_π is continuous, so $f_\pi \circ \gamma_k(t') \to f_\pi \circ \gamma(t')$ for all t'. Thus, using this particular value of k and (5.21), we conclude that

$$f_\pi \circ \gamma(t) - f_\pi \circ \gamma(t_0) \geq (c_0 - \epsilon)(t - t_0). \tag{5.22}$$

This holds for every $t \in (t_0, t_0+\delta)$, completing the proof. $\square$

We thus deduce the compactness of the set of broken bicharacteristics.

Proposition 5.5. *For any compact interval $I = [T_1, T_2]$, the set $\mathcal{R}$ of broken bicharacteristics $\gamma : I \to \dot\Sigma(\lambda)$ is compact in the topology of uniform convergence.*

Proof. Since $\mathcal{R}$ is equicontinuous and $\dot\Sigma(\lambda)$ is compact, any sequence of broken bicharacteristics in $\mathcal{R}$ has a convergent subsequence, converging uniformly over I, by the theorem of Ascoli-Arzelá. But the uniform limit of broken bicharacteristics is a broken bicharacteristic, proving the proposition. $\square$

Corollary 5.6. *(cf. Lebeau,* [19, Corollaire 7]*) If $\gamma : (T_1, T_2) \to \dot\Sigma(\lambda)$ is a generalized broken bicharacteristic then γ extends to a generalized broken bicharacteristic on $[T_1, T_2]$.*

Proof. Let $\gamma_n = [T_1, T_1+\delta] \to \dot\Sigma(\lambda)$ be given by $\gamma_n(t) = \gamma(t + 1/n)$, where $\delta > 0$ is chosen sufficiently small. By the previous proposition, there exists a subsequence of $\{\gamma_n\}$ that converges to a broken bicharacteristic $\tilde\gamma : [T_1, T_1+\delta] \to \dot\Sigma(\lambda)$. But then $\tilde\gamma|_{(T_1,T_1+\delta]} = \gamma$, so $\tilde\gamma$ gives the desired extension of γ to $[T_1, T_2)$. The other endpoint can be dealt with similarly. $\square$

Remark 5.7. This corollary shows that every generalized broken bicharacteristic $\gamma_0 : J \to \dot\Sigma(\lambda)$ can be extended to another one, γ, defined over $\mathbb{R}$ (meaning that $\gamma : \mathbb{R} \to \dot\Sigma(\lambda)$ and $\gamma|_J = \gamma_0$). Indeed, by the corollary we may assume that J is closed. It suffices to show that, say, γ can be extended to an interval that is unbounded from below; the extension in the other direction is similar. So suppose the lower endpoint of J is $T_1 \in \mathbb{R}$ (if it is $-\infty$, we are done), and suppose that $\gamma_0(T_1) \in {}^{\mathrm{sc}}T^*_{C'_a}\bar X_a \cap \pi_{ba}(\Sigma_b(\lambda))$; such a b exists by (4.25). Then choose $\tilde\xi \in \Sigma_b(\lambda)$ such that $\pi_{ba}(\tilde\xi) = \gamma_0(T_1)$, and define $\gamma|_{(-\infty,T_1]\cup J}$ by $\gamma(t) = \hat\pi(\exp((t-T_1)^{\mathrm{sc}}H^b_g)(\tilde\xi))$ for $t \leq T_1$, $\gamma(t) = \gamma_0(t)$ for $t \in J$. Directly from Definition (2.1), γ is a generalized broken bicharacteristic with the desired properties.

Since Lipschitz functions are differentiable almost everywhere, and they are equal to the integral of their a.e. defined derivative, we can analyze π-invariant functions such as τ in more detail.

In fact, the Hamilton vector field ${}^{\mathrm{sc}}H^b_g$ applied to $-\tau$ gives $2|\mu_b|^2 \geq 0$, so we deduce that $-\tau$ is monotone increasing, i.e. τ is monotone decreasing along broken bicharacteristics. In fact, writing $F = -\tau \circ \gamma$, note that $\tilde\xi = \hat\pi_b^{-1}(\xi)$ being in $\Sigma_b(\lambda)$ gives

$$\lambda - |\tilde\xi_b|^2 = \lambda - \tau^2 - |\mu_b|^2 \in \operatorname{spec}_{pp}(H^b). \tag{5.23}$$

Thus, $\lambda - \tau^2(\gamma(t_0)) \notin \operatorname{spec}_{pp}(H^b)$ for any b with $C_b \supset C_a$ implies that

$$D_\pm F(t_0) \geq c_0 > 0, \tag{5.24}$$

so there exist $c > 0$ and $\delta > 0$ such that

$$|\tau(\gamma(t)) - \tau(\gamma(t_0))| \geq c|t - t_0| \text{ if } |t - t_0| < \delta, \tag{5.25}$$

so the bicharacteristic γ is not constant. Conversely, if there exists b with $C_b \supset C_a$ such that $\lambda - \tau^2(\gamma(t_0)) \in \operatorname{spec}_{pp}(H^b)$, then the constant curve

$$\gamma_0 : \mathbb{R} \to {}^{\mathrm{sc}}\dot{T}^*\bar{X}, \ \gamma_0(t) = \gamma(t_0) \text{ for all } t \in \mathbb{R}, \tag{5.26}$$

is a broken bicharacteristic since for $\tilde{\xi} \in \hat{\pi}_b^{-1}(\gamma(t_0))$, we have $\mu_b = 0$, so ${}^{\mathrm{sc}}H_g^b(\tilde{\xi})$ vanishes.

Thus, we define the b-radial sets

$$R_\pm^b(\lambda) = \{\xi_b \in \Sigma_b(\lambda) : \ \mu_b = 0, \ \pm\tau \geq 0\}, \tag{5.27}$$

and their image by

$$R_\pm(\lambda) = \cup_b \pi_b(R_\pm^b(\lambda)). \tag{5.28}$$

We cannot expect a non-trivial propagation theorem at points in $R_\pm(\lambda)$ (since one of the broken bicharacteristics through them is stationary), but we can expect such results elsewhere. We emphasize that there can be (and usually there are, though not if there are no bound states in the subsystems) non-constant bicharacteristics through $R_\pm(\lambda)$; it is because there exists a constant bicharacteristic that we cannot expect an interesting propagation result.

Note that if over an interval $J \subset I$, the image of γ is disjoint from $R_+(\lambda) \cup R_-(\lambda)$, then $\gamma|_J$ can be reparameterized using τ as a parameter instead of t; Lipschitz functions on the reparameterized curve remain Lipschitz.

Another interesting π-invariant function is $\eta = \eta_a = z_a \cdot \nu_a$ defined near ${}^{\mathrm{sc}}T_p^*(C_a; \bar{X})$ for some $p \in C_a'$. Since ${}^{\mathrm{sc}}H_g^b\eta$ over $\Sigma_b(\lambda)$ is

$${}^{\mathrm{sc}}H_g^b\eta_a = \frac{x_a}{x}(2\tau_a\eta_a + 2|\nu_{ab}|^2), \tag{5.29}$$

where $\mu_b = (\mu_a, \nu_{ab})$ is the decomposition corresponding to that of X_b with respect to X_a and its orthocomplement, so

$$|\mu_b|^2 = |\mu_a|^2 + |\nu_{ab}|^2, \tag{5.30}$$

we can obtain a monotonicity result for $F = \eta_a \circ \gamma$, defined for t near t_0. First note that $F(t_0) = 0$ (as $z = 0$ at $\gamma(t_0) \in {}^{\mathrm{sc}}T_{C_a'}^*(C_a; \bar{X})$). Next, $F(t) \geq 0$ for $t \geq t_0$. Indeed, if $F(t_1) < 0$, let $t_0' = \sup\{t : \ F(t) = 0, \ t < t_1\}$, so $t_0 \leq t_0' < t_1$; since F is continuous, $F(t) < 0$ for $t \in (t_0', t_1]$. But by (5.29), $D_\pm F(t) \geq cF(t)$ for some $c > 0$ whenever $F \leq 0$, hence on $[t_0', t_1]$, so $D_\pm(e^{-c\cdot}F) \geq 0$ there, so $e^{-c\cdot}F$ is non-decreasing, so $F(t_1) \geq F(t_0') = 0$, a contradiction. Thus, $F(t) \geq 0$ for $t \geq t_0$, so by (5.29), $D_\pm F(t) \geq -c'F(t)$ for some $c' > 0$, so $D_\pm(e^{c'\cdot}F)(t) \geq 0$, hence $e^{c't}F(t)$ is non-decreasing. Thus, with $\eta_a(t) = \eta_a(\gamma(t)) = F(t)$, there exists $\delta > 0$ such that either η_a is identically 0 on $[t_0, t_0 + \delta)$, or $\eta_a(t) > 0$ for $t \in (t_0, t_0 + \delta)$. Since ${}^{\mathrm{sc}}H_g^b|z_a|^2 = 4(x_a/x)\eta_a$ (as η_a is π-invariant), we deduce that there exists $\delta > 0$ such that either $z_a = 0$ for all t in $(t_0, t_0 + \delta)$, or $z_a \neq 0$ for all t in $(t_0, t_0 + \delta)$. If the former holds, then $\gamma|_{(t_0, t_0+\delta)}$ is a differentiable curve in ${}^{\mathrm{sc}}T_{C_a'}^*\bar{X}_a$ with tangent vector given by ${}^{\mathrm{sc}}H_g^a$, by Remark 5.2. In other words, we have proved the following lemma.

Lemma 5.8. *Suppose γ is a broken bicharacteristic. Then there exists $\delta > 0$ such that either $\gamma(t) \in {}^{sc}T_{C_a'}^*(C_a; \bar{X})$ for all $t \in (t_0, t_0 + \delta)$, or $\gamma(t) \notin {}^{sc}T_{C_a'}^*(C_a; \bar{X})$*

for all $t \in (t_0, t_0+\delta)$. If the former holds, then $\gamma|_{(t_0,t_0+\delta)}$ is an integral curve of ${}^{sc}H_g^a$. A similar result holds for $(t_0-\delta, t_0)$. In the former case we say that γ is forward/backward tangential at t_0, in the latter that γ is forward/backward normal at t_0.

Remark 5.9. Note that tangential/normal behavior is the property of γ, not just of its value at t_0, unlike in the situation when there are no bound states in any subsystems. Indeed, in that case we only need to consider ${}^{\mathrm{sc}}H_g f(\tilde{\xi}_0)$ for $\tilde{\xi}_0 \in \hat{\pi}_0(\xi_0)$ in Definition 2.1, so in particular ${}^{\mathrm{sc}}H_g\eta_a(\tilde{\xi}_0) = |\nu_a|^2 = \lambda - \tau_a^2 - |\mu_a|^2$, so γ is tangential if and only if $\tau_a^2 + |\mu_a|^2 = \lambda$ at $\gamma(t_0) \in {}^{\mathrm{sc}}T^*_{C'_a}\bar{X}_a$. This remark also shows that our definition of broken bicharacteristics agrees with that of [37], which in turn corresponds to the analogous definition introduced by Lebeau in the study of the wave equation [19]. In particular, our general definition is equivalent to the one discussed in the introduction if $\Lambda_1 = \{0\}$.

We can give a more geometric description of the broken bicharacteristics, provided that the set of thresholds, Λ_1, is discrete, or if H is a four-body Hamiltonian, $\lambda \notin \Lambda_1$. Since this is improvement is not important for the propagation estimates, we only state the result below, and give the proof in the Appendix. Note that if there are no bound states in any subsystems, then $\Lambda_1 = \{0\}$ is certainly discrete, so in particular the proof applies in the setting of [37] (though it was already proved there, with the proof based on Lebeau's results).

Theorem 5.10. *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 ${}^{sc}H_g^a$ for some a. Similar results hold if the interval of definition, $\mathbb{R}$, is replaced by any interval.*

We end this section by analyzing the behavior of generalized broken bicharacteristics under the assumption that $\lambda \notin \Lambda_1$; this will be useful when studying the resolvent.

Lemma 5.11. *Suppose H is a many-body Hamiltonian, $\lambda \notin \Lambda_1$, and $\gamma : I \to \dot{\Sigma}(\lambda)$ is a generalized broken bicharacteristic where I is a closed unbounded interval. Then*

$$\overline{\gamma(I)} \subset \gamma(I) \cup R_+(\lambda) \cup R_-(\lambda). \tag{5.31}$$

Moreover, if I is not bounded above, $\tau(+\infty) = \lim_{t\to+\infty} \tau(\gamma(t))$ exists, $\lambda - \tau(+\infty)^2 \in \Lambda_1$, and there exists $\xi \in R_+(\lambda) \cup R_-(\lambda)$ and a sequence $t_j \to +\infty$ such that $\xi = \lim_{j\to\infty} \gamma(t_j)$ in $\dot{\Sigma}(\lambda)$ (hence in particular $\tau(\xi) = \tau(+\infty)$). Similar results hold as $t \to -\infty$ if I is not bounded below.

Proof. For the sake of definiteness we take $I = [t_0, +\infty)$, all other cases are very similar.

Since $\tau \circ \gamma$ is monotone decreasing, and τ is a bounded function on $\dot{\Sigma}(\lambda)$, $\tau(+\infty) = \lim_{t\to+\infty} \tau(t)$ exists (we wrote $\tau(t) = \tau(\gamma(t))$).

Now, let $t_n \to +\infty$ be any sequence such that $t_n \geq t_0$ for all n. Let $\gamma_n : [0,1] \to \dot{\Sigma}(\lambda)$ given by $\gamma_n(t) = \gamma(t+t_n)$. By Proposition 5.5, $\{\gamma_n\}$ has a subsequence, which we write as $\gamma'_n = \gamma_{k(n)}$, which converges uniformly to a generalized broken bicharacteristic $\gamma' : [0,1] \to \dot{\Sigma}(\lambda)$. Thus, for $t \in [0,1]$, $\tau(\gamma'(t)) = \lim_{n\to\infty} \tau(\gamma'_n(t)) = \lim_{n\to\infty} \gamma(t + t_{k(n)}) = \tau(+\infty)$, so τ is constant on γ'. Since $\tau \circ \gamma'$ is Lipschitz, it is equal to the integral of its a.e. defined derivative, $-2|\mu(t)|^2$, so we conclude that $|\mu(t)|^2 = 0$ a.e. along γ'. But then the arclength of the projection of γ' to $\mathbb{S}^{n-1}$, which is the integral of $|\mu(t)|$, is also zero, so γ' is a constant curve, and hence, as shown above, there exists $\xi \in R_+(\lambda) \cup R_-(\lambda)$ such that $\gamma'(t) = \xi$ for all $t \in [0,1]$. Thus,

$$\overline{\gamma([t_0,+\infty))} \cap (R_+(\lambda) \cup R_-(\lambda)) \neq \emptyset. \tag{5.32}$$

Also, $\tau(+\infty) = \tau(\xi)$, and $\xi \in R_+(\lambda) \cup R_-(\lambda)$, so $\lambda - \tau(+\infty)^2 \in \Lambda_1$.

We still need to show that if $\{t_n\}$ is a sequence in $[t_0,+\infty)$, and $\{\gamma(t_n)\}$ converges in $\dot\Sigma(\lambda)$, say $\xi_0 = \lim_{n\to\infty} \gamma(t_n)$, then either $\xi \in \gamma([t_0,+\infty))$, or $\xi \in R_+(\lambda) \cup R_-(\lambda)$. Now, if t_n has a subsequence converging to some $T \in [t_0,+\infty)$, then $\gamma(t_n)$ converges to $\gamma(T)$, so we are done. We may thus assume that $t_n \to +\infty$ as $n \to \infty$. By the argument of the previous paragraph, there is a subsequence $t_{k(n)}$ such that $\gamma'_n = \gamma(t + t_{k(n)})$ converges uniformly (over $[0,1]$) to a generalized broken bicharacteristic γ', which is a constant curve, $\gamma'(t) = \xi$ for $t \in [0,1]$, in $R_+(\lambda) \cup R_-(\lambda)$. In particular, $\gamma(t_{k(n)})$ converges to ξ. But on the other hand, $\xi_0 = \lim_{n\to\infty} \gamma(t_n)$, so $\xi_0 = \xi \in R_+(\lambda) \cup R_-(\lambda)$. This proves that

$$\overline{\gamma([t_0,+\infty))} \subset \gamma([t_0,+\infty)) \cup R_+(\lambda) \cup R_-(\lambda). \tag{5.33}$$

□

Remark 5.12. Note that under the assumptions of Theorem 5.10, $\gamma|_{[T,+\infty)}$ is an integral curve of ${}^{\mathrm{sc}}H_g^a$ for a sufficiently large T, so $\xi = \lim_{t\to+\infty} \gamma(t)$ exists in $\dot\Sigma(\lambda)$. Moreover, if $\xi \in R_+(\lambda)$ (i.e. it is incoming), then $\gamma|_{[T,+\infty)}$ is a constant curve, so $\xi \in \gamma([t_0,+\infty))$.

6. Positive commutators

Our approach to prove propagation of singularities along generalized broken bicharacteristics relies on positive commutator estimates. Just as in [36] and [37], we need to commute operators arising by quantization of π-invariant functions $q \in \mathcal{C}^\infty({}^{\mathrm{sc}}T^*_{\partial\bar X}\bar X)$, $\bar X = \mathbb{S}^n_+$ as usual. That q is π-invariant means that at C'_a, the regular part of C_a, given by $x_a = 0$, $z_a = 0$, $q(y_a, z_a, \xi_a, \xi^a)|_{z_a=0}$ is independent of ξ^a, i.e. $q(y_a, 0, \xi_a, \xi^a)$ is independent of ξ_a. This means that (except in some special cases) q is not symbolic at cotangent infinity, i.e. as $\xi \to \infty$, since typically ξ_a derivatives will not give any decay in the ξ^a direction. Recall here that a (non-polyhomogeneous) scattering symbol r of, say, multiorder $(0,0)$, $r \in \mathcal{A}^{(0,0)}(\mathbb{S}^n_+ \times \mathbb{S}^n_+)$, is an element of $\mathcal{C}^\infty(\mathbb{R}^n_w \times \mathbb{R}^n_\xi)$ that satisfies (product-type) symbol estimates in both sets of variables, i.e. for all $\alpha, \beta \in \mathbb{N}^n$ there exists $C_{\alpha\beta} > 0$ such that

$$|D_w^\alpha D_\xi^\beta r(w,\xi)| \leq C_{\alpha\beta} \langle w\rangle^{-|\alpha|} \langle \xi\rangle^{-|\beta|}. \tag{6.1}$$

However, in our arguments the failure of q to be in $\mathcal{A}^{(0,0)}(\mathbb{S}^n_+ \times \mathbb{S}^n_+)$ will never cause a problem, only an inconvenience, since we always localize in the spectrum of the elliptic operator H by composing our operators with $\psi_0(H) \in \Psi_{\mathrm{Sc}}^{-\infty,0}(\bar X, \mathcal{C})$ where $\psi_0 \in \mathcal{C}^\infty_c(\mathbb{R})$. Such operators $\psi_0(H)$ are smoothing – their amplitudes decay rapidly in ξ.

So fix $\psi_0 \in \mathcal{C}^\infty_c(\mathbb{R}; [0,1])$ which is identically 1 in a neighborhood of a fixed λ. Thus, $\psi_0(H) \in \Psi_{\mathrm{Sc}}^{-\infty,0}(\bar X, \mathcal{C})$, so it is smoothing. At the symbol level, $\psi_0(H)$ is locally the right quantization of some

$$p \in \mathcal{C}^\infty([\mathbb{S}^n_+;\mathcal{C}] \times \mathbb{S}^n_+) \tag{6.2}$$

which vanishes to infinite order at $[\mathbb{S}^n_+;\mathcal{C}] \times \partial\mathbb{S}^n_+$, i.e. it is Schwartz in ξ.

We are then interested in the following class of symbols q. We assume that $q \in \mathcal{C}^\infty(\mathbb{R}^n_w \times \mathbb{R}^n_\xi)$ and that for every multiindex α, $\beta \in \mathbb{N}^n$ there exist constants $C_{\alpha,\beta}$ and $m_{\alpha,\beta}$ such that

$$|(D^\alpha_w D^\beta_\xi q)(w,\xi)| \leq C_{\alpha,\beta}\langle w\rangle^{-|\alpha|}\langle\xi\rangle^{m_{\alpha,\beta}}. \tag{6.3}$$

This implies, in particular, that

$$q \in \mathcal{A}^0(\mathbb{S}^n_+ \times \mathbb{R}^n), \tag{6.4}$$

i.e. that q is a 0th order symbol in w, though it may blow up polynomially in ξ. Indeed, in the compactified notation, (6.3) becomes that for every $P \in \mathrm{Diff}_{\mathrm{b}}(\mathbb{S}^n_+)$, acting in the base ($w$) variables, and for every $\beta \in \mathbb{N}^n$ there exist $C_{P,\beta}$ and $m_{P,\beta}$ such that

$$|(PD^\beta_\xi)q| \leq C_{P,\beta}\langle\xi\rangle^{m_{P,\beta}}. \tag{6.5}$$

It is convenient to require in addition that q be polyhomogeneous on $\mathbb{S}^n_+ \times \mathbb{R}^n$:

$$q \in \mathcal{C}^\infty(\mathbb{S}^n_+ \times \mathbb{R}^n); \tag{6.6}$$

this stronger statement (implying (6.4)) automatically holds for the π-invariant symbols we are interested in.

We next introduce the product symbol

$$a(w,w',\xi) = q(w,\xi)p(w',\xi), \tag{6.7}$$

where $\psi_0(H)$ is given locally by the right quantization of p. The main point is

Lemma 6.1. *The symbol a defined by (6.7) is in $\mathcal{C}^\infty(\mathbb{S}^n_+ \times [\mathbb{S}^n_+;\mathcal{C}] \times \mathbb{S}^n_+)$ and it vanishes with all derivatives at $\mathbb{S}^n_+ \times [\mathbb{S}^n_+;\mathcal{C}] \times \partial\mathbb{S}^n_+$. Hence, it defines an operator $A \in \Psi^{-\infty,0}_{Sc}(\mathbb{S}^n_+,\mathcal{C})$ by the oscillatory integral*

$$Au(w) = (2\pi)^{-n}\int e^{i(w-w')\cdot\xi}a(w,w',\xi)\,u(w')\,dw'\,d\xi. \tag{6.8}$$

If in addition q is π-invariant, then for all $\xi \in {}^{sc}T^*(\tilde{C}_a;\bar{X})$ $\hat{A}_a(\xi) = q(\xi)\widehat{\psi_0(H)}_a(\xi)$. In particular, $\widehat{[A,H]}_{a,0}$ vanishes for all a, so $[A,H] \in \Psi^{-\infty,1}_{Sc}(\mathbb{S}^n_+,\mathcal{C})$.

The last statements can be seen directly, but they follow particularly easily from the forthcoming discussion in which we quantize q itself (without the factor p) to act on oscillatory functions, and from the oscillatory testing definition of the indicial operators that we have adopted.

Our immediate goal is now to prove that under certain conditions, the most important of which is that in a part of phase space, say $U \subset \dot{\Sigma}(\lambda)$, ${}^{\mathrm{sc}}H^b_g q$ is negative for all b,

$$i\psi(H)[A^*A,H]\psi(H) \geq B^*B + E + F \tag{6.9}$$

where $B, E \in \Psi^{-\infty,0}_{\mathrm{Sc}}(\mathbb{S}^n_+,\mathcal{C})$ (so they are bounded on $L^2_{\mathrm{sc}}(\mathbb{S}^n_+)$), $F \in \Psi^{-\infty,1}_{\mathrm{Sc}}(\mathbb{S}^n_+,\mathcal{C})$ (so F is compact on $L^2_{\mathrm{sc}}(\mathbb{S}^n_+)$), $\mathrm{WF}'_{\mathrm{Sc}}(E)$ disjoint from U and $\psi \in \mathcal{C}^\infty_c(\mathbb{R};[0,1])$ has sufficiently small support near λ. In view of B^*B, this says that the commutator $i[A^*A,H]$ is microlocally positive at U. The precise version of this statement is Proposition 6.5 at the end of this section.

Due to a square root construction in the ps.d.o. algebra, see [37, Corollary 9.7], this result follows immediately if we prove that all indicial operators of $i\psi(H)[A^*A, H]\psi(H)$ over U are positive. There are two closely related ways to proceed prove the positivity of the indicial operators. A general approach is to follow the proof of the Mourre estimate due to Froese and Herbst [5], but replace their global statements by the appropriate indicial operator ones. This approach is necessary in more general geometric settings. However, in the Euclidean setting it turns out that all one needs is the Mourre estimate in *all* the proper subsystems. We follow this path. Thus, we will need to evaluate some commutators quite explicitly, and use the Mourre estimate in the normal variables and the standard Hamilton vector field commutator estimate in the tangential variables.

Although the evaluation of the commutator appears (and is) rather obvious if we write $A = Q\psi_0(H)$, think of Q as a scattering ps.d.o. obtained by quantizing the symbol q, and use

$$[A, H] = [Q\psi_0(H), H] = [Q, H]\psi_0(H), \tag{6.10}$$

this argument is rather formal since q is not a scattering symbol. Here we follow [36] to make precise sense of this.

So let q be as in Lemma 6.1, and suppose that $f \in \mathcal{C}^\infty(\bar{X}; \mathbb{R})$, $u = e^{if/x}v$, $v \in \mathcal{C}^\infty([\bar{X}; \mathcal{C}])$. Thus, $u \in \cap_{r=0}^\infty H^{r,s}(\mathbb{R}^n)$ for $s < -n/2$. Using our indicial operator definition, $A \in \Psi_{\mathrm{Sc}}^{-\infty,0}(\bar{X}, \mathcal{C})$, the above calculation, (6.10), makes sense and gives the correct result if Q, defined by

$$Qu = (2\pi)^{-n} \int_{\mathbb{R}^n} e^{iw\cdot\xi} q(w,\xi)\hat{u}(\xi)\,d\xi, \tag{6.11}$$

acts on such oscillatory functions. But $u \in \cap_{r=0}^\infty H^{r,s}(\mathbb{R}^n)$, so $\hat{u} \in \cap_{r=0}^\infty H^{s,r}(\mathbb{R}^n)$, so the integral makes sense as a distributional pairing. The same holds if we replace $q(w,\xi)$ by $q^{(k)} = q(w,\xi)\langle\xi\rangle^{-2k}$, and in addition, by choosing k large enough, $q^{(k)}$ satisfies any fixed number of scattering symbol estimates as a scattering symbol of multiorder, say, $(0,0)$. In addition, $Qu = Q^{(k)}(\Delta+1)^k u$, and $(\Delta+1)^k : e^{if/x}\mathcal{C}^\infty([\bar{X}; \mathcal{C}]) \to e^{if/x}\mathcal{C}^\infty([\bar{X}; \mathcal{C}])$. Since any fixed symbol estimate of $e^{-if/x}Pu$, $u \in e^{if/x}\mathcal{C}^\infty([\bar{X}; \mathcal{C}])$, requires only a finite number of scattering symbol estimates on P, we conclude that

$$Q : e^{if/x}\mathcal{C}^\infty([\bar{X}; \mathcal{C}]) \to e^{if/x}\mathcal{C}^\infty([\bar{X}; \mathcal{C}]). \tag{6.12}$$

In addition, to calculate Ru, $R \in \Psi_{\mathrm{sc}}^{*,0}(\bar{X})$, modulo $x^l e^{if/x}\mathcal{C}^\infty([\bar{X}; \mathcal{C}])$ requires only a finite number of scattering symbol estimates on the amplitude r of R, we conclude that in all indicial operator calculations, as well as calculations of lower order terms, we can work as if Q were in $\Psi_{\mathrm{sc}}^{*,0}(\bar{X})$. We also note that if $R \in \Psi_{\mathrm{sc}}^{*,0}(\bar{X})$ has sc-principal symbol $r(y_a, z_a, \xi_a, \xi^a)$, its a-indicial operator, $\hat{R}_{a,0}(y_a, \xi_a)$ is the translation-invariant ps.d.o. $I(r) \in \Psi_{\mathrm{sc}}^{*,0}(\bar{X}^a)$ on X^a given by

$$I(r(y_a, 0, \xi_a, .))v = \mathcal{F}_{X^a}^{-1} r(y_a, 0, \xi_a, \xi^a)\mathcal{F}_{X^a} v,\ v \in \mathcal{S}'(X^a); \tag{6.13}$$

see [36, 37]. Here $\mathcal{F}_{X^a}$ denotes the Fourier transform on X^a. Correspondingly, when applied to $u \in e^{if/x}v$, $v \in \mathcal{C}^\infty([\bar{X}; \mathcal{C}])$, $e^{-if/x}Qu$ is given by $I(q(y_a, 0, \xi_a, .))v$ modulo $x\mathcal{C}^\infty([\bar{X}; \mathcal{C}])$, at C'_a. But q is π-invariant, so $q(y_a, 0, \xi_a, .)$ is independent of ξ^a, so $I(q(y_a, 0, \xi_a, .))$ is just multiplication by $q_\pi(y_a, 0, \xi_a)$, which we will simply write as $q(y_a, 0, \xi_a)$ as in Section 5. Simlarly, ${}^{\mathrm{sc}}H_g^a q|_{z=0}$ is also independent of ξ^a, since

$q|_{z=0}$ is and ${}^{\mathrm{sc}}H_g^a = 2|w_a|^{-1}\xi_a \cdot \partial_{w_a}$ is tangent to ${}^{\mathrm{sc}}T^*_{C_a}\mathbb{S}^n_+$, so $I(({}^{\mathrm{sc}}H_g^a q)(y_a, 0, \xi_a, .))$ is just multiplication by $({}^{\mathrm{sc}}H_g^a q)_\pi(y_a, 0, \xi_a, .) = ({}^{\mathrm{sc}}H_g^a q)(y_a, 0, \xi_a)$.

While the preceeding discussion was quite general, we will be interested in rather special choices of q, which will make the indicial operator calculation simpler. In particular, these choices will allow us to use the standard Mourre estimate on X^a, rather than essentially repeating its proof, as presented by Froese and Herbst [5], see also [3], to obtain a corresponding estimate for more general operators in the normal variables. Thus, we will make a first order assumption on q at the collision planes at infinity, i.e. at the C_a, as well, in addition to its π-invariance. Namely, we assume that for all clusters a, q has the structure

$$d_z q|_{z=0} = q_1\, \xi^a \cdot dz, \quad q_1\ \pi-\text{invariant}, \tag{6.14}$$

so for all a,

$$q = q_0 + q_1\eta_a + \sum_{i,j} z_i z_j q_{ij}, \tag{6.15}$$

with $q_0, q_1 \in \mathcal{C}^\infty({}^{\mathrm{sc}}T^*\bar{X}_a)$, $q_{ij} \in \mathcal{C}^\infty({}^{\mathrm{sc}}T^*\mathbb{S}^n_+)$.

We use this as follows. For $u \in e^{if/x}\mathcal{C}^\infty([\bar{X};\mathcal{C}])$ we can write

$$[A, H]u = AHu - HAu = Q\psi_0(H)Hu - HQ\psi_0(H)u = (QH - HQ)\psi_0(H)u. \tag{6.16}$$

As indicated above, during calculation the indicial operator of $[A, H]$, we can thus work as if Q were a scattering ps.d.o. Recall that our many-body Hamiltonians are of the form

$$H = H^a + \Delta_{X_a} + I_a,\ I_a \in x\,\mathrm{Diff}^2_{\mathrm{sc}}(U), \tag{6.17}$$

U a neighborhood of C'_a, disjoint from C_b such that $C_b \not\supset C_a$. Using (6.17) and (6.16), we write

$$[A, H]u = [Q, \Delta_{X_a}]\psi_0(H)u + [Q, I_a]\psi_0(H)u + [Q, H^a]\psi_0(H)u. \tag{6.18}$$

Since the principal symbol in the scattering calculus is given by the Poisson bracket, for $\tilde{u} = e^{if/x}\tilde{v}$, $\tilde{v} \in \mathcal{C}^\infty([\bar{X};\mathcal{C}])$, $p \in \mathrm{ff}([\bar{X};C_a])$ with $\beta[\bar{X};C_a](p) \in C'_a$,

$$ix^{-1}e^{-if/x}[Q, \Delta_{X_a}]\tilde{u}(p) = I((-{}^{\mathrm{sc}}H_g^a q)(\xi))\tilde{v}(p) = -({}^{\mathrm{sc}}H_g^a q_0)(\xi)\tilde{v}(p), \quad df(p) = \xi, \tag{6.19}$$

here we used that as ${}^{\mathrm{sc}}H_g^a q = {}^{\mathrm{sc}}H_g^a q_0$ is π-invariant, $I({}^{\mathrm{sc}}H_g^a q)$ is a multiplication operator. In addition, as $I_a \in x\,\mathrm{Diff}^2_{\mathrm{Sc}}(\bar{X}, \mathcal{C})$, we see that a priori $QI_a, I_aQ : e^{if/x}\mathcal{C}^\infty([\bar{X};\mathcal{C}]) \to xe^{if/x}\mathcal{C}^\infty([\bar{X};\mathcal{C}])$ with indicial operator given by the composition of the two indicial operators. Since that of Q is $I(q) = q\ \mathrm{Id}$, a multiple of the identity, we conclude that the $(a, 1)$-indicial operator of $[Q, I_a]$ vanishes, so in fact $[Q, I_a] : e^{if/x}\mathcal{C}^\infty([\bar{X};\mathcal{C}]) \to x^2e^{if/x}\mathcal{C}^\infty([\bar{X};\mathcal{C}])$.

The only remaining term is $[Q, H^a]\psi_0(H)$. Note that $z_j = |w_a|^{-1}(w^a)_j$ as usual, so $\eta_a = |w_a|^{-1}w^a \cdot \xi^a$. Thus, with Q_i, Q_{ij} denoting the quantization of q_i and q_{ij} respectively, the same way as Q is the quantization of q,

$$Q = Q_0 + |w^a|^{-1}Q_1 w^a \cdot D_{w^a} + \sum_{i,j} z_i z_j Q_{ij}. \tag{6.20}$$

Here Q_0, Q_1 depend on the ${}^{\mathrm{sc}}T^*\bar{X}_a$ variables only, so they commute with H^a. On the other hand, $[z_i, H^a] \in \Psi^{1,1}_{\mathrm{Sc}}(\mathbb{S}^n_+, \mathcal{C})$ (since all indicial operators of z_i are multiples of the indentity), and $Q_{ij} : e^{if/x}\mathcal{C}^\infty([\bar{X};\mathcal{C}]) \to e^{if/x}\mathcal{C}^\infty([\bar{X};\mathcal{C}])$, so the same holds for $[Q_{ij}, H^a]$. Thus,

$$[z_i z_j Q_{ij}, H^a] : e^{if/x}\mathcal{C}^\infty([\bar{X};\mathcal{C}]) \to |z|^2 e^{if/x}\mathcal{C}^\infty([\bar{X};\mathcal{C}]). \tag{6.21}$$

This proves that for oscillatory functions u,

$$[Q, H^a]\psi_0(H)u = |w_a|^{-1} q_1 [w^a \cdot D_{w^a}, H^a]\psi_0(H)u + u', \quad u' \in |z|^2 e^{if/x}\mathcal{C}^\infty([\bar{X};\mathcal{C}]), \tag{6.22}$$

where q_1 is evaluated at *df* as in (6.19). Thus, we conclude that

$$\begin{aligned} i\widehat{[A^*A, H]}_{a,1}(y_a, \xi_a) = & -2q^{\mathrm{sc}} H^a_g q_0(y_a, 0, \xi_a)\psi_0(H^a + |\xi_a|^2)^2 \\ & + i[B(y_a,\xi_a) + B(y_a,\xi_a)^*, H^a] \end{aligned} \tag{6.23}$$

where

$$B(y_a,\xi_a) = \psi_0(H^a + |\xi_a|^2) q q_1 \sum_j (w^a)_j D_{(w^a)_j} \psi_0(H^a + |\xi_a|^2) \in \Psi^{-\infty,-1}_{\mathrm{sc}}(\bar{X}^a) \tag{6.24}$$

is a ((y_a,ξ_a)-dependent) multiple of the generator of dilations on X^a. Although we worked at C'_a for the sake of convenience, $i\widehat{[A^*A, H]}_{a,1}$ is a well-defined element of $\mathcal{C}^\infty({}^{\mathrm{sc}}T^*(\tilde{C}_a;\bar{X}); \Psi^{-\infty,0}_{\mathrm{Sc}}(\bar{X}^a, \mathcal{C}^a))$; in particular it is continuous on ${}^{\mathrm{sc}}T^*(\tilde{C}_a;\bar{X})$, in which ${}^{\mathrm{sc}}T^*_{C'_a}(\tilde{C}_a;\bar{X})$ is dense, so (6.23) in fact gives $i\widehat{[A^*A, H]}_{a,1}$ on ${}^{\mathrm{sc}}T^*(\tilde{C}_a;\bar{X})$.

We also remark that if $\psi \in \mathcal{C}^\infty_c(\mathbb{R};[0,1])$, $\psi_0 \equiv 1$ on $\operatorname{supp}\psi$, then $\psi(H) = \psi_0(H)\psi(H)$, so $A\psi(H) = Q\psi_0(H)\psi(H) = Q\psi(H)$ on oscillatory functions. Thus,

$$\begin{aligned} i\psi(H)\widehat{[A^*A, H]}\psi(H)_{a,1}(y_a,\xi_a) = & -2q^{\mathrm{sc}} H^a_g q_0(y_a, 0, \xi_a)\psi(H^a + |\xi_a|^2)^2 \\ & + i[B_\psi(y_a,\xi_a) + B_\psi(y_a,\xi_a)^*, H^a] \end{aligned} \tag{6.25}$$

where

$$B(y_a,\xi_a) = \psi(H^a + |\xi_a|^2) q q_1 \sum_j (w^a)_j D_{(w^a)_j} \psi(H^a + |\xi_a|^2) \in \Psi^{-\infty,-1}_{\mathrm{sc}}(\bar{X}^a). \tag{6.26}$$

This also proves the following lemma.

Lemma 6.2. *(see also* [37, Lemma 9.4]*) Let q and A be as in Lemma 6.1, q being π-invariant. Suppose also that q is of the form* (6.15)*. For every seminorm in $\Psi^{-\infty,0}_{Sc}(\bar{X}^a, \mathcal{C}^a)$ and for every $l \in \mathbb{N}$ there exist $C > 0$ and $m \in \mathbb{N}$ such that for every a and every $\xi \in {}^{sc}T^*_p(\tilde{C}_a;\bar{X})$, $p \in \tilde{C}_a$, the seminorm of $\widehat{[A,H]}_{a,1}(\xi)$ in $\Psi^{-\infty,0}_{Sc}(\bar{X}^a, \mathcal{C}^a)$ is bounded by*

$$C(|q(\xi)| + |q_1(\xi)|). \tag{6.27}$$

Remark 6.3. Similar conclusions hold for every seminorm in $\mathcal{C}^\infty({}^{\mathrm{sc}}T^*(\tilde{C}_a;\bar{X}), \Psi^{-\infty,0}_{\mathrm{Sc}}(\bar{X}^a, \mathcal{C}^a))$, which can be seen directly from our calculations in the preceeding proof.

In view of (6.24), the Mourre estimate is immediately applicable; we first recall it. We present it essentially as stated in [3], statement $H_3(a)$, Section 6.4. Let

$$\begin{aligned} & d^a(\sigma) = \inf\{\sigma - \sigma' : \ \sigma' \le \sigma, \ \sigma' \in \Lambda'_a\} \ge 0, \text{ if } \sigma \ge \inf \Lambda'_a, \\ & d^a(\sigma) = 0, \text{ if } \sigma < \inf \Lambda'_a, \end{aligned} \tag{6.28}$$

$$d^{a,\kappa}(\sigma)=\inf\{d^a(\sigma'):\ \sigma'\in[\sigma-\kappa,\sigma+\kappa]\}. \tag{6.29}$$

Then given $\epsilon>0$, $\sigma_0\in\mathbb{R}$, there exists $\delta>0$ such that for all $\sigma\leq\sigma_0$ and for all $\psi_1\in\mathcal{C}_c^\infty(\mathbb{R};[0,1])$ supported in $(\sigma-\delta,\sigma+\delta)$,

$$\begin{aligned}&-i[\psi(H^a)(w^a\cdot D_{w^a}+D_{w^a}\cdot w^a)\psi(H^a+|\xi_a|^2),H^a]/2\\ &\qquad\geq 2(d^{a,\delta}(\sigma)-\epsilon)\psi_1(H^a)^2.\end{aligned} \tag{6.30}$$

Note that this definition of $d^a(\sigma)$ differs slightly from that of [3], namely our $d^a(\sigma)$ is bounded from above by theirs if $\sigma\geq\inf\Lambda_a$, and (6.30) is trivial if $\sigma<\inf\Lambda_a$.

We apply this with $\sigma=\lambda-|\xi_a|^2$, $\sigma_0=\lambda+1$. Thus, given $\epsilon>0$ there exists $\delta>0$ such that for all $\psi\in\mathcal{C}_c^\infty(\mathbb{R};[0,1])$ supported in $(\lambda-\delta,\lambda+\delta)$,

$$\begin{aligned}&-i[\psi(H^a+|\xi_a|^2)(w^a\cdot D_{w^a}+D_{w^a}\cdot w^a)\psi(H^a+|\xi_a|^2),H^a]/2\\ &\qquad\geq 2(d^{a,\delta}(\lambda-|\xi_a|^2)-\epsilon)\psi(H^a+|\xi_a|^2)^2.\end{aligned} \tag{6.31}$$

Note that if $\sigma\geq\inf\Lambda_a'$,

$$\begin{aligned}2d^a(\sigma)&=2\inf\{|\xi^a_b|^2:\ \sigma-|\xi^a_b|^2\in\operatorname{spec}_{pp}(H^b),\ C_b\supset C_a\}\\ &=\inf\{H^b_g(\xi^a\cdot w^a):\ \sigma-|\xi^a_b|^2\in\operatorname{spec}_{pp}(H^b),\ C_b\supset C_a\}\\ &=\inf\{{}^{\mathrm{sc}}H^b_g\eta_a(y_a,0,\xi_a,\xi^a_b):\ \sigma-|\xi^a_b|^2\in\operatorname{spec}_{pp}(H^b),\ C_b\supset C_a\}\geq 0;\end{aligned} \tag{6.32}$$

here ${}^{\mathrm{sc}}H^b_g\eta_a=|\xi^b_a|^2$ is independent of y_a and ξ_a, so the appearance of these on the last line is irrelevant. For the sake of convenience, in the next paragarphs, we write $\inf\emptyset=0$, then (6.32) holds for all $\sigma\in\mathbb{R}$. We remark that $\xi^a\cdot w^a$ is the principal symbol of $(w^a\cdot D_{w^a}+D_{w^a}\cdot w^a)/2$ in the scattering calculus (here the part at infinity is the one that matters), which explains how it arises in the commutator estimates. Thus, with $I=[\lambda-\delta,\lambda+\delta]$,

$$\begin{aligned}&2d^{a,\delta}(\lambda-|\xi_a|^2)\\ &\quad=\inf\{{}^{\mathrm{sc}}H^b_g\eta_a(\tilde\xi):\ \lambda'-|\xi_a|^2-|\xi^a_b|^2\in\operatorname{spec}_{pp}(H^b),\ C_b\supset C_a,\ \lambda'\in[\lambda-\delta,\lambda+\delta]\}\\ &\quad=\inf\{{}^{\mathrm{sc}}H^b_g\eta_a(\tilde\xi):\ \pi_b(\tilde\xi)=\xi,\ C_b\supset C_a,\ \exists\sigma\in\operatorname{spec}_{pp}(H^b),\ |\lambda-|\tilde\xi|^2-\sigma|\leq\delta\}\\ &\quad=\inf\{{}^{\mathrm{sc}}H^b_g\eta_a(\tilde\xi):\ \ C_b\supset C_a,\ \tilde\xi\in\hat\pi_{b,I}^{-1}(\{\xi\})\}.\end{aligned} \tag{6.33}$$

In our estimates, in the part of phase space where we wish to prove that the commutator is positive, we will have

$$q\geq 0,\ q_1\leq 0. \tag{6.34}$$

Note that due to (6.14), for b with $C_b\supset C_a$,

$${}^{\mathrm{sc}}H^b_g q|_{z=0}={}^{\mathrm{sc}}H^a_g q_0+q_1\,{}^{\mathrm{sc}}H^b_g\eta_a. \tag{6.35}$$

The Mourre estimate thus shows that

$$i\psi(H^a+|\xi_a|^2)[B+B^*,H^a]\psi(H^a+|\xi_a|^2)\geq -4qq_1(d^{a,\delta}(\lambda-|\xi_a|^2)-\epsilon)\psi(H^a+|\xi_a|^2)^2. \tag{6.36}$$

Substituting this into (6.23) yields

$$\begin{aligned}&i\psi(H^a+|\xi_a|^2)[\widehat{A^*A,H}]_{a,1}(\xi)\psi(H^a+|\xi_a|^2)\\ &\qquad\geq -2q({}^{\mathrm{sc}}H^a_g q_0+2q_1d^{a,\delta}(\lambda-|\xi_a|^2)-2\epsilon q_1)\psi(H^a+|\xi_a|^2)^2,\end{aligned} \tag{6.37}$$

with

$$-{}^{\mathrm{sc}}H_g^a q_0 - 2q_1 d^{a,\delta}(\lambda - |\xi_a|^2) = \inf\{-{}^{\mathrm{sc}}H_g^b q(\tilde{\xi}) : \quad C_b \supset C_a,\ \tilde{\xi} \in \hat{\pi}_{b,I}^{-1}(\{\xi\})\}, \tag{6.38}$$

where we used (6.33), (6.35). In (6.38), $\inf \emptyset$ must be understood as $-{}^{\mathrm{sc}}H_g^a q_0$, but due to the factors of $\psi(H^a + |\xi_a|^2)$ in (6.23), that equation holds for any value replacing ${}^{\mathrm{sc}}H_g^a q_0 + 2q_1 d^{a,\delta}(\lambda - |\xi_a|^2) - 2\epsilon q_1$ if $\lambda - |\xi_a|^2 < \inf \Lambda_a' - \delta$ (which is exactly when $\inf \emptyset$ arises above).

In order to estimate the commutator on some set $U \subset {}^{\mathrm{sc}}\dot{T}^*\mathbb{S}^n_+$, it is convenient to rewrite this as follows. Suppose that $b \in \mathcal{C}^\infty({}^{\mathrm{sc}}T^*\mathbb{S}^n_+)$ is π-invariant, $\delta_0 > 0$, $I = [\lambda - \delta_0, \lambda + \delta_0]$, for all clusters b,

$$\tilde{\xi} \in \hat{\pi}_{b,I}^{-1}(U) \Rightarrow {}^{\mathrm{sc}}H_g^b q(\tilde{\xi}) \leq -b(\tilde{\xi})^2, \tag{6.39}$$

and there exists $C > 0$ such that for all $\xi \in U$

$$|q_1(\xi)| \leq C b(\xi)^2. \tag{6.40}$$

Then for all $\epsilon' > 0$ there exists $\delta' > 0$ such that if $\operatorname{supp}\psi \subset (\lambda - \delta', \lambda + \delta')$ then

$$i\psi(H^a + |\xi_a|^2)\widehat{[A^*A, H]}_{a,1}\psi(H^a + |\xi_a|^2) \geq (2 - \epsilon')qb^2\psi(H^a + |\xi_a|^2)^2. \tag{6.41}$$

We have thus proved the following proposition.

Proposition 6.4. *(cf.* [37, Proposition 9.6]*) Suppose that H is a many-body Hamiltonian and $\lambda \in \mathbb{R}$. Suppose also that $q, b \in \mathcal{C}^\infty({}^{sc}T^*\mathbb{S}^n_+; \mathbb{R})$ are π-invariant, for all clusters a*

$$q = q_0 + q_1\eta_a + O(|z_a|^2),\ q_0, q_1\ \pi - \mathit{invariant}, \tag{6.42}$$

they satisfy the bounds (6.5)*, $q, b, -q_1 \geq 0$, and that there exist $\delta > 0$, $C > 0$, $C' > 0$, $U \subset \dot{\Sigma}(I)$, where $I = [\lambda - \delta, \lambda + \delta]$, such that for every index a and for all $\xi \in {}^{sc}T^*_{C_a}\bar{X}_a$,*

$$\xi \in \hat{\pi}_{a,I}^{-1}(U) \Rightarrow {}^{sc}H_g^a q(\xi) \leq -b(\xi)^2 \tag{6.43}$$

and

$$\xi \in \hat{\pi}_{a,I}^{-1}(U) \Rightarrow q(\xi) \leq C b(\xi)^2 \ \mathit{and}\ |q_1(\xi)| \leq C' b(\xi)^2. \tag{6.44}$$

Let $A \in \Psi_{Sc}^{-\infty,0}(\bar{X}, \mathcal{C})$ be as in Lemma 6.1. For any $\epsilon' > 0$ there exists $\delta' > 0$ such that if $\psi \in \mathcal{C}_c^\infty(\mathbb{R})$ is supported in $(\lambda - \delta', \lambda + \delta')$ and $\xi \in {}^{sc}T^*(\tilde{C}_a; \bar{X})$ for some a with $\tilde{\pi}(\xi) \in U$, then

$$i(\psi(H)\widehat{[A^*A, H]}\psi(H))_{a,1}(\xi) \geq (2 - \epsilon')b^2 q\psi(\hat{H}_{a,0}(\xi))^2. \tag{6.45}$$

We can now apply [37, Corollary 9.7] to obtain estimates on the original operators. Note that the proof of this corollary consists of a square root construction, [37, Proposition 8.3], for which the existence of L^2 eigenvalues in subsystems is irrelevant, and an indicial operator estimate, which was given in Proposition 9.6 in [37]; here its place is taken by the preceeding result, Proposition 6.4. Recall that the square root construction is via a ps.d.o. version of the functional calculus, and that (6.46) ensures that this can be done within the ps.d.o. calculus. Also, (6.46) might appear weaker than its analogue in [37], but due to (6.42), the other estimates of Corollary 9.7 of that paper follow automatically. Note that π-invariant (continuous) functions on ${}^{\mathrm{sc}}T^*\mathbb{S}^n_+$ can be regarded as (continuous) functions on ${}^{\mathrm{sc}}\dot{T}^*\mathbb{S}^n_+$, so it makes sense to talk about the support of these functions in ${}^{\mathrm{sc}}\dot{T}^*\mathbb{S}^n_+$.

Proposition 6.5. *(cf. [37, Corollary 9.7]) Suppose that the assumptions of Proposition 6.4 are satisfied and let C be as in (6.44), and U open. Suppose in addition that for any cluster a and any differential operator Q on ${}^{sc}T^*(\tilde{C}_a;\bar{X})$ there exists a constant C_Q such that*

$$\begin{aligned}&\tilde{\pi}(\xi)\in U \ \textit{and}\ b(\xi)\neq 0\\ &\ \Rightarrow |Q(b^{-2}q)(\xi)|\leq C_Q \ \textit{and}\ |Q(b^{-2}q_1)(\xi)|\leq C_Q.\end{aligned} \tag{6.46}$$

Then for any $\epsilon'>0$, $M>0$, and for any $K\subset {}^{sc}\dot{T}^*\bar{X}$ compact with $K\subset U$ there exists $\delta'>0$, $\psi\in\mathcal{C}_c^\infty(\mathbb{R})$ is supported in $(\lambda-\delta',\lambda+\delta')$, $\psi\equiv 1$ near λ, $B,E\in\Psi_{Sc}^{-\infty,0}(\bar{X},\mathcal{C})$, $F\in\Psi_{Sc}^{-\infty,1}(\bar{X},\mathcal{C})$ with $\mathrm{WF}'_{Sc}(B),\mathrm{WF}'_{Sc}(E),\mathrm{WF}'_{Sc}(F)\subset\dot{\Sigma}(I)$,

$$\mathrm{WF}'_{Sc}(E)\cap K=\emptyset,\ \mathrm{WF}'_{Sc}(F)\subset\operatorname{supp} q,\ \hat{B}_{a,0}(\xi)=b(\xi)q(\xi)^{1/2}\psi(\hat{H}_{a,0}(\xi)),\ \tilde{\pi}(\xi)\in K, \tag{6.47}$$

such that

$$i\psi(H)x^{-1/2}[A^*A,H]x^{-1/2}\psi(H)-M\psi(H)A^*A\psi(H)\geq(2-\epsilon'-MC)B^*B+E+F. \tag{6.48}$$

Remark 6.6. Multiplying both sides of (6.48) by $\psi_1(H)$ such that $\psi\equiv 1$ on $\operatorname{supp}\psi_1$ shows that ψ can be replaced by any such ψ_1.

7. Propagation of singularities

For our positive commutator estimates it is convenient to consider two scenarios separately, though we present them parallel to each other. Recall that we are interested in proving propagation estimates in $S=\dot{\Sigma}(\lambda)\setminus(R_+(\lambda)\cup R_-(\lambda))$. Note that $\bar{\xi}\in S\cap{}^{\mathrm{sc}}T^*_{C'_a}\bar{X}_a$, $\bar{\xi}=(\bar{y}_a,\bar{\tau}_a,\bar{\mu}_a)$, means that for all b with $C_a\subset C_b$, $\bar{\xi}_b\in\hat{\pi}_b^{-1}(\bar{\xi})$, $\mu_b(\bar{\xi}_b)\neq 0$. The two possibilities are:

(i) $\bar{\mu}_a\neq 0$. Then ${}^{\mathrm{sc}}H_g^a$ does not vanish at $\bar{\xi}$, so there is tangential propagation along C_a.

(ii) $\bar{\mu}_a=0$. Then there is no tangential propagation along C_a. (However, note that as $\bar{\xi}\in S$ this automatically gives $\bar{\xi}\notin\Sigma_a(\lambda)$, so certainly the particles cannot be in an a-bound state.) In this case, by (5.16),

$$^{\mathrm{sc}}H_g^b(z_a\cdot\nu_a)=(x_a/x)(2\tau_a(z_a\cdot\nu_a)+2|\nu_{ab}|^2)>0 \tag{7.1}$$

(near $\hat{\pi}_b^{-1}(\bar{\xi})$) since $\mu_b\neq 0$ there, so $\nu_{ab}\neq 0$ by (5.30). Thus, we can use $z_a\cdot\nu_a$ as a parameter along broken bicharacteristics.

The main technical result on the propagation of singularities is the following.

Proposition 7.1. *Suppose that H is a many-body Hamiltonian. Let $u\in\mathcal{C}^{-\infty}(\bar{X})$, $\lambda\notin\Lambda_1$. Let $\bar{\xi}\in S\cap{}^{sc}T^*_{C'_a}\bar{X}_a$, $\bar{\xi}=(\bar{y}_a,\bar{\tau}_a,\bar{\mu}_a)$, and suppose that $\bar{\xi}\notin\mathrm{WF}_{Sc}((H-\lambda)u)$. Let $\eta_a=z_a\cdot\nu_a$. Then there exists a neighborhood U_0 of $\bar{\xi}$ with the following properties.*

(i) *If $\bar{\mu}_a\neq 0$ and there exists a neighborhood $U\subset U_0$ of $\bar{\xi}$ in $\dot{\Sigma}(\lambda)$ and if there exists $s_0>0$ such that $\exp(-s_0\,{}^{sc}H_g^a)(\bar{\xi})\notin\mathrm{WF}_{Sc}(u)$ and for all s satisfying $0\leq s\leq s_0$, $\exp(-s\,{}^{sc}H_g^a)(\bar{\xi})\in U$ (i.e. the integral curve segment of ${}^{sc}H_g^a$ is completely inside U), and in addition*

$$\xi\in U\ \textit{and}\ \eta_a(\xi)<0\Rightarrow\xi\notin\mathrm{WF}_{Sc}(u), \tag{7.2}$$

then $\bar{\xi}\notin\mathrm{WF}_{Sc}(u)$.

(ii) *If $\bar\mu_a = 0$ and there exists a neighborhood $U \subset U_0$ of $\bar\xi$ in $\dot\Sigma(\lambda)$ such that*

$$\xi \in U \text{ and } \eta_a(\xi) < 0 \Rightarrow \xi \notin \mathrm{WF}_{Sc}(u), \tag{7.3}$$

then $\bar\xi \notin \mathrm{WF}_{Sc}(u)$.

Remark 7.2. Note that $\eta_a(\xi) < 0$ implies $z_a \neq 0$, so $\xi \notin {}^{\mathrm{sc}}T^*_{C'_a}\bar X_a$.

Proof. The main step in the proof is the construction of an operator which has a microlocally positive commutator with H near ξ_0. In fact, we construct the symbol of this operator. This symbol will not be a scattering symbol, i.e. it will not be in $\mathcal{C}^\infty(\mathbb{S}^n_+ \times \mathbb{S}^n_+)$, only due to its behavior as $\nu \to \infty$ corresponding to its π-invariance. This will be accommodated by composing its quantization with a cutoff in the spectrum of H, $\psi(H)$, $\psi \in \mathcal{C}^\infty_c(\mathbb{R})$ supported near λ, as discussed in Lemma 6.1. This approach simply extends the one taken in [36]-[37], though the actual construction is different due to the more complicated geometry.

We introduce some notation and then fix U_0. We define $c_0 > 0$ by

$$c_0 = \frac{1}{2}\inf\{-{}^{\mathrm{sc}}H^b_g\tau(\bar\xi_b) : \ \bar\xi_b \in \hat\pi_b^{-1}(\bar\xi),\ C_b \supset C_a\} > 0. \tag{7.4}$$

Note that at C_a, where $|w_a|/|w| = x/x_a = 1$,

$$\tau = \tau_a - \eta_a,\ \text{since } \tau = -\frac{w\cdot\xi}{|w|},\ \tau_a = -\frac{w^a\cdot\xi^a}{|w_a|},\ \eta_a = \frac{w_a\cdot\xi_a}{|w_a|}, \tag{7.5}$$

and if $\bar\mu_a = 0$, then ${}^{\mathrm{sc}}H_g\tau_a(\bar\xi_b) = 0$ when $\pi(\bar\xi_b) = \bar\xi$. Thus, if $\bar\mu_a = 0$, then

$$c_0 = \frac{1}{2}\inf\{{}^{\mathrm{sc}}H^b_g(z_a\cdot\nu_a)(\bar\xi_b) : \ \bar\xi_b \in \hat\pi_b^{-1}(\bar\xi)\} > 0. \tag{7.6}$$

Now fix $I = [\lambda - \delta_0, \lambda + \delta_0]$ and U_0 to a neighborhood of $\bar\xi$ in $\dot\Sigma(I)$ such that $U_0 \subset \bigcup\{{}^{\mathrm{sc}}T^*_{C'_b}\bar X_b : \ C_a \subset C_b\}$, $U_0 \cap \mathrm{WF}_{\mathrm{Sc}}((H-\lambda)u) = \emptyset$ (this is possible since $\mathrm{WF}_{\mathrm{Sc}}((H-\lambda)u)$ is closed), U_0 is inside a fixed system of local coordinates, and

$$\begin{aligned}&\text{if } \bar\mu_a \neq 0 \text{ then } \xi \in U_0,\ \bar\xi \in \hat\pi^{-1}_{b,I}(\xi),\ C_b \supset C_a \Rightarrow -{}^{\mathrm{sc}}H^b_g\tau(\xi_b) > 3c_0/2\\ &\text{if } \bar\mu_a = 0 \text{ then } \xi \in U_0,\ \xi_b \in \hat\pi^{-1}_{b,I}(\xi),\ C_b \supset C_a \Rightarrow {}^{\mathrm{sc}}H^b_g(z_a\cdot\nu_a)(\xi_b) > 3c_0/2.\end{aligned} \tag{7.7}$$

If $\bar\mu_a \neq 0$, we make an additional definition. Namely, we let $\delta > 0$ be given by

$$-\delta = \bar\tau - \tau(\exp(-s_0{}^{\mathrm{sc}}H^a_g)(\bar\xi)). \tag{7.8}$$

We will use $\epsilon \in (0,1)$ as a small parameter that microlocalizes in a neighborhood of $\bar\xi$ if $\bar\mu_a = 0$, and in a neighborhood of $\{\exp(-s{}^{\mathrm{sc}}H^a_g)(\bar\xi) : \ s \in [0, s_0]\}$ if $\bar\mu_a \neq 0$; if $\bar\mu_a \neq 0$ we will always take $\epsilon < \delta$.

Employing an iterative argument as usual, we may assume that $\bar\xi \notin \mathrm{WF}^{*,l}_{\mathrm{Sc}}(u)$ and we need to show that $\bar\xi \notin \mathrm{WF}^{*,l+1/2}_{\mathrm{Sc}}(u)$. (We can start the induction with an l such that $u \in H^{*,l}_{\mathrm{sc}}(\bar X)$.)

Our positive commutator estimates at a point $\bar\xi_a = (\bar y_a, \bar\tau, \bar\mu_a)$ will arise by considering functions

$$\begin{aligned}&\phi = \bar\tau - \tau + \epsilon^{-1}(|z_a|^2 + \omega),\ \text{if } \bar\mu_a \neq 0,\\ &\phi = z_a\cdot\nu_a + \frac{\beta}{\epsilon}(|z_a|^2 + \omega),\ \text{if } \bar\mu_a = 0,\end{aligned} \tag{7.9}$$

where ω localizes in the tangential variables y_a, τ_a, μ_a. In fact, if $\bar\mu_a \neq 0$, then ${}^{\mathrm{sc}}H^a_g(\bar\xi_a) \neq 0$, so we construct ω to be a 'quadratic distance' (in ${}^{\mathrm{sc}}T^*_{C_a}\bar X_a$) from the ${}^{\mathrm{sc}}H^a_g$ integral curve through $\bar\xi_a$ constructed so that ${}^{\mathrm{sc}}H^a_g\omega = 0$. That is, we define

ω on a hypersurface through $\bar{\xi}$ that is transversal to ${}^{\mathrm{sc}}H_g^a$, e.g. $\tau_a = \bar{\tau}_a$, to be given by a positive definite quadratic form in some local coordinates centered at $\bar{\xi}$, e.g. $(y_a - \bar{y}_a)^2 + (\mu_a - \bar{\mu}_a)^2$, and extend it to ${}^{\mathrm{sc}}T^*_{C_a}\bar{X}_a$ to be constant along the ${}^{\mathrm{sc}}H_g^a$ integral curves; cf. [37, Section 7]. We can then extend ω to a function on ${}^{\mathrm{sc}}T^*_{\partial\bar{X}}\bar{X}$ defined near C_a as discussed before (5.11), and then

$$ {}^{\mathrm{sc}}H_g\omega = 0, \text{ so } {}^{\mathrm{sc}}H_g^b\omega = 0 \text{ for all } b. \tag{7.10}$$

On the other hand, if $\bar{\mu}_a = 0$, we can take

$$\omega_0 = (\xi_a - \bar{\xi}_a)^2 + (y_a - \bar{y}_a)^2; \tag{7.11}$$

now

$$ {}^{\mathrm{sc}}H_g^a\omega_0 = 2(y_a - \bar{y}_a)\cdot {}^{\mathrm{sc}}H_g^a y_a = 4\mu_a\cdot(y_a - \bar{y}_a), \tag{7.12}$$

so $|{}^{\mathrm{sc}}H_g^a\omega_0| \leq C'\omega_0$. Thus, for C sufficiently large, we see that for

$$\omega = e^{-C\tau}\omega_0,\ {}^{\mathrm{sc}}H_g^a\omega \geq 0 \tag{7.13}$$

since $-{}^{\mathrm{sc}}H_g^a\tau > 0$ on S, hence near $\bar{\xi}$. Since ω depends on the tangential variables only, we conclude in either case that for all b,

$$ {}^{\mathrm{sc}}H_g^b\omega \geq 0. \tag{7.14}$$

Moreover, ${}^{\mathrm{sc}}H_g^b|z_a|^2 = 4z_{ab}\cdot\nu_{ab}$ under the decomposition $\mu_b = (\mu_a, \nu_{ab})$, so ${}^{\mathrm{sc}}H_g^b|z_a|^2 \leq C_1|z_a|$.

Now suppose that $\bar{\mu}_a \neq 0$,

$$\phi \leq 2\epsilon,\ \bar{\tau} - \tau \geq -\delta - \epsilon. \tag{7.15}$$

Since $\omega \geq 0$ and $|z_a|^2 \geq 0$, the first of these inequalities implies that $\bar{\tau} - \tau \leq 2\epsilon$, and the combination of these two gives $\phi - (\bar{\tau} - \tau) \leq \delta + 3\epsilon \leq 4\delta$ as $\epsilon < \delta$. Then we conclude that

$$-\delta - \epsilon \leq \bar{\tau} - \tau \leq 2\epsilon,\ |z_a| \leq 2(\epsilon\delta)^{1/2},\ \omega^{1/2} \leq 2(\delta\epsilon)^{1/2}. \tag{7.16}$$

Note that for all b with $C_b \supset C_a$, $z_{ab}\cdot\nu_{ab} = z_a\cdot\nu_a$ at ${}^{\mathrm{sc}}T^*_{C_b}\bar{X}_b$. Thus, if

$$z_a\cdot\nu_a \geq -C_3\epsilon c_0 \tag{7.17}$$

we see that

$$ {}^{\mathrm{sc}}H_g^b|z_a|^2 = 4z_a\cdot\nu_a \geq -4C_3\epsilon c_0. \tag{7.18}$$

Thus, using (7.7) as well, we deduce that there exists $C_4 > 0$ (independent of $\epsilon > 0$) such that

$$\text{if } z_a\cdot\nu_a \geq -C_4\epsilon, \text{ then } {}^{\mathrm{sc}}H_g^b\phi \geq -{}^{\mathrm{sc}}H_g^b\tau - c_0/2 > c_0. \tag{7.19}$$

Note that here $\epsilon \in (0,\delta)$ is arbitrary.

Similarly, suppose that $\bar{\mu}_a = 0$,

$$\phi \leq 2\epsilon,\ z_a\cdot\nu_a \geq -2\epsilon. \tag{7.20}$$

Then we conclude that

$$|z_a\cdot\nu_a| \leq 2\epsilon,\ |z_a| \leq 2\epsilon/\sqrt{\beta},\ \omega^{1/2} \leq 2\epsilon/\sqrt{\beta}. \tag{7.21}$$

Thus, from (7.7),

$$ {}^{\mathrm{sc}}H_g^b\phi \geq {}^{\mathrm{sc}}H_g^b(z_a\cdot\nu_a) - 2\sqrt{\beta}C_1 > c_0 \text{ if } \beta = (c_0/4C_1)^2. \tag{7.22}$$

The positive commutator estimate then arises by considering the following π-invariant symbol q and quantizing it as in Lemma 6.1. Let $\chi_0 \in \mathcal{C}^\infty(\mathbb{R})$ be equal to 0 on $(-\infty, 0]$ and $\chi_0(t) = \exp(-1/t)$ for $t > 0$. Thus, $\chi_0'(t) = t^{-2}\chi_0(t)$, $t > 0$, and $\chi_0'(t) = 0$, $t \leq 0$. Let $\chi_1 \in \mathcal{C}^\infty(\mathbb{R})$ be 0 on $(-\infty, 0]$, 1 on $[1, \infty)$, with $\chi_1' \geq 0$ and $\chi_1(t) = \exp(-1/t)$ on some small interval $(0, t_0)$, $t_0 > 0$. Furthermore, for $A_0 > 0$ large, to be determined, let

$$q = \chi_0(A_0^{-1}(2 - \phi/\epsilon))\chi_1((\bar{\tau} - \tau + \delta)/\epsilon + 1) \tag{7.23}$$

if $\bar{\mu}_a \neq 0$, and let

$$q = \chi_0(A_0^{-1}(2 - \phi/\epsilon))\chi_1((z_a \cdot \nu_a)/\epsilon + 2) \tag{7.24}$$

if $\bar{\mu}_a = 0$. Thus, $q(\tilde{\xi}) = \chi_0(2/A_0) > 0$, and on $\operatorname{supp} q$ we have

$$\phi \leq 2\epsilon \text{ and } \bar{\tau} - \tau \geq -\delta - \epsilon \text{ in case (i),} \tag{7.25}$$

and

$$\phi \leq 2\epsilon \text{ and } z_a \cdot \nu_a \geq -2\epsilon \text{ in case (ii),} \tag{7.26}$$

which are exactly (7.15) and (7.20), so $\operatorname{supp} q$ is a subset of (7.16) and (7.21) respectively. We also see that as ϵ decreases, so does $\operatorname{supp} q = \operatorname{supp} q_\epsilon$, in fact, if $0 < \epsilon' < \epsilon$ then $q_\epsilon > 0$ on $\operatorname{supp} q_{\epsilon'}$. Note that in case (i), by reducing ϵ, we can make q supported in an arbitrary small neighborhood of a compact backward bicharacteristic segment through $\bar{\xi}$, and in case (ii), by reducing ϵ, we can make q supported in an arbitrary small neighborhood of $\bar{\xi}$.

We at once obtain positivity estimates for ${}^{\mathrm{sc}}H_g^c q$. The following argument works similarly for both $\bar{\mu}_a = 0$ and $\bar{\mu}_a \neq 0$; we consider the slightly more complicated case $\bar{\mu}_a \neq 0$. Thus, if $\bar{\mu}_a \neq 0$, then

$$\begin{aligned} {}^{\mathrm{sc}}H_g^c q = &-A_0^{-1}\epsilon^{-1}\chi_0'(A_0^{-1}(2 - \phi/\epsilon))\chi_1((\bar{\tau} - \tau + \delta)/\epsilon + 1)\,{}^{\mathrm{sc}}H_g^c\phi \\ &- \epsilon^{-1}\chi_0(A_0^{-1}(2 - \phi/\epsilon))\chi_1'((\bar{\tau} - \tau + \delta)/\epsilon + 1)\,{}^{\mathrm{sc}}H_g^c\tau. \end{aligned} \tag{7.27}$$

We break up the first term by using a cutoff that ensures that the hypothesis in (7.19) is satisfied. Thus, let

$$\tilde{\chi} = \chi_1(4z_a \cdot \nu_a/(C_4\epsilon) + 2), \tag{7.28}$$

so

$$\text{on } \operatorname{supp}\tilde{\chi},\ z_a \cdot \nu_a \geq -C_4\epsilon/2, \tag{7.29}$$

$$\text{and on } \operatorname{supp}(1 - \tilde{\chi}),\ z_a \cdot \nu_a \leq -C_4\epsilon/4. \tag{7.30}$$

Then

$${}^{\mathrm{sc}}H_g^c q = -\tilde{b}_c^2 + e_c \tag{7.31}$$

with

$$\tilde{b}_c^2 = A_0^{-1}\epsilon^{-1}\chi_0'(A_0^{-1}(2 - \phi/\epsilon))\chi_1((\bar{\tau} - \tau + \delta)/\epsilon + 1)\tilde{\chi}\,{}^{\mathrm{sc}}H_g^c\phi. \tag{7.32}$$

Hence, with

$$b^2 = c_0 A_0^{-1}\epsilon^{-1}\chi_0'(A_0^{-1}(2 - \phi/\epsilon))\chi_1((\bar{\tau} - \tau + \delta)/\epsilon + 1)\tilde{\chi}, \tag{7.33}$$

using (7.19) and (7.29), we deduce that

$${}^{\mathrm{sc}}H_g^c q \leq -b^2 + e_c. \tag{7.34}$$

Moreover,

$$b^2 \geq (c_0 A_0/16) q \tag{7.35}$$

since $\phi \geq \bar\tau - \tau \geq -2\delta$ on $\operatorname{supp} q$, so

$$\begin{aligned}\chi_0'(A_0^{-1}(2-\phi/\epsilon)) &= A_0^2(2-\phi/\epsilon)^{-2}\chi_0(A_0^{-1}(2-\phi/\epsilon))\\ &\geq (A_0^2/16)\chi_0(A_0^{-1}(2-\phi/\epsilon)).\end{aligned} \tag{7.36}$$

On the other hand, e_c is supported where either

$$-\delta-\epsilon \leq \bar\tau-\tau \leq -\delta,\ \omega^{1/2} \leq 2(\epsilon\delta)^{1/2},\ |z_a| \leq 2(\epsilon\delta)^{1/2} \tag{7.37}$$

so near the backward direction along ${}^{\mathrm{sc}}H_g^a$ bicharacteristic through $\bar\xi$, or

$$z_a\cdot\nu_a \leq -C_4\epsilon/4, \text{ and } -\delta-\epsilon \leq \bar\tau-\tau \leq 2\epsilon,\ \omega^{1/2} \leq 2(\epsilon\delta)^{1/2},\ |z_a| \leq 2(\epsilon\delta)^{1/2}. \tag{7.38}$$

But by our assumption $\exp(-s_0{}^{\mathrm{sc}}H_g^a)(\bar\xi) \notin \mathrm{WF}_{\mathrm{Sc}}(u)$, $s_0 > 0$, so the same holds for a sufficiently small neighborhood of $\exp(-s_0{}^{\mathrm{sc}}H_g^a)(\bar\xi)$ as $\mathrm{WF}_{\mathrm{Sc}}(u)$ is closed. By choosing $\epsilon > 0$ sufficiently small, we can thus make sure that the region defined by (7.37) is disjoint from $\mathrm{WF}_{\mathrm{Sc}}(u)$. Moreover, by further reducing $\epsilon > 0$ if necessary and using our second assumption, we can also make sure that the region (7.38) is also disjoint from $\mathrm{WF}_{\mathrm{Sc}}(u)$, so that $\operatorname{supp} e_c$ is disjoint from $\mathrm{WF}_{\mathrm{Sc}}(u)$ for all c. Moreover, by (7.16), for $\epsilon > 0$ sufficiently small, we deduce from the inductive hypothesis that $\operatorname{supp} q$ (hence $\operatorname{supp} b$) is disjoint from $\mathrm{WF}_{\mathrm{Sc}}^{*,l}(u) \cap \dot\Sigma(I)$.

Moreover, with ∂ denoting a partial derivative with respect to one of (y, z, τ, μ, ν),

$$\begin{aligned}\partial q = &-A_0^{-1}\epsilon^{-1}\chi_0'(A_0^{-1}(2-\phi/\epsilon))\chi_1((\bar\tau-\tau+\delta)/\epsilon+1)\partial\phi\\ &-\epsilon^{-1}\chi_0(A_0^{-1}(2-\phi/\epsilon))\chi_1'((\bar\tau-\tau+\delta)/\epsilon+1)\partial\tau.\end{aligned} \tag{7.39}$$

At any C_b with $p \in C_b$, defined by $x = 0$, $z'' = 0$, as above, ϕ is independent of ν'' at $z'' = 0$ so outside $\operatorname{supp} e_c$

$$|\partial_{\nu''}^\beta dq| \leq C_\beta b^2 \text{ at } z'' = 0. \tag{7.40}$$

In fact, outside $\operatorname{supp} e_c$, but in the set where b is positive,

$$b^{-2}\partial q = c_0^{-1}\partial\phi, \tag{7.41}$$

so the uniform bounds of (6.46) also follow. In addition, at any cluster b, $|z_a|^2 = |z_{ab}|^2 + |z_a^b|^2$, $\eta_a = z_{ab}\cdot\nu_{ab} + z_a^b\cdot\nu_a^b = z_{ab}\cdot\nu_{ab} + \eta_b$, and z_{ab}, ν_{ab} are b-tangential variables, so ϕ, hence q has the form (6.42) around each C_b.

Let $\tilde\psi \in \mathcal{C}_c^\infty(\mathbb{R})$ be identically 1 near 0 and supported close to 0. We also define

$$\tilde q = \tilde\psi(x) q. \tag{7.42}$$

Thus, $\tilde q \in \mathcal{C}^\infty({}^{\mathrm{sc}}T^*\bar X)$ is a π-invariant function satisfying (6.5). Let A be the operator given by Lemma 6.1 with $\tilde q$ in place of q, so in particular its indicial operators are $q(\xi)\psi_0(\hat H_{b,0}(\xi))$. Note that (6.44) holds with $C = 16c_0^{-1}A_0^{-1}$. So suppose that $M > 0$ and $\epsilon' > 0$. Choose A_0 so large that $MC < \epsilon'$, and let U be the complement of $\cup_c\pi_c(\operatorname{supp} e_c)$ in $\dot\Sigma(I)$, and let $K = \mathrm{WF}_{\mathrm{Sc}}(u) \cap \dot\Sigma(I)$; so $K \subset U$ by our choice of $\epsilon > 0$. By Proposition 6.5 we deduce that there exists $\delta' > 0$,

$\psi \in \mathcal{C}_c^\infty(\mathbb{R})$ is supported in $(\lambda-\delta',\lambda+\delta')$, $\psi\equiv 1$ near λ, $B,E\in\Psi_{\mathrm{Sc}}^{-\infty,0}(\bar{X},\mathcal{C})$, $F\in\Psi_{\mathrm{Sc}}^{-\infty,1}(\bar{X},\mathcal{C})$ with $\mathrm{WF}'_{\mathrm{Sc}}(B),\mathrm{WF}'_{\mathrm{Sc}}(E),\mathrm{WF}'_{\mathrm{Sc}}(F)\subset\dot{\Sigma}(I)$,

(7.43)
$$\mathrm{WF}'_{\mathrm{Sc}}(E)\cap K=\emptyset,\ \mathrm{WF}'_{\mathrm{Sc}}(F)\subset\operatorname{supp} q,\ \hat{B}_{a,0}(\xi)=b(\xi)q(\xi)^{1/2}\psi(\hat{H}_{a,0}(\xi)),\ \tilde{\pi}(\xi)\in K,$$

such that

(7.44)
$$i\psi(H)x^{-1/2}[A^*A,H]x^{-1/2}\psi(H)-M\psi(H)A^*A\psi(H)\geq(2-2\epsilon')B^*B+E+F.$$

Let

$$\Lambda_r=x^{-l-1/2}(1+r/x)^{-1},\quad r\in(0,1),\tag{7.45}$$

so $\Lambda_r\in\Psi_{\mathrm{Sc}}^{0,-l+1/2}(X,\mathcal{C})$ for $r\in(0,1)$ and it is uniformly bounded in $\Psi_{\mathrm{Scc}}^{0,-l-1/2}(X,\mathcal{C})$. The last statement follows from $(1+r/x)^{-1}$ being uniformly bounded as a 0th order symbol, i.e. from $(x\partial_x)^k(1+r/x)^{-1}\leq C_k$ uniformly (C_k independent of r). In particular, note that

(7.46)
$$x\partial_x(1+r/x)^{-1}=rx^{-1}(1+r/x)^{-2}=\frac{r}{x+r}(1+r/x)^{-1}=(1-(1+r/x)^{-1})(1+r/x)^{-1}.$$

Since $0\leq\frac{r}{x+r}\leq 1$, $(x\partial_x)(1+r/x)^{-1}$ is a uniformly bounded multiple of $(1+r/x)^{-1}$, and in fact this bounded multiplier is uniformly bounded as a 0th order symbol. This also implies that

$$[(1+r/x)^{-1},H](1+r/x)\tag{7.47}$$

which is a priori uniformly bounded in $\Psi_{\mathrm{Scc}}^{1,0}(X,\mathcal{C})$ only, is in fact uniformly bounded in $\Psi_{\mathrm{Scc}}^{1,1}(X,\mathcal{C})$.

We also define

$$A_r=A\Lambda_r x^{-1/2}\psi(H),\ B_r=B\Lambda_r,\ E_r=\Lambda_r E\Lambda_r.\tag{7.48}$$

Then, with $\psi_0\in\mathcal{C}_c^\infty(\mathbb{R};[0,1])$ identically 1 near $\operatorname{supp}\psi$,

(7.49)
$$\begin{aligned}
&ix^{l+1/2}[A_r^*A_r,H]x^{l+1/2}\\
&=i(1+r/x)^{-1}\psi(H)x^{-1/2}[A^*A,H]x^{-1/2}\psi(H)(1+r/x)^{-1}\\
&+i(1+r/x)^{-1}\psi(H)A^*(1+r/x)x^{l+1/2}[\Lambda_r x^{-1/2},H]x^{-1/2}\psi_0(H)A\psi(H)(1+r/x)^{-1}\\
&+i(1+r/x)^{-1}\psi(H)A^*\psi_0(H)x^{-1/2}[\Lambda_r x^{-1/2},H](1+r/x)x^{l+1/2}A\psi(H)(1+r/x)^{-1}\\
&+H_r,
\end{aligned}$$

where H_r is uniformly bounded in $\Psi_{\mathrm{Scc}}^{-\infty,1}(X,\mathcal{C})$. Note that H_r arises by commuting A, powers of x and Λ_r through other operators, but as the indicial operators of A and x are a multiple of the identity, A, x and Λ_r commute with these operators to top order, and in case of Λ_r, the commutator is uniformly bounded as an operator of one lower order. Then, multiplying (7.44) by $(1+r/x)^{-1}$ from the left and right and rearranging the terms we obtain the following estimate of bounded self-adjoint operators on $L^2_{\mathrm{sc}}(X)$:

(7.50)
$$\begin{aligned} &ix^{l+1/2}[A_r^*A_r,H]x^{l+1/2}\\ &\qquad -(1+r/x)^{-1}(\psi(H)A^*(G_r^*+G_r)A\psi(H)+M\psi(H)A^*A\psi(H))(1+r/x)^{-1}\\ &\qquad \geq x^{l+1/2}((2-\epsilon')B_r^*B_r+E_r+F_r)x^{l+1/2}\end{aligned}$$

where

$$G_r=i\psi_0(H)x^{-1/2}[\Lambda_r x^{-1/2},H](1+r/x)x^{l+1/2}, \tag{7.51}$$

and $F_r\in\Psi_{\mathrm{Sc}}^{-\infty,-2l+1}(X,\mathcal{C})$ is uniformly bounded in $\Psi_{\mathrm{Scc}}^{-\infty,-2l}(X,\mathcal{C})$ as $r\to 0$. Since $[(1+r/x)^{-1},H](1+r/x)$ is uniformly bounded in $\Psi_{\mathrm{Scc}}^{1,1}(X,\mathcal{C})$, we conclude that G_r is uniformly bounded in $\Psi_{\mathrm{Scc}}^{-\infty,0}(X,\mathcal{C})$, hence as a bounded operator on $L^2_{\mathrm{sc}}(X)$. Thus, if $M>0$ is chosen sufficiently large, then $G_r+G_r^*\geq -M$ for all $r\in(0,1)$, so

$$(1+r/x)^{-1}\psi(H)A^*(G_r+G_r^*+M)A\psi(H)(1+r/x)^{-1}\geq 0. \tag{7.52}$$

Adding this to (7.50) shows that

$$ix^{l+1/2}[A_r^*A_r,H]x^{l+1/2}\geq x^{l+1/2}((2-\epsilon')B_r^*B_r+E_r+F_r)x^{l+1/2}. \tag{7.53}$$

The point of the commutator calculation is that in $L^2_{\mathrm{sc}}(\bar{X})$

$$\begin{aligned}\langle u,&[A_r^*A_r,H]u\rangle\\ &=\langle u,A_r^*A_r(H-\lambda)u\rangle-\langle u,(H-\lambda)A_r^*A_ru\rangle\\ &=2i\operatorname{Im}\langle u,A_r^*A_r(H-\lambda)u\rangle;\end{aligned} \tag{7.54}$$

the pairing makes sense for $r>0$ since $A_r\in\Psi_{\mathrm{Sc}}^{-\infty,-l}(\bar{X},\mathcal{C})$. Now apply (7.53) to $x^{-l-1/2}u$ and pair it with $x^{-l-1/2}u$ in $L^2_{\mathrm{sc}}(\bar{X})$. Then for $r>0$

$$\|B_ru\|^2\leq|\langle u,E_ru\rangle|+|\langle u,F_ru\rangle|+2|\langle u,A_r^*A_r(H-\lambda)u\rangle|. \tag{7.55}$$

Letting $r\to 0$ now keeps the right hand side of (7.55) bounded. In fact, $A_r(H-\lambda)u\in\dot{\mathcal{C}}^\infty(\bar{X})$ remains bounded in $\dot{\mathcal{C}}^\infty(\bar{X})$ as $r\to 0$. Similarly, by (7.43), E_ru remains bounded in $\dot{\mathcal{C}}^\infty(\bar{X})$ as $r\to 0$ since $\mathrm{WF}_{\mathrm{Sc}}(u)\cap\mathrm{WF}'_{\mathrm{Sc}}(E)=\emptyset$. Also, F_r is bounded in $\mathcal{B}(H^{m,l}_{\mathrm{sc}}(\bar{X}),H^{-m,-l}_{\mathrm{sc}}(\bar{X}))$, so $\langle u,F_ru\rangle$ stays bounded by (7.43) as well since $\operatorname{supp}q\cap\mathrm{WF}^{*,l}_{\mathrm{Sc}}(u)\cap\dot{\Sigma}(I)=\emptyset$. These estimates show that B_ru is uniformly bounded in $L^2_{\mathrm{sc}}(\bar{X})$. Since $(1+r/x)^{-1}\to\mathrm{Id}$ strongly on $\mathcal{B}(H^{m',l'}_{\mathrm{sc}}(\bar{X}),H^{m',l'}_{\mathrm{sc}}(\bar{X}))$, we conclude that $Bx^{-l-1/2}u\in L^2_{\mathrm{sc}}(\bar{X})$. By (7.43) and Proposition 4.2 this implies that for every m,

$$\bar{\xi}\notin\mathrm{WF}^{m,l+1/2}_{\mathrm{Sc}}(u); \tag{7.56}$$

in fact that $\xi\notin\mathrm{WF}^{m,l+1/2}_{\mathrm{Sc}}(u)$ for all $\xi\in K$ for which $q>0$. This is exactly the iterative step we wanted to prove. In the next step we decrease $\epsilon>0$ slightly to ensure that $\mathrm{WF}'_{\mathrm{Sc}}(F)\subset\operatorname{supp}\tilde{q}$ is disjoint from $\mathrm{WF}^{m,l+1/2}_{\mathrm{Sc}}(u)$, just as Hörmander decreases t in the proof of [12, Proposition 24.5.1]. □

Based on this proposition, we proceed inductively, assuming that propagation has been proved at C'_b with $C_a\subsetneq C_b$. Noting that $\eta_a=z_a\cdot\nu_a<0$ implies that a backward broken bicharacteristic through ξ must stay away from C_a, we can use Lebeau's argument, as presented in [37, Theorem 10.6], to prove propagation along broken bicharacteristics. The basic idea is that $\bar{\xi}\in\mathrm{WF}_{\mathrm{Sc}}(u)\cap{}^{\mathrm{sc}}T^*_{C'_a}\bar{X}_a$ implies that either every point on the non-constant backward ${}^{\mathrm{sc}}H_g^a$-bicharacteristic is in $\mathrm{WF}_{\mathrm{Sc}}(u)$ (in a neighborhood of $\bar{\xi}$), or there are points in $\mathrm{WF}_{\mathrm{Sc}}(u)\setminus{}^{\mathrm{sc}}T^*_{C'_a}\bar{X}_a$ arbitrarily close to $\bar{\xi}$ such that there is a backward broken bicharacteristic through these points which is completely in $\mathrm{WF}_{\mathrm{Sc}}(u)$ (by the inductive hypothesis). Using the compactness of the set of broken bicharacteristics, we can extract a sequence of backward broken bicharacteristics which converge to a backward broken bicharacteristic through $\bar{\xi}$, which will prove the propagation statement.

Theorem. *(Theorem 2.2) Let $u\in\mathcal{C}^{-\infty}(\bar{X})$, $\lambda\notin\Lambda_1$. Then*

$$\mathrm{WF}_{Sc}(u)\setminus\mathrm{WF}_{Sc}((H-\lambda)u) \tag{7.57}$$

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

Proof. As usual, broken bicharacteristic means *generalized* broken bicharacteristic in this proof.

We start by remarking that for every $V\subset\dot{\Sigma}(\lambda)$ and $\xi\in V$, the set $\mathcal{R}$ of generalized broken bicharacteristics γ defined on open intervals including 0, satisfying $\gamma(0)=\xi$, and with image in V, has a natural partial order, namely if $\gamma:(\alpha,\beta)\to V$, $\gamma':(\alpha',\beta')\to V$, then $\gamma\leq\gamma'$ if the domains satisfy $(\alpha,\beta)\subset(\alpha',\beta')$ and $\gamma=\gamma'|_{(\alpha,\beta)}$. Moreover, any non-empty totally ordered subset has an upper bound: one can take the generalized broken bicharacteristic with domain given by the union of the domains of those in the totally ordered subset, and which extends these, as an upper bound. Hence, by Zorn's lemma, if $\mathcal{R}$ is not empty, it has a maximal element. Note that we can also work with intervals of the form $(\alpha,0]$, $\alpha<0$, instead of open intervals.

We only need to prove that for every $\xi_0\in\mathrm{WF}_{\mathrm{Sc}}(u)\setminus\mathrm{WF}_{\mathrm{Sc}}((H-\lambda)u)$ there exists a generalized broken bicharacteristic $\gamma:[-\epsilon_0,\epsilon_0]\to\dot{\Sigma}$, $\epsilon_0>0$, with $\gamma(0)=\xi_0$ and such that $\gamma(t)\in\mathrm{WF}_{\mathrm{Sc}}(u)\setminus\mathrm{WF}_{\mathrm{Sc}}((H-\lambda)u)$ for $t\in[-\epsilon_0,\epsilon_0]$. In fact, once this statement is shown, taking $V=\mathrm{WF}_{\mathrm{Sc}}(u)\setminus\mathrm{WF}_{\mathrm{Sc}}((H-\lambda)u)$, $\xi=\xi_0$, in the argument of the previous paragraph, we see that $\mathcal{R}$ is non-empty, hence has a maximal element. We need to show that such an element, $\gamma:(\alpha,\beta)\to\dot{\Sigma}(\lambda)$, is maximal in $\dot{\Sigma}(\lambda)\setminus\mathrm{WF}_{\mathrm{Sc}}((H-\lambda)u)$ as well, i.e. if we take $V=\dot{\Sigma}(\lambda)\setminus\mathrm{WF}_{\mathrm{Sc}}((H-\lambda)u)$, $\xi=\xi_0$ in the first paragraph. But if $\gamma':(\alpha',\beta')\to\dot{\Sigma}(\lambda)$ is any proper extension of γ, with say $\alpha'<\alpha$, with image in $\dot{\Sigma}(\lambda)\setminus\mathrm{WF}_{\mathrm{Sc}}((H-\lambda)u)$, then $\gamma'(\alpha)\in\mathrm{WF}_{\mathrm{Sc}}(u)$ since $\mathrm{WF}_{\mathrm{Sc}}(u)$ is closed, and γ maps into it, hence by our assumption there is a generalized broken bicharacteristic $\tilde{\gamma}:(\alpha-\epsilon',\alpha+\epsilon')\to\mathrm{WF}_{\mathrm{Sc}}(u)\setminus\mathrm{WF}_{\mathrm{Sc}}((H-\lambda)u)$, $\epsilon'>0$, $\tilde{\gamma}(\alpha)=\gamma'(\alpha)$; piecing together $\tilde{\gamma}|_{(\alpha-\epsilon',\alpha]}$ and γ, directly from Definition 2.1, gives a generalized broken bicharacteristic which is a proper extension of γ, with image in $\mathrm{WF}_{\mathrm{Sc}}(u)\setminus\mathrm{WF}_{\mathrm{Sc}}((H-\lambda)u)$, contradicting the maximality of γ.

Indeed, it suffices to show that for any a, if

$$\bar{\xi}\in\mathrm{WF}_{\mathrm{Sc}}(u)\setminus\mathrm{WF}_{\mathrm{Sc}}((H-\lambda)u)\text{ and }\bar{\xi}\in{}^{\mathrm{sc}}T^*_{C'_a}(C_a;\bar{X}) \tag{7.58}$$

then

$$\begin{gathered}\text{there exists a broken bicharacteristic }\gamma:[-\epsilon_0,0]\to\dot{\Sigma}(\lambda),\ \epsilon_0>0,\\ \gamma(0)=\bar{\xi},\ \gamma(t)\in\mathrm{WF}_{\mathrm{Sc}}(u)\setminus\mathrm{WF}_{\mathrm{Sc}}((H-\lambda)u),\ t\in[-\epsilon_0,0],\end{gathered} \tag{7.59}$$

for the existence of a broken bicharacteristic on $[0,\epsilon_0]$ can be demonstrated similarly by replacing the forward propagation estimates by backward ones, and, directly from Definition 2.1, piecing together the two broken bicharacteristics gives one defined on $[-\epsilon_0,\epsilon_0]$.

We proceed to prove that (7.58) implies (7.59) by induction on a. This is certainly true for $a=0$ by Proposition 7.1: there are no normal variables z_a, ν_a, so $\eta_a = 0$ in the notation of that Proposition, showing that a segment of the backward bicharacteristic through $\bar\xi$ must be in $\mathrm{WF}_{\mathrm{Sc}}(u)$. Of course, this is simply Melrose's propagation theorem [23, Proposition 7].

In addition, if a is arbitrary and $\bar\xi\in R_+(\lambda)\cup R_-(\lambda)$, then the constant curve γ through $\bar\xi$ is a broken bicharacteristic, so (7.58)$\Rightarrow$(7.59) holds with this γ.

So suppose that (7.58)$\Rightarrow$(7.59) has been proved for all b with $C_a\subsetneq C_b$ and that $\bar\xi\in\dot\Sigma(\lambda)\cap{}^{\mathrm{sc}}T^*_{C'_a}(C_a;\bar X)$ satisfies (7.58). We use the notation of the proof of Proposition 7.1 below. Let U_0 be a neighborhood of $\bar\xi=(\bar y_a,\bar\tau_a,\bar\mu_a)$ in $\dot\Sigma(\lambda)$ as in Proposition 7.1; we may assume that $U_0\cap\mathrm{WF}_{\mathrm{Sc}}((H-\lambda)u)=\emptyset$. By reducing the size of U_0 if necessary, we may further choose $\epsilon_0>0$ such that every generalized broken bicharacteristic γ with $\gamma(0)\in U_0$ satisfies $\gamma(t)\in\cup_{C_a\subset C_b}{}^{\mathrm{sc}}T^*_{C'_b}\bar X_b$ for $t\in[-\epsilon_0,\epsilon_0]$. By Proposition 7.1, either every point on the non-constant backward ${}^{\mathrm{sc}}H^a_g$-bicharacteristic segment through $\bar\xi$ is in $\mathrm{WF}_{\mathrm{Sc}}(u)$ (in the neighborhood U_0 of $\bar\xi$), in which case we have proved (7.59), so we are done, or there is a sequence of points $\xi_n\in U_0$ such that $\xi_n\in\mathrm{WF}_{\mathrm{Sc}}(u)$, $\xi_n\to\bar\xi$ as $n\to\infty$, and $\eta_a(\xi_n)<0$ for all n. Since $\eta_a(\xi_n)<0$, $\xi_n\notin{}^{\mathrm{sc}}T^*_{C'_a}\bar X_a$. Thus, by the inductive hypothesis, for each n there exists a broken bicharacteristic $\tilde\gamma_n:(-\epsilon'_n,0]\to\dot\Sigma(\lambda)$, $\epsilon'_n>0$, with $\tilde\gamma_n(0)=\xi_n$, $\gamma_n(t)\in\mathrm{WF}_{\mathrm{Sc}}(u)\cap U_0\cap\cup_{C_a\subsetneq C_b}{}^{\mathrm{sc}}T^*_{C'_b}\bar X_b\cap\mathrm{WF}_{\mathrm{Sc}}(u)$ for all $t\in(-\epsilon'_n,0]$. We now use the argument of the first paragraph of the proof with $V=(\mathrm{WF}_{\mathrm{Sc}}(u)\setminus\mathrm{WF}_{\mathrm{Sc}}((H-\lambda)u))\cap\bigcup_{C_a\subsetneq C_b}{}^{\mathrm{sc}}T^*_{C'_b}(C_b;X)$, and $\xi=\xi_n$. Thus, $\tilde\gamma_n\in\mathcal R$, which is hence non-empty, hence has a maximal element. We let

$$\gamma_n:(-\epsilon_n,0]\to(\mathrm{WF}_{\mathrm{Sc}}(u)\setminus\mathrm{WF}_{\mathrm{Sc}}((H-\lambda)u))\cap\bigcup_{C_a\subsetneq C_b}{}^{\mathrm{sc}}T^*_{C'_b}(C_b;X)\tag{7.60}$$

be a maximal element of $\mathcal R$; it may happen that $-\epsilon_n=-\infty$.

We claim that $\epsilon_n\geq\epsilon_0$. For suppose that $\epsilon_n<\epsilon_0$. By Corollary 5.6, γ_n extends to a generalized broken bicharacteristic on $[-\epsilon_n,0]$, we continue to denote this by γ_n. Since $\epsilon_n<\epsilon_0$, γ_n is a generalized broken bicharacteristic with image in U_0; in fact, even the closure of the image is in this set. But $e^{Ct}\eta_a$ is non-decreasing (for sufficiently large $C>0$) along broken bicharacteristics by the argument that preceeds Lemma 5.8, so we conclude that

$$\eta_a(\gamma_n(t))\leq e^{C(t-t_0)}\eta_a(\gamma_n(0))<0\tag{7.61}$$

for $t\in[-\epsilon_0,0]$, hence $z_a(\gamma_n(t))\neq 0$. Thus, $\gamma_n(-\epsilon_n)\in\cup_{C_a\subsetneq C_b}{}^{\mathrm{sc}}T^*_{C'_b}(C_b;X)$. Moreover, $\gamma_n(-\epsilon_n)\in\mathrm{WF}_{\mathrm{Sc}}(u)$ since $\mathrm{WF}_{\mathrm{Sc}}(u)$ is closed, and $\gamma_n|_{(-\epsilon_n,0]}$ maps into it. Thus, by the inductive hypothesis, there is a generalized broken bicharacteristic,

$$\tilde\gamma_n:(\alpha,-\epsilon_n]\to(\mathrm{WF}_{\mathrm{Sc}}(u)\setminus\mathrm{WF}_{\mathrm{Sc}}((H-\lambda)u))\cap\bigcup_{C_a\subsetneq C_b}{}^{\mathrm{sc}}T^*_{C'_b}(C_b;X)\tag{7.62}$$

with $\alpha<-\epsilon_n$, $\tilde\gamma_n(-\epsilon_n)=\gamma_n(-\epsilon_n)$. Hence, piecing together $\tilde\gamma_n$ and γ_n gives a generalized broken bicharacteristic mapping into $(\mathrm{WF}_{\mathrm{Sc}}(u)\setminus\mathrm{WF}_{\mathrm{Sc}}((H-\lambda)u))\cap\bigcup_{C_a\subsetneq C_b}{}^{\mathrm{sc}}T^*_{C'_b}(C_b;X)$ and extending γ_n, which contradicts the maximal property of γ_n. Thus, $\epsilon_n\geq\epsilon_0$ as claimed.

By Proposition 5.5, there is a subsequence of $\gamma_n|_{[-\epsilon_0,0]}$ converging uniformly to a broken bicharacteristic $\gamma:[-\epsilon_0,0]\to\dot\Sigma(\lambda)$. Since $\mathrm{WF}_{\mathrm{Sc}}(u)$ is closed, $\gamma:[-\epsilon_0,0]\to\mathrm{WF}_{\mathrm{Sc}}(u)$. In particular, $\gamma(0)=\bar\xi$ and $\gamma(t)\in\mathrm{WF}_{\mathrm{Sc}}(u)$ for all $t\in[-\epsilon_0,0]$, providing the inductive step. □

Remark 7.3. As expected, the theorem does not provide any interesting information at the radial sets $R_+(\lambda)\cup R_-(\lambda)$.

This theorem essentially says that the propagation of quantum particles, modulo 'trivial' (i.e. Schwartz) terms can be understood as a series of collisions in which the total energy and the external momentum are preserved.

8. The resolvent

Before we can turn Theorem 2.2 into a result on the wave front relation of the S-matrix, we need to analyze the resolvent. More precisely, we need to understand the boundary values

$$R(\lambda\pm i0)=(H-(\lambda\pm i0))^{-1} \tag{8.1}$$

of the resolvent at the real axis in a microlocal sense. To do so, we also need estimates at the radial sets $R_\pm(\lambda)$. Since some of the Hamilton vector fields ${}^{\mathrm{sc}}H_g^a$ of the metric g vanish at $R_+(\lambda)\cup R_-(\lambda)$, the estimates must utilize the weights x^{-l-1} themselves. In this sense they are delicate, but on the other hand they only involve x and its sc-microlocal dual variable τ, so they do not need to reflect the geometry of $\mathcal{C}$. The best known positive commutator estimate is the Mourre estimate, originally proved by Perry, Sigal and Simon in Euclidean many-body scattering [27], in which one takes $q=x^{-1}\tau$ with the notation of Section 6. Since it is easy to analyze the commutator of powers of x with H (in particular, they commute with V), the functional calculus allows one to obtain microlocal estimates from these, as was done by Gérard, Isozaki and Skibsted [6, 7]. Thus, nearly all the technical results in this section can be proved, for example, by using the Mourre estimate and Theorem 2.2. In particular, apart from the propagation statements, they are well-known in our Euclidean many-body setting.

We first recall the limiting absorption principle.

Theorem 8.1. *Suppose that H is a many-body Hamiltonian, and $\lambda\notin\Lambda$. Let $f\in\dot{\mathcal{C}}^\infty(\bar X)$, $u_t^\pm=R(\lambda\pm it)f$, $t>0$. Then $u_t^\pm$ has a limit $u_\pm=R(\lambda\pm i0)f$ in $H_{sc}^{m,l}(\bar X)$, $l<-1/2$, as $t\to 0$. In addition,*

$$\mathrm{WF}_{Sc}(u_\pm)\subset\Phi_\pm(R_\mp(\lambda)). \tag{8.2}$$

Remark 8.2. The first statement in the theorem also holds if we merely assume $f\in H_{\mathrm{sc}}^{m,l'}(\bar X)$ with $l'>1/2$, but then $\mathrm{WF}_{\mathrm{Sc}}(u_\pm)$ has to be replaced by the filtered wave front set $\mathrm{WF}_{\mathrm{Sc}}^{m,l'-1}(u_\pm)$. Moreover, $R(\lambda\pm i0)$ give continuous operators from $H_{\mathrm{sc}}^{m,l'}(\bar X)$ to $H_{\mathrm{sc}}^{m+2,l}(\bar X)$.

Proof. The existence of $u_\pm$ in $H_{\mathrm{sc}}^{m,l}(\bar X)$, $l<-1/2$ follows from the Mourre estimate, as presented in [27]. That $\xi\in\mathrm{WF}_{\mathrm{Sc}}(u_+)$ implies $\tau(\xi)<0$ (in fact, $\tau(\xi)\le-\sqrt{a(\lambda)}$ where $a(\lambda)=\inf\{\lambda-\sigma:\sigma\in\Lambda,\ \sigma<\lambda\}$), follows from the work of Gérard, Isozaki and Skibsted [6]; see [37] to see how the proof would proceed with our notation. By Theorem 2.2, $\mathrm{WF}_{\mathrm{Sc}}(u_+)\setminus\mathrm{WF}_{\mathrm{Sc}}(f)=\mathrm{WF}_{\mathrm{Sc}}(u_+)$ is a union of maximally extended generalized broken bicharacteristics. So suppose that $\xi\in\mathrm{WF}_{\mathrm{Sc}}(u_+)$, and let $\gamma : \mathbb{R} \to \dot{\Sigma}(\lambda)$ be a generalized broken bicharacteristic in $\mathrm{WF}_{\mathrm{Sc}}(u_+)$ with $\gamma(t_0) = \xi$. Then, by Lemma 5.11, $\tau(-\infty) = \lim_{t\to-\infty} \tau(\gamma(t))$ exists. If $\tau(-\infty) \geq 0$ then $\tau(\gamma(t)) > -\sqrt{a(\lambda)}$ for large negative t, contradicting that $\tau \leq -\sqrt{a(\lambda)}$ on $\mathrm{WF}_{\mathrm{Sc}}(u_+)$. Thus, $\tau(-\infty) < 0$, and hence by Lemma 5.11, $\overline{\gamma((-\infty, t_0])} \cap R_-(\lambda) \neq \emptyset$, so $\xi \in \Phi_+(R_-(\lambda))$. We thus conclude that (8.2) holds. □

A pairing argument immediately shows $R(\lambda \pm i0)v$ also exists for distributions $v \in \mathcal{C}^{-\infty}(\bar{X})$ with wave front set disjoint from the incoming and outgoing radial set respectively. Combining it with the propagation theorem, Theorem 2.2, we can deduce the following result.

Theorem (Theorem 2.4). *Suppose that H is a many-body Hamiltonian, and $\lambda \notin \Lambda$. Suppose also that $v \in \mathcal{C}^{-\infty}(\bar{X})$ and $\mathrm{WF}_{Sc}(v) \cap \Phi_-(R_+(\lambda)) = \emptyset$. Let $u_t^+ = R(\lambda + it)v$, $t > 0$. Then u_t^+ has a limit $u_+ = R(\lambda + i0)v$ in $\mathcal{C}^{-\infty}(\bar{X})$ as $t \to 0$ and $\mathrm{WF}_{Sc}(u_+) \cap \Phi_-(R_+(\lambda)) = \emptyset$. Moreover, $\mathrm{WF}_{Sc}(u_+) \subset \Phi_+(R_-(\lambda)) \cup \Phi_+(\mathrm{WF}_{Sc}(v))$. The result also holds with $R_+(\lambda)$ and $R_-(\lambda)$ interchanged, $R(\lambda + it)$ replaced by $R(\lambda - it)$, Φ_+ and Φ_- interchanged.*

Proof. As mentioned above, the first part follows from the self-adjointness of H, so that for $t > 0$, $v \in \mathcal{C}^{-\infty}(\bar{X})$, $f \in \dot{\mathcal{C}}^\infty(\bar{X})$, we have $v(R(\lambda + it)f) = R(\lambda + it)v(f)$; recall that the distributional pairing is the real pairing, not the complex (i.e. L^2) one. The wave front statement of Theorem 8.1 and the assumption on v show the existence of the limit $u_+ = R(\lambda+i0)v$ in $\mathcal{C}^{-\infty}(\bar{X})$ and that in addition $\mathrm{WF}^{m,l}_{\mathrm{Sc}}(u_+) \cap \Phi_-(R_+(\lambda)) = \emptyset$ for every $l < -1/2$. The statement $\mathrm{WF}_{\mathrm{Sc}}(u_+) \cap \Phi_-(R_+(\lambda)) = \emptyset$ follows from a microlocalized version of the Mourre estimate due to Gérard, Isozaki and Skibsted [7]; see [11] or [37] for a detailed argument. The final part of the conclusion follows from Theorem 2.2, much as in the previous proof. □

9. Poisson operators

The propagation of singularities theorem, especially in its form for the resolvent, Theorem 2.4, has immediate consequences for the wave front relation of all S-matrices. To see this, recall the definition of the Poisson operator from (2.29). First, let

$$I_a = \sum_{C_a \not\subset C_b} V_b, \quad \tilde{I}_a = (I_a/x_a)|_{C_a} \in \mathcal{C}^\infty(C_a), \tag{9.1}$$

so I_a is $\mathcal{C}^\infty$ near C_a' with simple vanishing at C_a', so I_a/x_a is $\mathcal{C}^\infty$ there. Then, for $\lambda \in (\epsilon_\alpha, \infty) \setminus \Lambda$ and $g \in \mathcal{C}_c^\infty(C_a')$, there is a unique $u \in \mathcal{C}^{-\infty}(\bar{X})$ such that $(H - \lambda)u = 0$, and u has the form

$$\begin{aligned} u =& e^{-i\sqrt{\lambda-\epsilon_\alpha}/x} x^{\dim C_a/2} x^{i\tilde{I}_a/2\sqrt{\lambda-\epsilon_\alpha}} \tilde{v}_- + R(\lambda + i0)f, \\ \tilde{v}_- =& ((\pi^a)^*\psi_\alpha)(\pi_a^* g) + x\tilde{v}_-', \ f \in \dot{\mathcal{C}}^\infty(\bar{X}), \end{aligned} \tag{9.2}$$

and $\tilde{v}_-'$ is conormal to the boundary of $[\bar{X}; C_a]$, with infinite order vanishing off the front face (the inverse image of C_a under the blow-down map), and has a full asymptotic expansion at the front face of the form

$$\sum_{k=0}^{\infty} \sum_{s=0}^{2k+2} x^k (\log x)^s a_j(y, Z), \tag{9.3}$$

a_j smooth in y and Schwartz in Z where we used the notation of (3.8)-(3.9) for the coordinates in the interior of the front face of $[\bar{X}; C_a]$. (Uniqueness holds if we merely require that $f \in H_{\mathrm{sc}}^{0,1/2+\epsilon'}(\bar{X})$, $\epsilon' > 0$, due to Isozaki's results [16, 15] applied to the difference of two solutions of the form (9.2), see [35]; existence is a direct consequence of the following parametrix construction.) The Poisson operator $P_{\alpha,+}(\lambda)$ is the map

$$P_{\alpha,+}(\lambda) : \mathcal{C}_c^{\infty}(C_a') \to \mathcal{C}^{-\infty}(\bar{X}) \text{ defined by } P_{\alpha,+}(\lambda)g = u. \tag{9.4}$$

The scattering matrix is then given by the following formula, which is related to the representation formula of Isozaki and Kitada [17]:

$$S_{\beta\alpha}(\lambda) = \frac{1}{2i\sqrt{\lambda - \epsilon_\beta}}((H-\lambda)\tilde{P}_{\beta,-}(\lambda))^* P_{\alpha,+}(\lambda), \tag{9.5}$$

$\lambda > \max(\epsilon_\alpha, \epsilon_\beta)$, $\lambda \notin \Lambda$ where $\tilde{P}_{\beta,-}(\lambda)$ is a microlocalized version of $P_{\beta,-}(\lambda)$, microlocalized near the outgoing radial set (see the following paragraphs for details).

This formula reduces the understanding of the structure of the S-matrices to that of the Poisson operators. These in turn can be described in two steps. First, one constructs the Poisson operators approximately in the incoming region of phase space, and then one uses the propagation results for the resolvent to obtain the wave front relation of the Poisson operators.

A very good parametrix, which we here denote by $\tilde{P}_{\alpha,+}(\lambda)$, for $P_{\alpha,+}(\lambda)$ in the incoming region of phase space, i.e. where τ is close to $\sqrt{\lambda - \epsilon_\alpha}$, has been constructed by Skibsted [32] in the short-range and by Bommier [1] in the long-range setting using a WKB-type construction under the assumption that $\epsilon_\alpha \in \operatorname{spec}_d(H^a)$, i.e. ϵ_α is below the thresholds of H^a. Thus, writing their construction explicitly for the class of potentials that we are considering and using the notation of (3.8)-(3.9) for the coordinates in the interior of the front face of $[\bar{X}; C_a]$, they construct an operator

$$\tilde{P}_{\alpha,+}(\lambda) : \mathcal{C}_c^{-\infty}(C_a') \to \mathcal{C}^{-\infty}(\bar{X}) \tag{9.6}$$

by constructing its kernel

$$K^\flat_{\alpha,+} = e^{-i\sqrt{\lambda-\epsilon_\alpha}\cos\operatorname{dist}(y,y')/x} x^{i\tilde{I}_a(y')/2\sqrt{\lambda-\epsilon_\alpha}} a_+(x,y,Z,y'), \tag{9.7}$$

$a_+ \in \mathcal{C}^\infty([\bar{X}; C_a] \times C_a)$ vanishes to infinite order at the 'main face' (the lift of $C_0 = \partial\bar{X}$ to $[\bar{X}; C_a]$; this means that a_+ is Schwartz in the fibers of the blow-down map, which are X^a, i.e. it is Schwartz in Z), and a_+ is supported where y is near y', which in turn implies (by looking at the phase of the exponential) that τ is near $\sqrt{\lambda - \epsilon_\alpha}$. Note that the phase is a multiple of $\cos\operatorname{dist}(y,y') = y \cdot y'$, where we consider C_a as the unit sphere in X_a, $y, y' \in C_a$. In terms of Euclidean variables $w_a = y/x$ on X^a,

$$K^\flat_{\alpha,+} = e^{-i\sqrt{\lambda-\epsilon_\alpha}w_a\cdot y'} |w_a|^{-i\tilde{I}_a(y')/2\sqrt{\lambda-\epsilon_\alpha}} \tilde{a}_+(w_a, y', Z), \tag{9.8}$$

with $\tilde{a}_+$ polyhomogeneous, of degree 0 in w_a, smooth in y', Schwartz in Z.

The construction of $K^\flat_{\alpha,+}$, i.e. finding an oscillatory function of the form (9.7) satisfying that $(H-\lambda)K^\flat_{\alpha,+}$ is in $\dot{\mathcal{C}}^\infty(\bar{X} \times C_a')$ at least near $y = y'$, where $H - \lambda$ is applied to $K^\flat_{\alpha,+}$ in the left factor $\bar{X}$, is essentially given by a non-commutative WKB-type procedure. Since one already has the correct phase function, one only needs to solve transport equations starting at the diagonal $y = y'$, which, however, are operator-valued. To remove the errors in these equations, $H^a - \epsilon_\alpha$ has to be inverted on the orthocomplement of its L^2 null space. Since $H^a - \epsilon_\alpha$ has a parametrix in $\Psi_{\mathrm{Sc}}^{-2,0}(\bar{X}^a, \mathcal{C}^a)$ (because ϵ_α is below the set of thresholds), this is possible with the resulting (generalized) inverse being in $\Psi_{\mathrm{Sc}}^{-2,0}(\bar{X}^a, \mathcal{C}^a)$. This gives a kernel K_0 of the form (9.7), defined near $y = y'$, $x = 0$, and satisfying $(H - \lambda)K_0$ is in $\dot{\mathcal{C}}^\infty(\bar{X} \times C'_a)$ in the region where the transport equations have been solved (see [32, 1] for more details). Multiplying it by a cut-off function $\phi \in \mathcal{C}^\infty(C'_a \times C'_a)$ supported near the diagonal, identically 1 in a smaller neighborhood of the diagonal, we obtain a kernel K which is still of the form (9.7), now globally defined, and $(H - \lambda)K$ is in $\dot{\mathcal{C}}^\infty(\bar{X} \times C'_a)$ near $y = y'$. Finally, we take $\psi \in \mathcal{C}_c^\infty(\mathbb{R})$ identically 1 near λ, and apply $\psi(H) \in \Psi_{\mathrm{Sc}}^{-\infty,0}(\bar{X}, \mathcal{C})$ to K in the left factor $\bar{X}$, i.e. we compose the operator P given by the kernel K with $\psi(H)$, so that $\tilde{P}_{\alpha,+}(\lambda) = \psi(H)P$. Writing out the composition explicitly, similarly to how one shows that $\Psi_{\mathrm{Sc}}(\bar{X}, \mathcal{C})$ preserves oscillatory functions, see [37, Section 4], shows that $K^\flat_{\alpha,+}$ is indeed of the required form, (9.7). (Recall that this is based on conjugating an Sc-ps.d.o. by an oscillatory function, observing that the resulting kernel is that of an Sc-ps.d.o, and using that Sc-ps.d.o's map smooth functions on $\bar{X}$ to smooth functions, which is quite straightforward to see by an explicit integral representation of the kernel.) In addition, $(H - \lambda)\tilde{P}_{\alpha,+}(\lambda)g = \psi(H)(H - \lambda)Pg$ for all $g \in \mathcal{C}_c^{-\infty}(C'_a)$, which will allow us to use that $(H - \lambda)K$ is in $\dot{\mathcal{C}}^\infty(\bar{X} \times C'_a)$ near $y = y'$. Also, $(P - \tilde{P}_{\alpha,+}(\lambda))g = (\mathrm{Id} - \psi(H))Pg = \tilde{\psi}(H)(H - \lambda)Pg$ where $\tilde{\psi}(s) = (1 - \psi(s))/(s - \lambda)$ so $\tilde{\psi} \in S^{-1}_{\mathrm{phg}}(\mathbb{R})$, $\tilde{\psi}(H) \in \Psi_{\mathrm{Sc}}^{-2,0}(\bar{X}, \mathcal{C})$. In view of the corresponding property of $(H - \lambda)K$, $K^\flat_{\alpha,+} - K$ vanishes to infinite order near $y = y'$, $x = 0$, i.e. $K^\flat_{\alpha,+}$ and K are 'microlocally equal' there.

We note that in fact the construction of the kernel can be continued up to $C_{a,\mathrm{sing}}$; we just need to cut off a_+ shortly beforehand. In particular, if a is a 2-cluster, then the construction works until reaching the outgoing radial set. We also remark that if the V_b are Schwartz, then a product decomposition immediately gives $\tilde{P}_{\alpha,+}(\lambda)$, without a need to remove errors, so in that case one can allow ϵ_α to be arbitrary.

The main properties of $\tilde{P}_{\alpha,+}(\lambda)$ are that for any $g \in \mathcal{C}_c^{-\infty}(C'_a)$, $h \in \mathcal{C}_c^\infty(C'_a)$, $\epsilon' > 0$,

$$\mathrm{WF}_{\mathrm{Sc}}(\tilde{P}_{\alpha,+}(\lambda)g) \subset {}^{\mathrm{sc}}T^*_{C'_a}(C_a; \bar{X}), \tag{9.9}$$

$$\begin{aligned}\tilde{P}_{\alpha,+}(\lambda)h = e^{-i\sqrt{\lambda - \epsilon_\alpha}/x} x^{\dim C_a/2} x^{i\tilde{I}_a/2\sqrt{\lambda-\epsilon_\alpha}} (((\pi^a)^*\psi_\alpha)((\pi_a^* h) + xv'),\\ v' \text{ as in (9.3)},\end{aligned} \tag{9.10}$$

$$(H - \lambda)\tilde{P}_{\alpha,+}(\lambda)h \in \dot{\mathcal{C}}^\infty(\bar{X}), \tag{9.11}$$

(9.12)
$$\begin{aligned}\mathrm{WF}_{\mathrm{Sc}}(\tilde{P}_{\alpha,+}(\lambda)g) \subset &\{(y, \tau, \mu) :\ y \in \operatorname{supp} g,\ \tau = \sqrt{\lambda - \epsilon_\alpha},\ \mu = 0\}\\ &\cup \{\xi \in \dot{\Sigma}(\lambda) \setminus (R_+(\lambda) \cup R_-(\lambda)) :\ \exists\zeta \in \mathrm{WF}(g),\ \xi \in \gamma_{\alpha,-}(\zeta)\},\end{aligned}$$

$$\begin{aligned}&\mathrm{WF}_{\mathrm{Sc}}((H - \lambda)\tilde{P}_{\alpha,+}(\lambda)g)\\ &\quad\subset \{\xi \in \dot{\Sigma}(\lambda) \setminus (R_+(\lambda) \cup R_-(\lambda)) :\ \exists\zeta \in \mathrm{WF}(g),\ \xi \in \gamma_{\alpha,-}(\zeta)\}.\end{aligned} \tag{9.13}$$

See [36, Appendix A] for a discussion of these mapping properties if α is the free cluster; the general case is similar since we are working in the regular part of C_a, and a_+ is rapidly decreasing in X^a. However, since the notion of wave front set is more complicated than at the free cluster, we briefly indicate how to prove these statements. Before doing this, we discuss the consequences of (9.9)-(9.13) for the actual Poisson operator $P_{\alpha,+}(\lambda)$.

The Poisson operator, first defined on $\mathcal{C}_c^\infty(C_a')$ by (9.4), is given by

$$P_{\alpha,+}(\lambda) = \tilde{P}_{\alpha,+}(\lambda) - R(\lambda + i0)(H-\lambda)\tilde{P}_{\alpha,+}(\lambda). \tag{9.14}$$

Note that for $g \in \mathcal{C}_c^\infty(C_a')$, $(H-\lambda)\tilde{P}_{\alpha,+}(\lambda)g \in \dot{\mathcal{C}}^\infty(\bar{X})$ by (9.11), so the resolvent can certainly be applied to it. For $g \in \mathcal{C}_c^\infty(C_a')$, the right hand side of (9.14) is of the form (9.2) by (9.10), so it indeed yields the Poisson operator by its definition, (9.4). Similar results hold for the Poisson operator $P_{\beta,-}(\lambda)$ with outgoing initial data. Theorem 2.4, (9.13) and (9.14) immediately show the following proposition.

Proposition. *(Proposition 2.6) Suppose that H is a many-body Hamiltonian, $\lambda \notin \Lambda$, and* (2.34) *holds. Suppose also that $g \in \mathcal{C}_c^\infty(C_a')$. Then*

$$\mathrm{WF}_{Sc}(P_{\alpha,+}(\lambda)g) \setminus R_+(\lambda) \subset \Phi_+(R_-(\lambda)). \tag{9.15}$$

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 $(R_+(\lambda) \times \mathrm{WF}(g)) \cap \mathcal{R}_{\alpha,+} = \emptyset$ (i.e. $\mathcal{R}_{\alpha,+}(\mathrm{WF}(g)) \cap R_+(\lambda) = \emptyset$). If g is such a distribution, then

$$\mathrm{WF}_{Sc}(P_{\alpha,+}(\lambda)g) \setminus R_+(\lambda) \subset \Phi_+(R_-(\lambda)) \cup \mathcal{R}_{\alpha,+}(\mathrm{WF}(g)). \tag{9.16}$$

We now return to the proof of (9.9)-(9.13). First note that (9.9) follows from the fact that $\operatorname{supp} a_+$ is disjoint from $C_{a,\mathrm{sing}} \times D \times \bar{X}^a$ for any $D \subset C_a'$ compact. Next, (9.10)-(9.11) are direct consequences of the stationary phase lemma. The $\log x$ factors appear in the lower order terms (i.e. in v') due to the derivatives falling on $x^{i\tilde{I}_a(y')/2\sqrt{\lambda-\epsilon_\alpha}}$ as stated in (9.3); see [37, Sections 11-12] for a detailed description. Note that in addition to the stationary phase lemma, (9.11) uses that $(H-\lambda)\tilde{P}_{\alpha,+}(\lambda)h = \psi(H)(H-\lambda)Ph$, and the kernel of $(H-\lambda)P$ is rapidly decreasing near $y = y'$, where the phase is stationary. The stationary phase lemma also shows (9.12) with $h \in \mathcal{C}_c^\infty(C_a')$ in place of g (with the second set on the right hand side empty), since all terms in the stationary phase expansion arise by differentiating h and evaluating the result at y, so we obtain rapid decay away from $\operatorname{supp} h$.

Concerning (9.12) (for $g \in \mathcal{C}_c^{-\infty}(C_a')$), we are done if we show that for any ξ that is not in the right hand side of (9.12), we can write $u = Bv + f$ with $B \in \Psi_{\mathrm{Sc}}^{-\infty,0}(\bar{X},\mathcal{C})$, $v \in \mathcal{C}^{-\infty}(X)$, $f \in \dot{\mathcal{C}}^\infty(\bar{X})$, $\xi \notin \mathrm{WF}_{\mathrm{Sc}}'(B)$. For the sake of simplicity, and since we only need this weaker statement here, we only state the proof with $\{(y, \sqrt{\lambda - \epsilon_\alpha}, 0) :\ y \in \operatorname{supp} g\}$ in the right hand side of (9.12) replaced by $\{(y, \sqrt{\lambda - \epsilon_\alpha}, 0) :\ y \in C_a'\}$; the improved statement only requires a more careful consideration of supports in (9.19).

To find such B, v, f, we consider $q \in \mathcal{C}_c^\infty({}^{\mathrm{sc}}T^*\bar{X}_a)$ as in Section 6, $\rho \in \mathcal{C}^\infty(\bar{X})$ supported near C_a, identically 1 in a small neighborhood of C_a, and take $\psi_0 \in \mathcal{C}_c^\infty(\mathbb{R})$ is identically 1 on $\operatorname{supp}\psi$ (recall that $\tilde{P}_{\alpha,+}(\lambda) = \psi(H)P$), and let $A = \rho Q\psi_0(H) \in \Psi_{\mathrm{Sc}}^{-\infty,0}(\bar{X},\mathcal{C})$ as in Section 6. Then, as discussed above (with $\psi(H)$ in place of A), the kernel K' of $A\tilde{P}_{\alpha,+}(\lambda)$ has the form (9.7), i.e.

$$K' = e^{-i\sqrt{\lambda-\epsilon_\alpha}\, y\cdot y'/x} x^{i\tilde{I}_a(y')/2\sqrt{\lambda-\epsilon_\alpha}} a'(x, y, Z, y'), \tag{9.17}$$

$a' \in \mathcal{C}^\infty([\bar{X};C_a]\times C_a)$, and in addition

$$\begin{aligned}(\bar{y}, d_{(y/x)}(-\sqrt{\lambda-\epsilon_\alpha}\, y\cdot y'/x)|_{(0,\bar{y},\bar{y}')}) &\notin \operatorname{supp} q\\ &\Rightarrow a' \text{ vanishes to infinite order near } (\bar{y},\bar{y}')\in C_a\times C'_a.\end{aligned} \tag{9.18}$$

Suppose also that

$$y\in C'_a \Rightarrow (y,\sqrt{\lambda-\epsilon_\alpha},0)\notin \operatorname{supp} q, \tag{9.19}$$

so by (9.18), the diagonal $y=y'$ is disjoint from $\operatorname{supp} a'$. This means that, with $\mathcal{F}_{X_a}$ denoting the Fourier transform in X_a, $\mathcal{F}_{X_a} A\tilde{P}_{\alpha,+}(\lambda)$ is a Fourier integral operator in the usual sense (on $X_a^*\times C'_a$ where X_a^* is the dual of X_a, which we identify with X_a for the sake of convenience), with values in Schwartz functions on X^a, and with canonical relation in

$$(T^*X_a\setminus 0)\times (T^*C'_a\setminus 0) \tag{9.20}$$

due to the previous remark. We also take $C\in\Psi^0(C'_a)$ with compactly supported kernel and amplitude (full symbol) c, and suppose that

$$\begin{aligned}(y,\xi)\in \operatorname{supp} q \text{ and } (y',\zeta)&\in \operatorname{cone\,supp} c\cap S^*C'_a\\ \Rightarrow (y,\xi)\notin \overline{\gamma_{\alpha,-}(y',\zeta)} &= \gamma_{\alpha,-}(y',\zeta)\cup\{(y',\sqrt{\lambda-\epsilon_\alpha},0\}.\end{aligned} \tag{9.21}$$

(N.B. $(y,\xi)\in\operatorname{supp} q$ automatically implies that (y,ξ) is not in the second set on the right hand side, i.e. it is not incoming, by (9.19).) We claim that under these conditions $A\tilde{P}_{\alpha,+}(\lambda)C$ has a smooth rapidly decreasing kernel $K_{APC}\in\dot{\mathcal{C}}^\infty(\bar{X}\times C'_a)$. This can be seen from the standard FIO calculus (with values in Schwartz functions on X^a if stated this way) if we perform Fourier transform in X_a. Namely, as remarked above $\mathcal{F}_{X_a}A\tilde{P}_{\alpha,+}(\lambda)$ is a Fourier integral operator, with canonical relation satisfying (9.20). Thus, $\mathcal{F}_{X_a}A\tilde{P}_{\alpha,+}(\lambda)C$ is also an FIO. But by (9.18) and (9.21), $(y',\zeta)\in\mathrm{WF}'(C)$ implies that for no $(\xi,y')\in T^*X_a$ is (ξ,y',y,ζ) in the canonical relation of $\mathcal{F}_{X_a}A\tilde{P}_{\alpha,+}(\lambda)$, hence smoothness of the kernel of $\mathcal{F}_{X_a}A\tilde{P}_{\alpha,+}(\lambda)C$ follows. Rapid decay at infinity of the kernel of $\mathcal{F}_{X_a}A\tilde{P}_{\alpha,+}(\lambda)C$ being automatic, this shows that $K_{APC}\in\dot{\mathcal{C}}^\infty(\bar{X}\times C'_a)$. This can also be seen more directly, writing out the composition as an oscillatory integral, in the uncompactified notation, with $w_a=y/x$,

$$\begin{aligned}K_{APC}(w_a,Z,y'') = \int e^{-i\sqrt{\lambda-\epsilon_\alpha}w_a\cdot y'}e^{i(y'-y'')\cdot\zeta}|w_a|^{-i\tilde{I}_a(y')/2\sqrt{\lambda-\epsilon_\alpha}}\\ a'(w_a,y',Z)c(y',\zeta)\,dy'\,d\zeta,\end{aligned} \tag{9.22}$$

where $w_a\cdot y'$ stands for the X_a-scalar product of $w_a\in X_a$ and $y'\in C_a$, we see that the phase of the y' integral is only stationary if $(y,\xi_a)\in\overline{\gamma_{\alpha,-}(y',\zeta)}$, but $a'c$ is rapidly decreasing there.

Now, given any $g\in\mathcal{C}_c^{-\infty}(C'_a)$, and any $U\subset S^*C'_a$ open such that $\mathrm{WF}(g)\subset U$, we can find $C\in\Psi^0(C'_a)$ with compactly supported kernel such that $\mathrm{WF}'(C)\subset U$, $\mathrm{WF}'(\mathrm{Id}-C)\cap\mathrm{WF}(g)=\emptyset$. Thus, $(\mathrm{Id}-C)g\in\mathcal{C}_c^\infty(C'_a)$. Choosing q as above, i.e. satisfying (9.19) and (9.21), we see that

$$Au = A\tilde{P}_{\alpha,+}(\lambda)Cg + A\tilde{P}_{\alpha,+}(\lambda)(\mathrm{Id}-C)g\in\dot{\mathcal{C}}^\infty(\bar{X}). \tag{9.23}$$

As $(\mathrm{Id}-\psi_0(H))u=0$, this shows that

$$u=\psi_0(H)u = Q\psi_0(H)u + (\psi_0(H)-Q\psi_0(H))u = Au + (\psi_0(H)-A)u, \tag{9.24}$$

so if $q \equiv 1$ near (y,ξ), so $(y,\xi) \notin \mathrm{WF}'_{\mathrm{Sc}}(B)$, $B = \psi_0(H) - A \in \Psi_{\mathrm{Sc}}^{-\infty,0}(\bar{X},\mathcal{C})$, then $(y,\xi) \notin \mathrm{WF}_{\mathrm{Sc}}(u)$. But U, hence $\operatorname{supp} c$, can be chosen arbitrarily small around $\mathrm{WF}(g)$; correspondingly for any (y,ξ) such that $(y,\xi) \notin \overline{\gamma_{\alpha,-}(y',\zeta)}$ for any $(y',\zeta) \in \mathrm{WF}(g)$, and (y,ξ) is not incoming, we deduce that $(y,\xi) \notin \mathrm{WF}_{\mathrm{Sc}}(u)$. The estimate for $\mathrm{WF}_{\mathrm{Sc}}((H-\lambda)u)$ works the same way; now $(H-\lambda)u = \psi_0(H)(H-\lambda)Pg$, with $(H-\lambda)P$ of the same form as P but with smaller (cone) support. This gives the improved estimate.

Note if we only required finitely many of the symbol estimates on, say, the symbol whose left quantization is B, a conclusion analogous to (9.12) would easily follow for any operator with kernel given by an oscillatory function as in (9.7), i.e. we could allow a_+ to be arbitrary, and there would be no need for the factor $\psi(H)$ in the definition of $\tilde{P}_{\alpha,+}(\lambda)$. (Of course, (9.13) could not hold then.) Indeed, $v = (\Delta+1)^k u$ is of the same form as u, so $u = (\Delta+1)^{-k}v$. Choosing $q \in \mathcal{C}_c^\infty({}^{\mathrm{sc}}T^*\bar{X}_a)$, $C \in \Psi^0(C'_a)$ as above, so $Q \in \Psi_{\mathrm{sc}}^{-\infty,0}(\bar{X}_a)$, regarded as an operator on $\bar{X}$, we deduce just as above that $Q\tilde{P}_{\alpha,+}(\lambda)C$ has a smooth rapidly decreasing kernel, so (9.23) holds with Q in place of A. Let $\rho \in \mathcal{C}^\infty(\bar{X})$ be a cutoff function supported near C_a as above. Then $u = (\mathrm{Id} - \rho Q)(\Delta+1)^{-k}v + f$, $f = \rho Q u \in \dot{\mathcal{C}}^\infty(\bar{X})$, so if $B = (\mathrm{Id} - \rho Q)(\Delta+1)^{-k}$ were in $\Psi_{\mathrm{Sc}}^{-\infty,0}(\bar{X},\mathcal{C})$, we would be able to deduce that $\xi \notin \mathrm{WF}'_{\mathrm{Sc}}(B)$ implies $\xi \notin \mathrm{WF}_{\mathrm{Sc}}(u)$. The problem is that q is not a symbol in (ξ_a,ξ^a) jointly since it is independent of the latter. However, note that k can be chosen arbitrarily large, so it can be arranged that B satisfies an arbitrary, but finite, number of the symbol estimates corresponding to $\Psi_{\mathrm{Sc}}^{-\infty,0}(\bar{X},\mathcal{C})$, while keeping v in a fixed weighted Sobolev space. While this is sufficient for any ps.d.o. argument based on weighted Sobolev space estimates, etc., to go through, it is not sufficient for ensuring that B is in $\Psi_{\mathrm{Sc}}^{-\infty,0}(\bar{X},\mathcal{C})$; that was the reason for the somewhat more complicate argument of the previous paragraphs.

10. Scattering matrices

In view of the pairing formula (9.5) for the S-matrix, which we restate below, Proposition 2.6 allows us to describe the wave front relation of the S-matrices rather directly. Recall that the S-matrix from an incoming cluster α to an outgoing cluster β is given by

$$S_{\beta\alpha}(\lambda) = \frac{1}{2i\sqrt{\lambda - \epsilon_\beta}}((H-\lambda)\tilde{P}_{\beta,-}(\lambda))^* P_{\alpha,+}(\lambda), \tag{10.1}$$

$\lambda > \max(\epsilon_\alpha,\epsilon_\beta)$, $\lambda \notin \Lambda$. This formula defines $S_{\beta\alpha}(\lambda)$ as a map $\mathcal{C}_c^\infty(C'_a) \to \mathcal{C}^{-\infty}(C'_b)$. Namely if $g \in \mathcal{C}_c^\infty(C'_a)$ then $S_{\beta\alpha}(\lambda)g$ is given by the formula

$$\langle S_{\beta\alpha}(\lambda)g, h\rangle = \frac{1}{2i\sqrt{\lambda-\epsilon_\beta}}\langle P_{\alpha,+}(\lambda)g, (H-\lambda)\tilde{P}_{\beta,-}(\lambda)h\rangle, \quad h \in \mathcal{C}_c^\infty(C'_b), \tag{10.2}$$

where the pairing makes sense since, by (9.13) with $\tilde{P}_{\beta,-}$ in place of $\tilde{P}_{\alpha,+}$, $(H-\lambda)\tilde{P}_{\beta,-}(\lambda)h \in \mathcal{S}(\mathbb{R}^n)$. (Note that $\langle\cdot,\cdot\rangle$ denotes the complex L^2 pairing, linear in the first variable, not the real distributional pairing; the two are related by taking the complex conjugate of the second term.)

Before stating the full results on the wave front relation of $S_{\beta\alpha}(\lambda)$, we first address the question whether $S_{\beta\alpha}(\lambda)$ maps $\mathcal{C}_c^\infty(C'_a)$ to $\mathcal{C}^\infty(C'_b)$ and extends to a map $\mathcal{C}_c^{-\infty}(C'_a) \to \mathcal{C}^{-\infty}(C'_b)$. This is closely related to the question whether the wave front set of the kernel of $S_{\beta\alpha}(\lambda)$ is a subset of $T^*(C'_b \times C'_a)\setminus((0\times T^*C'_a)\cup(T^*C'_b\times 0))$, as we discussed in Section 2. By a pairing argument we can answer the first question affirmatively if for all $g \in \mathcal{C}_c^\infty(C'_a)$, $h \in \mathcal{C}_c^{-\infty}(C'_b)$, the two terms being paired in (10.2), that is $P_{\alpha,+}(\lambda)g$ and $(H-\lambda)\tilde{P}_{\beta,-}(\lambda)h$, have disjoint wave front sets. Indeed, suppose that $K_1 = \mathrm{WF}_{\mathrm{Sc}}(P_{\alpha,+}(\lambda)g)$ and $K_2 = \mathrm{WF}_{\mathrm{Sc}}((H-\lambda)\tilde{P}_{\beta,-}(\lambda)h)$ are disjoint. Being wave front sets, they are closed, and as $\psi(H)P_{\alpha,+}(\lambda)g = P_{\alpha,+}(\lambda)g$ if $\psi \equiv 1$ near λ, $\psi \in \mathcal{C}_c^\infty(\mathbb{R})$, we see that K_1 is compact, and K_2 is also compact by (9.13) applied for $\tilde{P}_{\beta,-}(\lambda)$. As discussed in Section 4, there exists $q \in \mathcal{C}^\infty({}^{\mathrm{sc}}T^*\bar{X})$, q π-invariant, such that $q \equiv 1$ on K_1, $q \equiv 0$ on K_2, and q satisfies estimates (6.3), so we can define an operator $A \in \Psi_{\mathrm{Sc}}^{-\infty,0}(\bar{X},\mathcal{C})$ as in Lemma 6.1 which is of the form $Q\psi(H)$, ψ as above, and Q acts on oscillatory functions. Then $\mathrm{WF}'_{\mathrm{Sc}}(\psi(H)-A) \cap K_1 = \emptyset$ by construction, so $(\psi(H)-A)P_{\alpha,+}(\lambda)g \in \dot{\mathcal{C}}^\infty(\bar{X})$. In addition, $\mathrm{WF}'_{\mathrm{Sc}}(A^*) \cap K_2 = \emptyset$, so $A^*(H-\lambda)\tilde{P}_{\beta,-}(\lambda)h \in \dot{\mathcal{C}}^\infty(\bar{X})$ as well. Then

(10.3)
$$\begin{aligned}&\langle P_{\alpha,+}(\lambda)g, (H-\lambda)\tilde{P}_{\beta,-}(\lambda)h\rangle\\ &= \langle(\psi(H)-A)P_{\alpha,+}(\lambda)g, (H-\lambda)\tilde{P}_{\beta,-}(\lambda)h\rangle + \langle P_{\alpha,+}(\lambda)g, A^*(H-\lambda)\tilde{P}_{\beta,-}(\lambda)h\rangle,\end{aligned}$$

with the equality a priori valid for g, h smooth, for then the second factor is Schwartz, shows that the pairing (10.2) makes sense (i.e. extends by continuity from smooth data) if K_1 and K_2 are disjoint.

This is certainly the case if α and β are either the free channel or 2-cluster channels satisfying (2.34) (including the possibility that one is free, the other is such a two cluster channel). In fact, if $\beta = 0$ is the free channel, α is arbitrary (but satisfies (2.34)), $\lambda > 0$ (so with the notation of Theorem 8.1 $a(\lambda) = \lambda$) then on $\mathrm{WF}_{\mathrm{Sc}}((H-\lambda)\tilde{P}_{\beta,-}(\lambda)h)$, $-\sqrt{\lambda} < \tau < \sqrt{\lambda}$ by (9.13), while $\mathrm{WF}_{\mathrm{Sc}}(P_{\alpha,+}(\lambda)g) \subset \Phi_+(R_-(\lambda))$ by Proposition 2.6, so as τ is a decreasing function along generalized broken bicharacteristics, $\tau \leq -\sqrt{a(\lambda)} = -\sqrt{\lambda}$ on it, so these two sets are indeed disjoint. On the other hand, if β is a 2-cluster channel satisfying (2.34), α arbitrary, then one can arrange (by continuing the kernel construction until close to the $-$ outgoing, i.e. $+$ incoming, set) that on $\mathrm{WF}_{\mathrm{Sc}}((H-\lambda)\tilde{P}_{\beta,-}(\lambda)h)$, τ is arbitrarily close to $\sqrt{\lambda-\epsilon_\beta}$, which is again disjoint from the set $\tau \leq -\sqrt{a(\lambda)}$, hence from $\mathrm{WF}_{\mathrm{Sc}}(P_{\alpha,+}(\lambda)g) \subset \Phi_+(R_-(\lambda))$. This suffices to prove that $S_{\beta\alpha}(\lambda) : \mathcal{C}^\infty(C'_a) \to \mathcal{C}^\infty(C'_b)$ in this case. By a similar argument, or by duality, $S_{\beta\alpha}(\lambda)$ extends to a map $\mathcal{C}^{-\infty}(C'_a) \to \mathcal{C}^{-\infty}(C'_b)$ if either α is a 2-cluster channel or the free channel. In other cases Proposition 2.6 and (9.13) do not allow us to conclude that the wave front sets of the two terms are disjoint, and correspondingly we cannot expect that $S_{\beta\alpha}(\lambda)$ either preserves smoothness or extends to distributional data. We summarize these results in the following corollary.

Corollary 10.1. *Suppose that H is a many-body Hamiltonian, $\lambda \notin \Lambda$, and* (2.34) *holds. If β is a two-cluster channel or the free cluster then $S_{\beta\alpha}(\lambda)$ preserves smoothness: $S_{\beta\alpha}(\lambda) : \mathcal{C}_c^\infty(C'_a) \to \mathcal{C}_c^\infty(C'_b)$. If α is a two-cluster channel or the free cluster then $S_{\beta\alpha}(\lambda)$ extends to a map on distributions: $S_{\beta\alpha}(\lambda) : \mathcal{C}_c^{-\infty}(C'_a) \to \mathcal{C}_c^{-\infty}(C'_b)$*

The pairing argument of course allows us to describe the wave front relation of the S-matrices in general. If $g \in \mathcal{C}_c^{-\infty}(C'_a)$ satisfies $\mathcal{R}_{\alpha,+}(\mathrm{WF}(g)) \cap R_+(\lambda) = \emptyset$, then $P_{\alpha,+}(\lambda)g$ is defined, and its wave front set is given by Proposition 2.6. Similarly, if $h \in \mathcal{C}_c^{-\infty}(C'_b)$, then $\tilde{P}_{\beta,-}(\lambda)h$ is always defined and the wave front set of its 'error as a generalized eigenfunction' is given by (9.13). Thus, under the additional assumption that these two wave front sets are disjoint, which holds if

$$\{\gamma_{\beta,+}(\zeta) : \zeta \in \mathrm{WF}(h)\} \cap (\mathcal{R}_{\alpha,+}(\mathrm{WF}(g)) \cup \Phi_+(R_-(\lambda))) = \emptyset, \tag{10.4}$$

we see that $\langle S_{\beta\alpha}(\lambda)g, h\rangle$ is defined via (10.2). Since h is arbitrary, except that its wave front set satisfies (10.4), this allows us to conclude that if $K \subset S^*C'_a$ is such that

$$\{\gamma_{\beta,+}(\zeta) : \zeta \in K\} \cap (\mathcal{R}_{\alpha,+}(\mathrm{WF}(g)) \cup \Phi_+(R_-(\lambda))) = \emptyset, \tag{10.5}$$

then $\mathrm{WF}(S_{\beta\alpha}(\lambda)g) \cap K = \emptyset$. But by the definition of $\mathcal{R}_{\beta\alpha}$ and $\mathcal{R}_{\beta,-}$, (10.5) is equivalent to

$$\mathcal{R}_{\beta\alpha}(\mathrm{WF}(g)) \cap K = \emptyset \text{ and } \mathcal{R}_{\beta,-}^{-1}(R_-(\lambda)) \cap K = \emptyset. \tag{10.6}$$

(See the proof of Theorem 12.4 in [37] for a more detailed version of the pairing argument.) We have thus completed the proof of Theorem 2.8.

Theorem. *(Theorem 2.8) Suppose that H is a many-body Hamiltonian, $\lambda \notin \Lambda$, and (2.34) holds. Then $S_{\beta\alpha}(\lambda)$ 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*

$$\mathrm{WF}(S_{\beta\alpha}(\lambda)g) \subset \mathcal{R}_{\beta,-}^{-1}(R_-(\lambda)) \cup \mathcal{R}_{\beta\alpha}(\mathrm{WF}(g)). \tag{10.7}$$

Appendix A. Geometric description of broken bicharacteristics

The purpose of the appendix is to give a more geometric description of the generalized broken bicharacteristics, provided that the set of thresholds, Λ_1, is discrete, that is to prove Theorem 5.10. We also analyze four-body scattering, where we can also obtain a similar simple geometric description for generalized broken bicharacteristics.

It is convenient to break up the analysis of the structure of the generalized broken bicharacteristics into a local and a global step. Although until now we used the expression 'broken bicharacteristic' as a synonym for the cumbersome term 'generalized broken bicharacteristic', we now give a stronger definition for the former *which is only valid in this Appendix.*

Definition A.1. Suppose I is compact, $\gamma : I \to \dot{\Sigma}(\lambda)$ is a generalized broken bicharacteristic. We say that it is a broken bicharacteristic if there exist $t_0 < t_1 < \ldots < t_k$, $I = [t_0, t_k]$, such that for each j, $\gamma|_{[t_j,t_{j+1}]}$ is the projection of an integral curve of ${}^{\mathrm{sc}}H_g$ to $\dot{\Sigma}(\lambda)$. In general, if I is not compact, we say that γ is a broken bicharacteristic if $\gamma|_J$ is a broken bicharacteristic for all compact intervals $J \subset I$.

Definition A.2.

(i) An N-body Hamiltonian has a locally broken bicharacteristic relation if for all I compact, and for all generalized broken bicharacteristics $\gamma : I \to \dot{\Sigma}(\lambda)$, there exist $t_0 < t_1 < \ldots < t_k$, $I = [t_0, t_k]$, such that for each j, $\gamma|_{[t_j,t_{j+1}]}$ is the projection of an integral curve of ${}^{\mathrm{sc}}H_g$ to $\dot{\Sigma}(\lambda)$.

(ii) We say that an N-body Hamiltonian has a globally broken bicharacteristic relation if for all generalized broken bicharacteristics $\gamma : \mathbb{R} \to \dot{\Sigma}(\lambda)$, there exist $t_0 < t_1 < \ldots < t_k$, such that $\gamma|_{(-\infty,t_0]}$, $\gamma_{[t_k,+\infty)}$, as well as for each j, $\gamma|_{[t_j,t_{j+1}]}$, are the projections of integral curves of ${}^{\mathrm{sc}}H_g$ to $\dot{\Sigma}(\lambda)$.

When we talk about the length $\ell(\gamma)$ of a generalized broken bicharacteristic γ, we mean the length of its projection to $\mathbb{S}^{n-1}$ (recall that the projection is Lipschitz).

Lemma A.3. *Suppose that H is a many-body Hamiltonian. Then there exists $l > 0$ such that for every generalized broken bicharacteristic $\gamma : [\alpha, \beta] \to \dot{\Sigma}(\lambda)$ of length $\ell(\gamma) \leq l$ there exists a cluster a such that the image of γ lies in $\cup_{C_a \subset C_b} {}^{sc}T^*_{C'_b}\bar{X}_b$.*

Proof. For each point $p \in \mathbb{S}^{n-1}$ there exists a unique a such that $p \in C'_a$. Also, there exists $l_p > 0$ such that $\exp_p(B_{l_p}(0))$ lies in $\cup_{C_a \subset C_b} {}^{\text{sc}}T^*_{C'_b}\bar{X}_b$, where $B_{l_p}(0)$ denotes the open ball of radius l_p in $T_p\mathbb{S}^{n-1}$ with respect to the standard metric. Now, $\{\exp_p(B_{l_p/2}(0)) : \ p \in \mathbb{S}^{n-1}\}$ is an open cover of the compact set $\mathbb{S}^{n-1}$, so it has a finite subcover corresponding to some points, say, p_j, $j = 1, \ldots, m$. Let $l = \min\{l_{p_j}/2 : 1 \leq j \leq m\}$. If γ is as above, let j be such that $\gamma(\alpha) \in \exp_{p_j}(B_{l_{p_j}/2}(0))$. For any $t \in [\alpha, \beta]$, the distance of $\gamma(t)$ and $\gamma(\alpha)$ is bounded by the length of γ, hence by $l \leq l_{p_j}/2$, so the image of γ lies in $\exp_{p_j}(B_{l_{p_j}}(0))$ which in turn lies in $\cup_{C_a \subset C_b} {}^{\text{sc}}T^*_{C'_b}\bar{X}_b$ for some a. $\square$

We next give an upper bound for the length of a broken bicharacteristic if Λ_1 is discrete. Note that Λ_1 is bounded, so under this assumption it is finite.

Lemma A.4. *Suppose that Λ_1 is discrete, and let C_1 be the number of its elements. Suppose that $\gamma : I \to \dot{\Sigma}(\lambda)$ is a broken bicharacteristic, I an interval. Then $\ell(\gamma) \leq C_1\pi$.*

Proof. We recall from [25] the explicit arclength parametrization, $s = s(t)$, of the integral curves of ${}^{\text{sc}}H_g$ with kinetic energy $\sigma > 0$. In terms of this parameterization for $\gamma|_{[t_j,t'_j]}$, $\tau(s) = \sqrt{\sigma_j}\cos(s - s_0)$ where s varies in a subinterval of $(s_0, s_0 + \pi)$, and $[t_j, t'_j]$ is such that $\gamma|_{[t_j,t'_j]}$ is an integral curve of ${}^{\text{sc}}H_g$ with kinetic energy σ_j. Since $\tau \circ \gamma$ (which we usually just write as τ) is monotone decreasing, this shows that the total length of the segments of γ which are integral curves of ${}^{\text{sc}}H_g$ with any given kinetic energy $\sigma > 0$, is at most π. If $\sigma = 0$, the bicharacteristic segment is constant. Since σ must be such that $\lambda - \sigma \in \Lambda_1$, there are C_1 possible values of σ, which proves our estimate. $\square$

Next, we note that in three-body scattering the uniform upper bound π holds without any assumptions on the structure of Λ_1,

Lemma A.5. *Suppose that H is a three-body Hamiltonian. Suppose that $\gamma : I \to \mathbb{R}$ is a broken bicharacteristic, I an interval. Then $\ell(\gamma) \leq \pi$.*

Proof. In three-body scattering kinetic energy is constant along generalized broken bicharacteristics (essentially because there are no positive energy bound states), so the proof of the previous lemma applies and gives the desired conclusion. $\square$

Our strategy to analyze generalized broken bicharacteristics is to divide them into pieces of length $\leq l$, and reduce the analysis to that in a subsystem, by virtue of Lemma A.3.

Lemma A.6. *Suppose H is an N-body hamiltonian all of its proper subsystems have a globally broken bicharacteristic relation. Then every generalized broken bicharacteristic of H of length $\leq l$, l as in Lemma A.3, is a broken bicharacteristic. In addition, if in all of the proper subsystems the maximum number of breaks in a broken bicharacteristic (defined over $\mathbb{R}$ and of* arbitrary energy*) is at most M_{N-1}, then every generalized broken bicharacteristic of H of length $\leq l$ has at most $2M_{N-1} + 2$ breaks.*

Proof. Let $\gamma : [\alpha, \beta] \to \dot{\Sigma}(\lambda)$ be a generalized broken bicharacteristic of length $\ell(\gamma) \leq l$, so the image of γ lies in a region $\cup_{C_a \subset C_b} {}^{\mathrm{sc}}T^*_{C'_b} \bar{X}_b$ for some a. Thus, we can use local coordinates around a for describing γ. By Lemma 5.8 and the argument preceeding it (showing that η_a cannot change sign more than once), there exist some points α', β' such that on $[\alpha, \alpha')$ and on $(\beta', \beta]$ the image of γ is disjoint from ${}^{\mathrm{sc}}T^*_{C'_a} \bar{X}_a$, and on $[\alpha', \beta']$, γ is an integral curve of ${}^{\mathrm{sc}}H^a_g$, where some intervals may be empty or reduce to a point. Consider the interval $(\beta', \beta]$ for the sake of definiteness, and assume that it is non-empty. Let $S(t)$ be given by

$$S(t) = -\int_t^\beta (1 + |z_a(t')|^2)^{1/2} |z_a(t')|^{-1} \, dt', \tag{A.1}$$

so $S(t)$ is the solution of the ODE

$$dS/dt = (1 + |z_a(t)|^2)^{1/2} / |z_a(t)|, \ t \in (\beta', \beta], \ S(\beta) = 0, \tag{A.2}$$

where we wrote $|z_a(t)| = |z_a(\gamma(t))|$. Thus, S is $\mathcal{C}^1$ and its derivative is positive, so the same holds for its inverse function, S^{-1}, defined on an interval J. We denote by $\dot{\Sigma}_{H^a}(\lambda - |\bar{\xi}_a|^2)$ the characteristic variety of the (proper) subsystem Hamiltonian H^a at energy $\lambda - |\bar{\xi}_a|^2$. Now let $\tilde{\gamma} : J \to \dot{\Sigma}_{H^a}(\lambda - |\bar{\xi}_a|^2)$, given by

$$\tilde{\gamma}(s) = (z_a(S^{-1}(s)) / |z_a(S^{-1}(s))|, \nu_a(S^{-1}(s))), \tag{A.3}$$

so in terms of Euclidean coordinates,

$$\tilde{\gamma}(s) = (w^a(S^{-1}(s)) / |w^a(S^{-1}(s))|, \xi^a(S^{-1}(s))), \tag{A.4}$$

It is straightforward to check that $\tilde{\gamma}$ is a generalized broken bicharacteristic of H^a; the change of parameters accounts for the change in normalization of the rescaled Hamilton vector fields. In fact, ${}^{\mathrm{sc}}H_g = \langle w \rangle H_g$, while its analog in the subsystem is $\langle w^a \rangle H_{g^a}$, and the quotient $\langle w^a \rangle / \langle w \rangle$ is $|z_a| / (1 + |z_a|^2)^{1/2}$. Thus, by the hypothesis, $\tilde{\gamma}$ is a broken bicharacteristic. Since ξ_a is constant along generalized broken bicharacteristics, we conclude that on $(\beta', \beta]$, $\gamma|_{(\beta', \beta]}$ is a broken bicharacteristic if and only if $\tilde{\gamma}$ is, so by the hypothesis it is a broken bicharacteristic, and it has as many breaks as $\tilde{\gamma}$, so if we assume uniform bounds in the proper subsystems, at most M_{N-1}.

A similar estimate holds for $[\alpha, \alpha')$, so on $[\alpha, \beta]$, γ is a broken bicharacteristic, and if we also assume uniform bounds in the proper subsystems, it can have at most $2M_{N-1} + 2$ breaks, proving the lemma. □

Corollary A.7. *Suppose H is an N-body hamiltonian, and all of its proper subsystems have a globally broken bicharacteristic relation. Then H has a locally broken bicharacteristic relation.*

Proof. If $\gamma : I \to \dot{\Sigma}(\lambda)$ is a generalized broken bicharacteristic, I compact, then its total arclength is finite, so dividing it up into segments of length $\leq l$ and applying the previous lemma proves the proposition. □

Proposition A.8. *Suppose H is an N-body hamiltonian with Λ_1 discrete, all of its proper subsystems have a globally broken bicharacteristic relation, and in all of these subsystems the maximum number of breaks in a broken bicharacteristic (defined over $\mathbb{R}$ and* of any energy*) is at most M_{N-1}. Then H has a globally broken bicharacteristic relation and there is a constant M_N such that every broken bicharacteristic of H* of any energy *has at most M_N breaks.*

Proof. Due to the previous corollary, every generalized broken bicharacteristic of H is a broken bicharacteristic. By Lemma A.4, its length $\ell(\gamma)$ satisfies the inequality $\ell(\gamma) \leq C_1\pi$. Dividing it up into pieces of length $\leq l$, of which (we can arrange that) there are at most $C_1\pi/l+1$, shows that the total number of breaks is at most $(C_1\pi/l+1)(2M_{N-1}+3)$ which is independent of γ, proving the proposition. $\square$

An inductive argument completes the proof of Theorem 5.10, which we restate.

Theorem A.9. *Suppose that H is a many-body Hamiltonian and Λ_1 is discrete. Then H has a globally broken bicharacteristic relation, and there is a constant M such that every generalized broken bicharacteristic of H has at most M breaks.*

We next discuss what happens if Λ_1 is not discrete.

In the following we let $C_0>0$ be a constant such that for $s,s'\in(0,\pi)$,

$$|\cos s-\cos s'|\geq C_0^{-2}|s-s'|^2. \tag{A.5}$$

Thus, C_0^2 is essentially the Hölder constant in the Hölder of order $\frac{1}{2}$ estimate for arccos.

Lemma A.10. *Suppose that $\gamma: I\to\mathbb{R}$ is a broken bicharacteristic, I compact, $[t_j,t_j']$, $j=1,\dots,k$, are subintervals of I such that the open intervals (t_j,t_j') are disjoint. Suppose that the kinetic energy over the interval $[t_j,t_j']$ is σ_j, and let*

$$\Delta\tau=\sum_{j=1}^{k}\tau(\gamma(t_j'))-\tau(\gamma(t_j)). \tag{A.6}$$

Let $\ell(\gamma_j)$ be the length of $\gamma_j=\gamma|_{[t_j,t_j']}$. Then

$$\begin{aligned}\sum_{j=1}^{k}\ell(\gamma_j)&\leq C_0(\sum_{j=1,\ \sigma_j>0}^{k}\sigma_j^{-1})^{1/2}|\Delta\tau|\\&\leq C_0(\min\{\sigma_j:\ \sigma_j\neq 0,\ j=1,\dots,k\})^{-1/2}\,k^{1/2}|\Delta\tau|.\end{aligned} \tag{A.7}$$

Proof. We again use the explicit arclength parametrization, $s=s(t)$, of the integral curves of ${}^{\mathrm{sc}}H_g$ with $\sigma_j>0$. Thus, $\tau(s)=\sqrt{\sigma_j}\cos(s-s_0)$ for γ_j where s varies in a subinterval of $(s_0,s_0+\pi)$. This gives

$$C_0\sigma_j^{-1/2}|\tau(s(t_j'))-\tau(s(t_j))|^{1/2}\geq s(t_j')-s(t_j). \tag{A.8}$$

If $\sigma_j=0$ then both $\tau(s(t_j'))-\tau(s(t_j))$ and $s(t_j')-s(t_j)$ vanish. Summing over j and applying the Cauchy-Schwartz inequality to the left hand side proves the lemma. $\square$

Note that in Lemma A.6, we really only need to assume that the estimates M_{N-1} in the subsystems are uniform over bounded sets of energy to obtain a uniform estimate M_N over bounded sets of energy for H.

Corollary A.11. *Suppose H is an N-body hamiltonian all of its proper subsystems have a globally broken bicharacteristic relation, and in all of the proper subsystems the maximum number of breaks in a broken bicharacteristic (defined over $\mathbb{R}$) is at most M_{N-1}. Suppose that $\gamma: I\to\dot{\Sigma}(\lambda)$ is a generalized broken bicharacteristic of H (hence a broken bicharacteristic under these assumptions), and suppose that there exist $c_0>0$, $m>0$, such that the kinetic energy assumes at most m values which are less than c_0. Then there is a constant M_N that depends only on c_0, m, and H, such that γ has at most M_N breaks.*

Proof. We only need to show that there exists M_N as above such that for every compact interval $J \subset I$, $\gamma|_J$ has at most M_N breaks. Let n denote the number of breaks in $\gamma|_J$. Note that $\tau \circ \gamma$ is monotone decreasing and it is bounded, with a bound given by $(\lambda - \inf \Lambda_1)^{1/2}$ (since $\lambda - \tau^2 - |\mu|^2 \in \Lambda_1$ in $\dot{\Sigma}(\lambda)$). By Lemma A.10, the total length of bicharacteristic segments with kinetic energy at least c_0 is at most $2C_0 c_0^{-1/2} n^{1/2} (\lambda - \inf \Lambda_1)^{1/2}$, while by the proof of Lemma A.4, the total length of bicharacteristic segments with kinetic energy less than c_0 is at most $m\pi$. Thus,

$$\ell(\gamma|_J) \leq 2C_0 c_0^{-1/2} n^{1/2} (\lambda - \inf \Lambda_1)^{1/2} + m\pi. \tag{A.9}$$

On the other hand, dividing $\gamma|_J$ into segments of length $\leq l$, of which we can arrange that there are at most $\ell(\gamma|_J)/l + 1$, and applying Lemma A.6, shows that

(A.10)

$$\begin{aligned} n &\leq (2M_{N-1} + 2)(\ell(\gamma|_J)/l + 1) \\ &\leq (2M_{N-1} + 2)(1 + m\pi/l) + 2(2M_{N-1} + 2) C_0 c_0^{-1/2} n^{1/2} (\lambda - \inf \Lambda_1)^{1/2}/l. \end{aligned}$$

Dividing through by $n^{1/2}$ gives the desired estimate for n, uniform in the energy λ as long as λ stays in a bounded set. $\square$

Proposition A.12. *Suppose that H is as in Corollary A.11, and $\lambda \notin \Lambda_1$. Then there exists M_N depending only on H and $\inf\{\lambda - E : \ \lambda - E > 0,\ E \in \Lambda_1\}$ such that every generalized broken bicharacteristic $\gamma : I \to \dot{\Sigma}(\lambda)$ has at most M_N breaks.*

Proof. Note first that Λ_1 is closed, so for $\lambda \notin \Lambda_1$, $\inf\{\lambda - E : \ \lambda - E > 0,\ E \in \Lambda_1\} > 0$. The kinetic energy $\sigma \geq 0$ on any bicharacteristic segment satisfies $\lambda - \sigma \in \Lambda_1$, so $\sigma \geq \inf\{\lambda - E : \ \lambda - E > 0,\ E \in \Lambda_1\} > 0$. Applying Corollary A.11 with $c_0 = \inf\{\lambda - E : \ \lambda - E > 0,\ E \in \Lambda_1\}$, $m = 0$, completes the proof. $\square$

Combining this result with Lemma A.5 yields the following theorem.

Theorem A.13. *Suppose that H is a 4-body Hamiltonian, and $\lambda \notin \Lambda_1$. Then there exists M depending only on H and $\inf\{\lambda - E : \ \lambda - E > 0,\ E \in \Lambda_1\}$ such that every generalized broken bicharacteristic $\gamma : I \to \dot{\Sigma}(\lambda)$ has at most M breaks.*

While in 4-body scattering one is mostly interested in $\lambda \notin \Lambda_1$, making this result useful, in the inductive step, to analyze 5-body scattering, the 4-body thresholds must be understood as well, as indicated by the proof of Lemma A.6, in particular by $\tilde{\gamma} : J \to \dot{\Sigma}_{H^a}(\lambda - |\bar{\xi}_a|^2)$ (the notation is the same as in the Lemma), for $\lambda - |\bar{\xi}_a|^2$ can be a threshold of the subsystem H^a.

Appendix B. Lagrangian structure of the forward broken bicharacteristic relation

In this section we show that if the set of thresholds of H is discrete, then the part of the forward broken bicharacteristic relation corresponding to non-tangentially breaking broken bicharacteristics is the finite union of Lagrangian submanifolds, and it maps the outgoing radial set to a finite union of Lagrangian submanifolds as well. Together with Theorem 2.8, (a simple modification of) this immediately implies the corresponding result, stated in Theorem 2.10, about the wave front relation of the various scattering matrices with incoming and outgoing channels satisfying the assumptions (2.34).

First, recall that if Λ_1 is discrete, every generalized broken bicharacteristic γ consists of a finite number of bicharacteristic segments (with a uniform bound on the number of these segments). Let a_j be the cluster and α_j the channel in which the jth segment propagates. Also, let c_j be the cluster at which γ breaks between propagation along the clusters a_j and a_{j+1}, so $C_{c_j} \subset C_{a_j} \cap C_{a_{j+1}}$ and the 'break point' is in ${}^{\mathrm{sc}}T^*_{C'_{c_j}} \bar{X}_{c_j}$, i.e. over the regular part of C_{c_j}. Thus, we can associate a string

$$a_1, \alpha_1, c_1, a_2, \alpha_2, c_2, \dots, c_m, a_{m+1}, \alpha_{m+1} \tag{B.1}$$

to γ, where each term has the same meaning as above. Since there is a uniform bound on the finite number of breaks that γ has, there are only finitely many such permissible strings. Moreover, since we are assuming that there is a break at c_j, $j = 1, \dots, m$, we can impose that either the segment in a_j, or the segment in a_{j+1}, is not tangential to c_j; in particular, $a_j \neq c_j$ or $a_{j+1} \neq c_j$.

Our additional assumption, on non-tangential breaking, is then that we only consider the contribution of broken bicharacteristics to the relation for which, for all j, *both* of the segments in a_j and a_{j+1} are *not* tangential to c_j. As discussed before the statement of Theorem 2.10, this holds for every generalized broken bicharacteristic when there are no bound states in any subsystems, and it implies, in particular, that $a_j \neq c_j$ and $a_{j+1} \neq c_j$. In fact, it suffices for our arguments that for all j, the segment in a_{j+1} is not tangential to c_j (which is what we use from now on), or instead, by 'duality', that for all j, the segment in a_j is not tangential to c_j; it is the combination that neither of these two statements holds that causes trouble.

It will be convenient to use the linear structure of the collision planes in this discussion. Thus, we will think of the relations, just as of the wave front sets, as conic sets, invariant under a natural $\mathbb{R}^+$ action *in the base variables* (i.e. in configuration space). Correspondingly, we talk about conic Lagrangian rather than Legendre submanifolds. Since multiplying a vector field by a non-zero function simply reparameterizes the integral curves, the bicharacteristics of ${}^{\mathrm{sc}}H^a_g$ and H_{g_a} agree after reparamaterization, so the former are given by the ($\mathbb{R}^+$-quotient induced) projection of straight lines in $T^*X_a = X_a \times X_a^*$ whose projection to X_a^* is constant, say ξ, such that $|\xi|_a^2 = g_a(\xi) = \lambda - \epsilon_\alpha$ where ϵ_α is the energy of the bound state the particle is propagating in. We sometimes write $|\xi|$ for $|\xi|_a$ to simplify the notation. We often identify X_a^* with X_a via the metric g_a (induced by g); we do so in particular when talking about $T^*X_a = X_a \times X_a^*$.

We show that the forward broken bicharacteristic relation is given by a finite union of Lagrangians, one for each string as in (B.1). To see this, we write the part of the forward broken bicharacteristic relation corresponding to such a string as the composite of elementary relations, each of which is Lagrangian, and which intersect transversally in the usual sense. Thus, we let $\tilde{\Lambda}^{\mathrm{in}} = \tilde{\Lambda}^{\mathrm{in}}_{c_j,a_j}$ to be the relation on $T^*X_{c_j} \times T^*X_{a_j}$ corresponding to projection from $T^*_{X_{c_j}} X_{a_j}$ to $T^*X_{c_j}$, and we let $\tilde{\Lambda}^{\mathrm{out}} = \tilde{\Lambda}^{\mathrm{out}}_{a_{j+1},\alpha_{j+1},c_j}$ to be the relation on $T^*X_{a_{j+1}} \times T^*X_{c_j}$ corresponding to bicharacteristics emanating from cluster c_j, and then propagating along cluster a_{j+1} in channel α_{j+1}. We also introduce the propagating Lagrangian $\tilde{\Lambda}^{\mathrm{prop}} = \tilde{\Lambda}^{\mathrm{prop}}_{a_j,\alpha_j}$ corresponding to the Hamilton flow inside channel α_j in the characteristic set; thus,

$$\tilde{\Lambda}^{\mathrm{prop}}_{a_j,\alpha_j} = \tilde{\Lambda}^{\mathrm{out}}_{a_j,\alpha_j,a_j}. \tag{B.2}$$

To simplify the notation, we write $c = c_j$, $a = a_j$, and suppose $X_{c_j} \subset X_{a_j}$ Then $\tilde{\Lambda}^{\mathrm{in}} = \tilde{\Lambda}^{\mathrm{in}}_{ca}$ is the Lagrangian corresponding to projection $T^*_{X_c} X_a \to T^*X_c$, so

$(w, \xi, w', \xi') \in \tilde{\Lambda}^{\text{in}}_{ca}$ means that

$$\xi = \pi_{ac}(\xi'),\ w = w' \in X_c. \tag{B.3}$$

Thus, $\tilde{\Lambda}^{\text{in}}$ is smoothly parameterized by $w \in X_c$, $\xi' \in X_a^*$. The tangent space $T_q\tilde{\Lambda}^{\text{in}}$ is spanned by

$$v \cdot \partial_w + v \cdot \partial_{w'},\ v \in X_c, \quad \pi_{ac}(v') \cdot \partial_\xi + v' \cdot \partial_{\xi'},\ v' \in X_a. \tag{B.4}$$

Here, as in what follows, the center dot $\cdot$, e.g. when writing $v \cdot \partial_{\xi'}$, etc., simply denotes the $\partial_{\xi'}$, etc., component of the tangent vector. Note that $\tilde{\Lambda}^{\text{in}}$ is indeed a Lagrangian submanifold of $T^*X_c \times T^*X_a$ with respect to the usual twisted symplectic form $\omega_c - \omega_a$, where ω_c denotes the canonical symplectic form on T^*X_c as well as its lift to the product (by an abuse of notation).

Next, suppose that $X_c \subset X_a$. Then the propagating Lagrangian $\tilde{\Lambda}^{\text{out}} = \tilde{\Lambda}^{\text{out}}_{a\alpha c}$, from X_c to X_a in channel α, is defined as follows. A point $(w, \xi, w', \xi') \in \tilde{\Lambda}^{\text{out}}$ means that

$$w = w' + c\xi,\ \xi' = \pi_{ac}(\xi),\ |\xi|^2 = \lambda - \epsilon_\alpha,\ c > 0. \tag{B.5}$$

This means that

$$\xi = \sqrt{\lambda - \epsilon_\alpha}\,\frac{w - w'}{|w - w'|}, \xi' = \pi_{ac}(\xi). \tag{B.6}$$

In particular, w, w' are coordinates on $\tilde{\Lambda}^{\text{out}}$, hence $\tilde{\Lambda}^{\text{out}}$ is a smooth graph over $X_a \times X_c$. Thus, the tangent space of $\tilde{\Lambda}^{\text{out}}$ at some point $p \in \tilde{\Lambda}^{\text{out}}$, given by (w, w') as above, is spanned by

$$\begin{aligned} &v \cdot \partial_w + Bv \cdot \partial_\xi + Cv \cdot \partial_{\xi'}, \quad v \in X_a, \\ &v' \cdot \partial_{w'} + B'v' \cdot \partial_{\xi'} + C'v' \cdot \partial_\xi, \quad v' \in X_c, \end{aligned} \tag{B.7}$$

where $B \in \text{End}(X_a)$, $B'_j \in \text{End}(X_c)$ are given by

$$\begin{aligned} B &= \frac{\sqrt{\lambda - \epsilon_\alpha}}{|w - w'|^3}(|w - w'|^2 \operatorname{Id} - (w - w') \otimes (w - w')), \\ B' &= \pi_{ac} \circ C' = -\frac{\sqrt{\lambda - \epsilon_{\alpha_j}}}{|w - w'|^3}(|w - w'|^2 \operatorname{Id} - (w' - \pi_{ac}(w)) \otimes (w' - \pi_{ac}(w))), \end{aligned} \tag{B.8}$$

and $C \in \text{Hom}(X_a, X_c)$, $C' \in \text{Hom}(X_c, X_a)$ are given by

$$\begin{aligned} C &= \pi_{ac} \circ B = \frac{\sqrt{\lambda - \epsilon_\alpha}}{|w - w'|^3}(|w - w'|^2\, \pi_{ac} - (\pi_{ac}(w) - w') \otimes (w - w')) \\ C' &= -\frac{\sqrt{\lambda - \epsilon_\alpha}}{|w - w'|^3}(|w - w'|^2 \operatorname{Id} - (w - w') \otimes (\pi_{ac}(w) - w')). \end{aligned} \tag{B.9}$$

Again, $\tilde{\Lambda}^{\text{out}}$ is indeed a Lagrangian submanifold of $T^*X_a \times T^*X_c$ with respect to the usual twisted symplectic form $\omega_a - \omega_c$. Note that B, B' are self-adjoint, $B \geq 0$, $-B' \geq 0$, $C' = -C^*$. In addition, if $w \notin X_c$, then B' is negative definite; if $w \in X_c$, $\text{Ker}(B') = \text{span}(w - w')$.

Before continuing, we make some general remarks about Lagrangian submanifolds Λ of T^*X_a. Suppose that Λ is (locally) a smooth graph over X_a; i.e. that for every $p \in \Lambda$, the bundle projection $T^*X_a \to X_a$ has a surjective differential at p (which is thus an isomorphism). Then Λ is (locally) the image of a smooth bundle map $F : X_a \to T^*X_a$, i.e. the composite of F with the projection to the base is the identity map. Since $T^*X_a = X_a \times X_a^*$ naturally, F has the form

$F(w) = (w, F_2(w))$ where $F_2 : X_a \to X_a^*$. Moreover, $T_pT^*X_a$ can be naturally identified with the vector space T^*X_a itself; so for each $w \in X_a$, $(F_2)_*|_w = (F_2)_*$ is a linear map from X_a to X_a^*. Let $A = A_w$ be the induced endomorphism of X_a via the metric identification of X_a and X_a^*. That Λ is Lagrangian means that for any two tangent vectors $V, V' \in T_p\Lambda$, $\omega(V, V') = 0$, where $\omega = \omega_a$ is the standard symplectic form given by $d\xi \wedge dw$, so writing $V, V' \in T_pT^*X_a = X_a \times X_a^*$ as $V = (v, v^*)$, $V' = (v', (v')^*)$, $\omega(V, V') = v^*(v') - (v')^*(v)$, so in our case, with $V = F_*v$, $V' = F_*v'$, the Lagrangian condition becomes $(F_2)_*v(v') - (F_2)_*v'(v) = 0$. Since the metric identification means that $(F_2)_*v(v') = g_a(Av, v') = Av \cdot v'$, the Lagrangian condition amounts to the statement that A is self-adjoint.

A similar discussion also applies to $T^*X_{a_{j+1}} \times T^*X_{c_j}$ with the twisted symplectic form $\omega_{a_{j+1}} - \omega_{c_j}$, and shows that for $\tilde{\Lambda}^{\text{out}}_{a_{j+1},\alpha_{j+1},c_j}$, which is a graph by (B.6), with the notation of (B.7), B and B' are self-adjoint on $X_{a_{j+1}}$ and X_{c_j} respectively, while $C' = -C^*$ (this of course follows from (B.8) as well).

We introduce the following notation.

Definition B.1. We say that a Lagrangian $\Lambda \subset T^*X_b$ is spreading if the projection to X_b is a local diffeomorphism, and, with the notation of the preceeding paragraphs, for all $p = (w, \xi) \in \Lambda$, $A = A_p \geq 0$.

The reason for the word 'spreading' is that in the forward flowout of a spreading Lagrangian, the distance between bicharacteristics is increasing. Namely, if $(w, \xi) \in \Lambda$, then so are $(w + \Delta w, \xi + A\Delta w + f(w, \Delta w))$, where $f(w, \Delta w) = O(|\Delta w|^2)$, for small Δw, and the forward flowout of these is $(w + t\xi, \xi)$ and $(w + \Delta w + t(\xi + A\Delta w) + O(|\Delta w|^2), \xi + A\Delta w + O(|\Delta w|^2))$, $t > 0$, respectively. Thus, up to $O(|\Delta w|^2)$ terms, the distance between these after time t is $|(\mathrm{Id} + tA)\Delta w|$, which is increasing if $A \geq 0$. This also indicates that if A has a non-trivial kernel, there may be various complications.

The idea in describing broken bicharacteristic propagation in Lagrangian terms is that, by their very definition, spreading Lagrangians will remain spreading under propagation; in fact this is true even after the breaks that happen when bicharacteristics hit some cluster sets. The only time when the strict positivity of A may be lost is when broken bicharacteristics propagating tangentially to a cluster c leave it to propagate in some other cluster a with $X_c \subsetneq X_a$. Dually, the only time when the lack of strict positivity of A may cause trouble is when a broken bicharacteristic propagating in a cluster a hits another cluster c, and starts propagating tangentially to c. It is such combinations we avoid by our non-tangentially breaking assumption.

We now show that both $\tilde{\Lambda}^{\text{in}}_{ca}$ and $\tilde{\Lambda}^{\text{out}}_{ac}$ map spreading Lagrangians to spreading Lagrangians. We start with the simpler case, $\tilde{\Lambda}^{\text{in}}_{ca}$.

Lemma B.2. *Suppose that Λ' is spreading. Then $\Lambda = \tilde{\Lambda}^{in} \circ \Lambda'$ is a smooth Lagrangian and it is spreading.*

Proof. Note that as a set,

$$\Lambda = \pi_1((T^*X_c \times \Lambda') \cap \tilde{\Lambda}^{\text{in}}), \tag{B.10}$$

where π_1 denotes projection to the first factor, T^*X_c, of $T^*X_c \times T^*X_a$.

We first remark that the submanifolds $T^*X_c \times \Lambda'$ and $\tilde{\Lambda}^{\text{in}}$ of $T^*X_c \times T^*X_a$ intersect transversally, i.e. for all q in their intersection,

$$T_q(T^*X_c \times \Lambda') + T_q\tilde{\Lambda}^{\text{in}} = T_q(T^*X_c \times T^*X_a). \tag{B.11}$$

Indeed, taking into account (B.4), vectors of the form $v' \cdot \partial_{\xi'}$ are in the range of the differential of the projection of $\tilde{\Lambda}^{\text{in}}$ to T^*X_a. Moreover, Λ' has full rank projection to X_a since it is spreading, so the intersection is indeed transversal. Thus, $(T^*X_c \times \Lambda') \cap \tilde{\Lambda}^{\text{in}}$ is a smooth submanifold of $T^*X_c \times T^*X_a$. Since $\tilde{\Lambda}^{\text{in}}$ is Lagrangian, $\omega_c - \omega_a$ vanishes on its tangent space, since Λ' is Lagrangian, ω_a vanishes on its tangent space, hence we see that ω_c also vanishes on its tangent space.

Next, we need to find the tangent space of the intersection at some point $q \in (T^*X_c \times \Lambda') \cap \tilde{\Lambda}^{\text{in}}$. Dimension counting shows that we have found the full tangent space provided we find a $\dim X_c$ dimensional subspace. So let $v \in X_c$, and let A' be the map in $\text{End}(X_a)$ as in the above definition. Then

$$(v \cdot \partial_w + v \cdot \partial_{w'}) + (\pi_{ac}(A'v) \cdot \partial_\xi + A'v \cdot \partial_{\xi'}) \in T_q(T^*X_c \times \Lambda') \cap T_q\tilde{\Lambda}^{\text{in}}; \tag{B.12}$$

hence these vectors give the whole tangent space of the intersection at q as v varies in X_c. Note that the ∂_w component is only zero if $v = 0$. Thus, $(\pi_1)_*$ has trivial kernel when restricted to the tangent space of the intersection at q, so Λ is a smooth manifold. Since ω_c vanishes on the intersection, it will also vanish on Λ, so Λ is Lagrangian (since it has dimension $\dim X_c$). Moreover, the tangent space of Λ at $\pi_1(q)$ is given by vectors $v \cdot \partial_w + \pi_{ac}(A'v) \cdot \partial_\xi$, $v \in X_c$. Thus, Λ is a smooth Lagrangian manifold. Moreover, the tangent vectors of Λ are of the form $v \cdot \partial_w + Av \cdot \partial_\xi$, $v \in X_c$, where

$$A \in \text{End}(X_c),\ A = \pi_{ac}A'\pi_{ac}, \tag{B.13}$$

so $A' \geq 0$ implies $A \geq 0$. This also shows that $\text{Ker}(A) = \text{Ker}(A') \cap X_c$. □

Lemma B.3. *Suppose that Λ' is spreading. Then $\Lambda = (\tilde{\Lambda}^{out}_{ac} \circ \Lambda') \setminus T^*_{X_c}X_a$ is a smoooth Lagrangian and it is spreading.*

Proof. As in the proof of the previous lemma, we first need to show that for $p = (w, \xi, w', \xi') \in (T^*X_a \times \Lambda') \cap \tilde{\Lambda}^{\text{out}}$

$$T_p(T^*X_a \times \Lambda') + T_p\tilde{\Lambda}^{\text{out}} = T_p(T^*X_a \times T^*X_c), \tag{B.14}$$

under the assumption that $w \notin X_c$, hence in particular $w \neq w'$. Note that $w \notin X_c$ implies that B' is negative definite. But, due to the first summand, ∂_w, ∂_ξ are in the left hand side, hence so is $v' \cdot \partial_{w'} + B'v' \cdot \partial_{\xi'}$, $v' \in X_c$, due to (B.7). Since the vectors $v_0 \cdot \partial_{w'} + A'v_0 \cdot \partial_{\xi'}$, $v_0 \in X_a$, are also in the left hand side due to the first summand, (B.14) will follow if the block matrix $\begin{bmatrix} I & I \\ B' & A' \end{bmatrix}$ is invertible, i.e. if $B' - A'$ is invertible. But B' is negative definite, so we conclude that $A' - B'$ is positive definite, hence invertible. This proves (B.14).

Next, we need to find

$$T_p(T^*X_a \times \Lambda') \cap T_p\tilde{\Lambda}^{\text{out}}. \tag{B.15}$$

Dimension counting shows that we will have found the whole intersection if for every $v \in X_a$ we find an element of the intersection which is of the form

$$v \cdot \partial_w + Av \cdot \partial_\xi + v_1 \cdot \partial_{w'} + v_2 \cdot \partial_{\xi'}. \tag{B.16}$$

To do so, fix $v \in X_a$, and consider elements of $T_p\tilde{\Lambda}^{\text{out}}$ which are of the form

$$v \cdot \partial_w + Bv \cdot \partial_\xi + Cv \cdot \partial_{\xi'} + v' \cdot \partial_{w'} + B'v' \cdot \partial_{\xi'} + C'v' \cdot \partial_\xi, \quad v' \in X_c. \tag{B.17}$$

For these to be in the intersection (B.15), we need that there exist $v_0 \in X_c$ such that the projection of (B.17) to $T_{(w',\xi')}T^*X_c$ is equal to $v_0 \cdot \partial_{w'} + A'v_0 \cdot \partial_{\xi'}$, i.e. such that

$$v' = v_0, \quad Cv + B'v' = A'v_0. \tag{B.18}$$

The existence of such v' and v_0 thus again follows from the invertibility of $\begin{bmatrix} I & -I \\ B' & -A' \end{bmatrix}$, which holds since $A' - B'$ is positive definite, and we see that in particular $v' = (A' - B')^{-1}Cv$. The projection of the corresponding tangent vector in (B.15) to $T_{(w,\xi)}T^*X_a$ is given by

$$v \cdot \partial_w + (Bv + C'v') \cdot \partial_\xi = v \cdot \partial_w + (B - C^*(A' - B')^{-1}C)v \cdot \partial_\xi \tag{B.19}$$

where we used $C' = -C^*$. Note in particular that the ∂_w component is non-zero. Thus, the projection of the intersection $(T^*X_a \times \Lambda') \cap \tilde{\Lambda}$ to T^*X_a is a smooth Lagrangian Λ with tangent vectors of the form

$$v \cdot \partial_w + Av \cdot \partial_\xi, \quad A = B - C^*(A' - B')^{-1}C. \tag{B.20}$$

We need to show that the composite Lagrangian is spreading; in particular $A \geq 0$. To see this, we take the following orthogonal decomposition of X_a:

$$X_a = \operatorname{span}(w - w') \oplus ((w - w')^\perp \cap X_c^\perp) \oplus P_{w-w'}^\perp X_c. \tag{B.21}$$

Here, as in what follows, for any vector v, $P_v^\perp$ denotes orthogonal projection to the orthocomplement of the span of v.

First, consider $v = w - w'$. Since $Bv = 0$, $Cv = 0$, we conclude that $Av = 0$, so $v \in \operatorname{Ker}(A)$.

Next, consider $v \in (w - w')^\perp \cap X_c^\perp$. Then $Cv = 0$, and $Bv = \frac{\sqrt{\lambda - \epsilon_\alpha}}{|w - w'|}v$. Thus,

$$v \in (w - w')^\perp \cap X_c^\perp \Rightarrow Av = \frac{\sqrt{\lambda - \epsilon_\alpha}}{|w - w'|}v. \tag{B.22}$$

Hence, $(w - w')^\perp \cap X_c^\perp$ is an eigenspace of A with eigenvalue $\frac{\sqrt{\lambda - \epsilon_\alpha}}{|w - w'|} > 0$.

It remains to analyze the restriction of A to $P_{w-w'}^\perp X_c$. Note that since its orthocomplement is a union of eigenspaces of A, $P_{w-w'}^\perp X_c$ has the same property; in particular, A indeed maps it into itself. Note that we only need to prove that for all v in this space, $v \cdot Av \geq 0$. But for such v, $Bv = \sqrt{\lambda - \epsilon_\alpha}|w - w'|^{-1}v$, so we need to show that

$$\sqrt{\lambda - \epsilon_\alpha}|w - w'|^{-1}\|v\|^2 \geq Cv \cdot ((A' - B')^{-1}Cv). \tag{B.23}$$

Now, $-B'$ is positive definite, $A' \geq 0$, so $0 \leq (A' - B')^{-1} \leq (-B')^{-1}$. Thus, to prove the above inequality, it suffices to show that for such v,

$$\sqrt{\lambda - \epsilon_\alpha}|w - w'|^{-1}\|v\|^2 \geq Cv \cdot ((-B')^{-1}Cv), \tag{B.24}$$

i.e. $\sqrt{\lambda - \epsilon_\alpha}|w - w'|^{-1} \geq C^*(-B')^{-1}C$ as elements of $\operatorname{End}(P_{w-w'}^\perp X_c)$. Note that for any such v, $Cv = \sqrt{\lambda - \epsilon_\alpha}|w - w'|^{-1}\pi_{ac}v$. To prove (B.24), we further split the problem.

First, suppose $v \in (w - w')^\perp \cap X_c \subset P_{w-w'}^\perp X_c$. Then, $\pi_{ac}v = v$, so

$$Cv = \sqrt{\lambda - \epsilon_\alpha}|w - w'|^{-1}v \in (w - w')^\perp \cap X_c = (\pi_{ac}(w) - w')^\perp \cap X_c. \tag{B.25}$$

But $(\pi_{ac}(w)-w')^\perp\cap X_c$ is an eigenspace of $-B'$ with eigenvalue $\sqrt{\lambda-\epsilon_\alpha}|w-w'|^{-1}$, so $(-B')^{-1}Cv=v$. Hence, $C^*(-B')^{-1}Cv=\sqrt{\lambda-\epsilon_\alpha}|w-w'|^{-1}v$ for such v. In particular, $(w-w')^\perp\cap X_c$ is an eigenspace of $C^*(-B')^{-1}C$.

On the other hand, suppose

$$v=P_{w-w'}(\pi_{ac}(w)-w')=(\pi_{ac}(w)-w')-\frac{|\pi_{ac}(w)-w'|^2}{|w-w'|^2}(w-w'). \tag{B.26}$$

so

(B.27)

$$Cv=\sqrt{\lambda-\epsilon_\alpha}|w-w'|^{-1}\pi_{ac}v=\sqrt{\lambda-\epsilon_\alpha}|w-w'|^{-1}(1-\frac{|\pi_{ac}(w)-w'|^2}{|w-w'|^2})(\pi_{ac}(w)-w'),$$

which is in the span of $\pi_{ac}(w)-w'$. But

(B.28)

$$-B'(\pi_{ac}(w)-w')=\sqrt{\lambda-\epsilon_\alpha}|w-w'|^{-1}(1-\frac{|\pi_{ac}(w)-w'|^2}{|w-w'|^2})(\pi_{ac}(w)-w'),$$

so $(-B')^{-1}Cv=\pi_{ac}(w)-w'$. Hence,

(B.29)

$$C^*(-B')^{-1}Cv=\sqrt{\lambda-\epsilon_\alpha}|w-w'|^{-1}(1-\frac{|\pi_{ac}(w)-w'|^2}{|w-w'|^2})=P_{w-w'}(\pi_{ac}(w)-w')=v.$$

Thus, $C^*(-B')^{-1}Cv=\sqrt{\lambda-\epsilon_\alpha}|w-w'|^{-1}v$ for all $v\in P^\perp_{w-w'}X_c$. As indicated above, this proves that

$$\sqrt{\lambda-\epsilon_\alpha}|w-w'|^{-1}\|v\|^2\geq Cv\cdot((A'-B')^{-1}Cv). \tag{B.30}$$

Combining these results proves that $A\geq 0$, proving the lemma. We remark that our calculations also show that

$$\mathrm{Ker}(A)=\mathrm{Ker}(A')+\mathrm{span}(w-w'). \tag{B.31}$$

□

This proof also shows what goes wrong if $w\in X_c$: the intersection of $T^*X_a\cap\Lambda'$ and $\tilde\Lambda^{\mathrm{out}}_{ac}$ need not be transversal, unless A' is positive definite.

With this notation, every element of the part of the forward generalized broken bicharacteristic relation corresponding to the string (B.1) is in the composite relation

$$\tilde\Lambda^{\mathrm{out}}_{a_{m+1},\alpha_{m+1},c_m}\circ\tilde\Lambda^{\mathrm{in}}_{c_m,a_m}\circ\tilde\Lambda^{\mathrm{out}}_{a_m,\alpha_m,c_{m-1}}\circ\ldots\circ\tilde\Lambda^{\mathrm{out}}_{a_2,\alpha_2,c_1}\circ\tilde\Lambda^{\mathrm{in}}_{c_1,a_1}\circ\tilde\Lambda^{\mathrm{prop}}_{a_1,\alpha_1}, \tag{B.32}$$

and conversely, every element of the composite relation certainly corresponds to an element of the forward generalized broken bicharacteristic relation. We now prove that (B.32) is a smooth Lagrangian. As indicated in the first paragraphs, a simple modification yields Theorem 2.10 if we also prove that the composite relation maps $R_-(\lambda)\cap{}^{\mathrm{sc}}T^*_{C'_{a_1}}X_{a_1}$ to a finite union of smooth Lagrangians. We do not state this mapping property explicitly to avoid an overburdened notation, but we indicate in Remark B.6 how it is proved by a simple modification of the following argument.

Proposition B.4. *For each string as in* (B.1) *the composite relation* (B.32) *is a smooth Lagrangian submanifold of* $T^*X_{a_{m+1}}\times T^*X_{a_1}$.

The rest of this appendix is denoted to the proof of this proposition and to the indication of the minor changes required for the proof of Theorem 2.10. Before proceeding with the proof, we make a definition analogous to Definition B.1.

Definition B.5. A Lagrangian relation $\tilde{\Lambda} \subset T^*X_a \times T^*X_c$ is forward-spreading if for each $q \in \tilde{\Lambda}$, there is a Lagrangian plane $V \subset T_{\pi_1(q)}T^*X_a$, in the image of the differential of the projection $\tilde{\Lambda} \mapsto T^*X_a$ at q, such that V is spreading; here π_1 denotes projection to the first factor.

Proof. The proof proceeds by induction. Thus, let

$$\begin{aligned} \Lambda_j^{\mathrm{in}} &= \tilde{\Lambda}^{\mathrm{in}}_{c_j,a_j} \circ \ldots \circ \tilde{\Lambda}^{\mathrm{out}}_{a_2,\alpha_2,c_1} \circ \tilde{\Lambda}^{\mathrm{in}}_{c_1,a_1} \circ \tilde{\Lambda}^{\mathrm{prop}}_{a_1,\alpha_1}, \\ \Lambda_j^{\mathrm{out}} &= \tilde{\Lambda}^{\mathrm{out}}_{a_j,\alpha_j,c_{j-1}} \circ \ldots \circ \tilde{\Lambda}^{\mathrm{out}}_{a_2,\alpha_2,c_1} \circ \tilde{\Lambda}^{\mathrm{in}}_{c_1,a_1} \circ \tilde{\Lambda}^{\mathrm{prop}}_{a_1,\alpha_1}. \end{aligned} \tag{B.33}$$

For the sake of convenience, we also write $\Lambda_1^{\mathrm{out}} = \tilde{\Lambda}^{\mathrm{prop}}_{a_1,\alpha_1}$. We need to show that Λ_1^{out} is forward-spreading, as well as the following inductive statement. For each $j \leq m$, given that Λ_j^{in} is a forward-spreading smooth Lagrangian, so is $\Lambda_{j+1}^{\mathrm{out}} = \tilde{\Lambda}^{\mathrm{out}}_{a_{j+1},\alpha_{j+1},c_j} \circ \Lambda^{\mathrm{in}}_{j-1}$, and also that provided that Λ_j^{out} is a forward-spreading smooth Lagrangian, so is $\Lambda_j^{\mathrm{in}} = \tilde{\Lambda}^{\mathrm{in}}_{c_j,a_j} \circ \Lambda_j^{\mathrm{out}}$. These results essentially follow from the two lemmas we have proved in this section, Lemma B.3 and Lemma B.2 respectively; we discuss the details below.

First, note that $\tilde{\Lambda}^{\mathrm{prop}} = \tilde{\Lambda}^{\mathrm{prop}}_{a_1,\alpha_1}$ is forward spreading. Indeed, for all $q \in \tilde{\Lambda}^{\mathrm{prop}}$ and for all $v \in X_{a_1}$, $v \cdot \partial_w + Bv \cdot \partial_\xi$ is in the image of the differential of the projection $\tilde{\Lambda}^{\mathrm{prop}} \mapsto T^*X_{a_1}$ at q by (B.7). Since $B \geq 0$, we can take $A = B$ in Definition B.1. This particular choice of Lagrangian subspace of $T_{\pi_1(q)}T^*X_a$ is analogous to considering mapping properties of the forward bicharacteristic relation on outgoing spherical waves; see Remark B.6 below. Since in this case $C' = -B$, it is easy to see that we could also consider the Lagrangian subspace spanned by $v \cdot \partial_w$, $v \in X_{a_1}$; this would be analogous to considering mapping properties of the forward bicharacteristic relation on plane waves.

Next, suppose, say, that Λ_j^{in} is a smooth forward-spreading Lagrangian; the proof under the assumption that Λ_j^{out} is a smooth forward-spreading Lagrangian is similar. To prove that $\Lambda_{j+1}^{\mathrm{out}}$ is also a smooth forward-spreading Lagrangian, it suffices to show that $T^*X_{a_{j+1}} \times \Lambda_j^{\mathrm{in}}$ and $\tilde{\Lambda}^{\mathrm{out}}_{a_{j+1},\alpha_{j+1},c_j} \times T^*X_{a_1}$ intersect transversally in $T^*X_{a_{j+1}} \times T^*X_{c_j} \times T^*X_{a_1}$, find the intersection of the tangent spaces, show that its push-forward by π, the map projecting to the first and third factors, $T^*X_{a_{j+1}} \times T^*X_{a_1}$, has trivial kernel, and find a spreading Lagrangian subspace in the range of the differential of the projection of $\Lambda_{j+1}^{\mathrm{out}}$ to $T^*X_{a_{j+1}}$.

Let V' be a spreading Lagrangian subspace of $TT^*X_{c_j}$ such that V' is in the range of the differential of the projection $\Lambda_j^{\mathrm{in}} \to T^*X_{c_j}$. To show transversality, it suffices to prove that

$$T\tilde{\Lambda}^{\mathrm{out}} + TT^*X_{a_{j+1}} \times V' = TT^*X_{a_{j+1}} \times TT^*X_{c_j}, \tag{B.34}$$

and in this case the Lagrangian subspace

$$V = T\tilde{\Lambda}^{\mathrm{out}} \circ V' \subset TT^*X_{a_{j+1}}, \tag{B.35}$$

given by the projection of $T\tilde{\Lambda}^{\mathrm{out}} \cap (TT^*X_{a_{j+1}} \times V')$ to $TT^*X_{a_{j+1}}$, is in the range of the differential of the projection $\Lambda_{j+1}^{\mathrm{out}} \to T^*X_{a_{j+1}}$. Since the previous statements involving V' referred to tangent vectors, they are essentially equivalent to mapping properties of $\tilde{\Lambda}^{\mathrm{out}}$ on Lagrangian submanifolds Λ' of $T^*X_{c_j}$. But this is exactly what we have proved in Lemma B.3. Thus, we conclude that $\Lambda^{\mathrm{out}}_{j+1}$ is smooth forward-spreading Lagrangian, completing the inductive proof. $\square$

Remark B.6. The outgoing radial set, $R_-(\lambda)\cap {}^{\mathrm{sc}}T^*_{C'_{c_1}}X_{c_1}$ gives another example of a spreading Lagrangian Λ'. (Strictly speaking, $R_-(\lambda)\cap {}^{\mathrm{sc}}T^*_{C'_{c_1}}X_{c_1}$ needs to be 'homogenized' using the $\mathbb{R}^+$ action, i.e. the conic structure, to extend it to a Lagrangian submanifold of $T^*X_{c_1}$.) Namely, the Lagrangian in ${}^{\mathrm{sc}}T^*_{X_{c_1}}X_{c_1}$ corresponding to $R_-(\lambda)$ is a union of the Lagrangians

$$\Lambda = \Lambda_\sigma = \{(w, \sqrt{\lambda-\sigma}\frac{w}{|w|}) : w \in X_c\},\ \sigma \in \Lambda_1, \tag{B.36}$$

so, with the notation of Definition B.1, A is given by

$$A = \frac{\sqrt{\lambda-\sigma}}{|w|^3}(|w|^2 \operatorname{Id} - w\otimes w), \tag{B.37}$$

hence $A \geq 0$. Moreover, $\operatorname{Ker}(A)$ is exactly $\operatorname{span}(w)$. Thus, the proof of Proposition B.4 actually shows that the forward broken bicharacteristic relation maps it to a finite union of smooth Lagrangian submanifolds.

We now indicate the changes required to prove the S-matrix result, Theorem 2.10.

Proof. (Proof of Theorem 2.10.) With the notation of (B.1), if $m=0$, then γ is an unbroken bicharacteristic, so the endpoints of γ are related by the antipodal relation, which is certainly Lagrangian. So we may assume $m \geq 1$. In addition, due to the assumptions (2.34), the ${}^{\mathrm{sc}}H^a_g$ bicharacteristics will only break upon hitting C_{c_1} with $c_1 \neq a$ (i.e. a-tangential bicharacteristics cannot become normal to a without hitting $C_{a,\mathrm{sing}}$). Similarly, $c_m \neq b$.

The only change from the proof of Proposition B.4 is that we need to replace the first, respectively the last two, Lagrangians in the composition (B.32) by the Lagrangians $\tilde{\Lambda}_\beta \subset T^*C'_b \times T^*X_{c_m}$ and $\tilde{\Lambda}_\alpha \subset T^*X_{c_1} \times T^*C'_a$ given by the (twisted) graphs of $d(-\sqrt{\lambda-\epsilon_\beta}\,\omega\cdot w')$ and $d(-\sqrt{\lambda-\epsilon_\alpha}\,\omega'\cdot w)$ respectively; here we wrote (ω,ζ,w',ξ') and (w,ξ,ω',ζ') for the coordinates on $T^*C'_b \times T^*X_{c_m}$ and $T^*X_{c_1} \times T^*C'_a$ respectively. Thus, on $\tilde{\Lambda}_\alpha$, $\xi = -\sqrt{\lambda-\epsilon_\alpha}\,\pi_{a,c_1}(\omega')$, so the differential of the projection of $\tilde{\Lambda}_\alpha$ to $T^*X_{c_1}$ is surjective since $a \neq c_1$. In particular, we can choose a Lagrangian subspace V' of $T_{(w,\xi)}T^*X_{c_1}$ which is in the range of the differential of this projection, and which is a graph over X_{c_1} of the form (w, Aw) with A positive definite (e.g. the identity). Then the proof of Proposition B.4 shows that the composite relation

$$\tilde{\Lambda}^{\mathrm{out}}_{a_{m+1},\alpha_{m+1},c_m} \circ \tilde{\Lambda}^{\mathrm{in}}_{c_m,a_m} \circ \tilde{\Lambda}^{\mathrm{out}}_{a_m,\alpha_m,c_{m-1}} \circ \ldots \circ \tilde{\Lambda}^{\mathrm{out}}_{a_2,\alpha_2,c_1} \circ \tilde{\Lambda}^{\mathrm{in}}_{c_1,a_1} \circ \tilde{\Lambda}_\alpha \tag{B.38}$$

is a smooth Lagrangian. Since the differential of the projection of $\tilde{\Lambda}_\beta$ to $T^*X_{c_m}$ is also surjective as $b \neq c_m$, the composition of $\tilde{\Lambda}_\beta$ with (B.38) is transversal, so the result is a smooth Lagrangian submanifold of $T^*C'_b \times T^*C'_a$. In view of Theorem 2.8, this and Remark B.6 complete the proof. $\square$

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