SMOOTHNESS AND HIGH ENERGY ASYMPTOTICS OF THE SPECTRAL SHIFT FUNCTION IN MANY-BODY SCATTERING

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Abstract. Let $H = \Delta + \sum_{\#a=2} V_a$ be a 3-body Hamiltonian, H_a the subsystem Hamiltonians, $\Delta \geq 0$ the Laplacian of the Euclidean metric g on $X_0 = \mathbb{R}^n$, V_a real-valued. Buslaev and Merkurev [5, 4, 3] have shown that, if the pair potentials decay sufficiently fast, for $\phi \in \mathcal{C}_c^\infty(\mathbb{R})$, the operator $\phi(H) - \phi(H_0) - \sum_{\#a=2}(\phi(H_a) - \phi(H_0))$ is trace class. Hence, one can define a modified spectral shift function σ, as a distribution on $\mathbb{R}$, by taking its trace. In this paper we show that if V_a are Schwartz, then σ is in fact $\mathcal{C}^\infty$ away from the thresholds, and obtain its high energy asymptotics. In addition, we generalize this result to N-body scattering, N arbitrary.

Contents

1. Introduction

In scattering theory the spectral shift function plays a role which is analogous to the counting function of the eigenvalues of the Laplacian on compact manifolds without boundary or on bounded domains. Since the operators one considers have a rather large continuous spectrum, the spectral data are not discrete any more, and any generalization of the counting function has to be defined 'relative to' operators that are considered well understood – such as the free Laplacian in two-particle potential scattering. This generalization, the spectral shift function, is well understood in two-body scattering, see e.g. [2, 30, 7, 28, 20, 6]. In this paper we study a modification of the spectral shift function, adapted to many-body scattering. We

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analyze both its smoothness properties and its high energy asymptotics, which corresponds to the Weyl asymptotics of the counting function on compact manifolds. The spectral shift function also plays a role in quantum statistical physics, see [4].

So let $H = \Delta + \sum_{\#a=2} V_a$ be a 3-body Hamiltonian, H_a the subsystem Hamiltonians, $\Delta \geq 0$ the Laplacian of the Euclidean metric g on $X_0 = \mathbb{R}^n$, V_a real-valued. Buslaev and Merkurev [5, 4, 3] have shown that, if the pair potentials decay sufficiently fast, and under a spectral assumption, for $\phi \in \mathcal{C}_c^\infty(\mathbb{R})$, the operator $\phi(H) - \phi(H_0) - \sum_{\#a=2}(\phi(H_a) - \phi(H_0))$ is trace class. Indeed, this follows from the adoptation of the Helffer-Sjöstrand functional calculus [17], see [34], even without the spectral assumption. Hence, one can define a modified spectral shift function, which is really a distribution on $\mathbb{R}_\lambda$, by

$$\sigma(\phi) = \mathrm{tr}(\phi(H) - \phi(H_0) - \sum_{\#a=2} (\phi(H_a) - \phi(H_0))). \tag{1.1}$$

In the two-body setting, σ is often denoted by ξ'. The purpose of this paper is to show that σ is in fact $\mathcal{C}^\infty$ away from the thresholds, and to obtain its high energy asymptotics. Namely, we prove the following theorem.

Theorem. *(See Theorem 5.2.) Suppose that the pair potentials V_a are Schwartz (on X^a). Then the spectral shift function σ is $\mathcal{C}^\infty$ on $\mathbb{R} \setminus \Lambda$, where Λ is the set of thresholds and L^2 eigenvalues of H. Moreover, σ is a symbol outside a compact set, and it has a full asymptotic expansion as $\lambda \to +\infty$:*

$$\sigma(\lambda) \sim \sum_{j=0}^{\infty} \lambda^{\frac{n}{2}-3-j} c_j.$$

In addition,

$$c_0 = C_0 \sum_a \sum_{b \neq a} \int_{X_0} V_a V_b \, dg,$$

where $C_0 = \frac{1}{16}(n-2)(n-4)(2\pi)^{-n} \operatorname{vol}(\mathbb{S}^{n-1})$ depends only on $n = \dim X_0$, and dg is the Riemannian density of the metric g.

Buslaev and Merkurev had shown previously [5] that σ is given by a continuous function, under the assumption that 0 is not an eigenvalue or resonance of any two-body subsystem, and that the bottom of the essential spectrum is not an eigenvalue of the whole Hamiltonian. We remark that the leading term has an additional λ^{-1} decay as compared to the corresponding formulae in two-body scattering, see [2, 30, 7, 28, 20, 6]. This is due to the fact that $\phi(H) - \phi(H_0) - \sum_{\#a=2}(\phi(H_a) - \phi(H_0))$ is lower order in a high-energy sense than $\phi(H) - \phi(H_0)$ is in the two-body setting. Correspondingly, if we include a three-particle interaction V_1 in H, i.e. allow $\#a = 1$, the leading term will have its usual order $\lambda^{\frac{n}{2}-2}$.

In fact, this is not the only modified spectral shift function one can consider. For example, let χ_a, $\#a \geq 2$, be a partition of unity by $\mathcal{C}^\infty$ functions on the radial (or geodesic) compactification $\bar{X}_0$ of the configuration space X_0 that correspond to the collision plane structure. Then $\phi(H) - \sum_{\#a\geq 2} \phi(H_a)\chi_a$ is also trace class, and one can define a modified spectral shift function by taking its trace. This spectral shift function will depend on the choice of the partition of unity, and it may be argued that it is less natural than the one adopted above. This trace is also smooth away from the thresholds and its high energy asymptotics can also be calculated. In fact, this expression generalizes without changes to many-body scattering with arbitrarily many particles, and our proof shows its smoothness. Even the Buslaev-Merkurev expression can be adopted to N-body scattering, N arbitrary, with combinatorial complexity being the only additonal issue. The corresponding result is stated in Theorem 6.3 in the last section.

The main reason why these statements hold is that the corresponding expressions for the spectral measure, or for the high-energy cutoff outgoing (or incoming) resolvents $\psi(H)(H-(\lambda+i0))^{-1}$, $\psi \in \mathcal{C}_c^\infty(\mathbb{R})$, ψ identically 1 near λ, already make sense pointwise in λ. While these operators are not necessarily trace class, the trace makes sense as an oscillatory integral since it can be regarded as a pairing of the Schwartz kernel of these operators with the delta distribution δ_{diag} associated to the diagonal, both being tempered distributions on $X_0 \times X_0$. Indeed, the latter only requires that the scattering wave front set of these two distributions (on the radial compactification $\overline{X_0 \times X_0}$ of $X_0 \times X_0$, in the terminology of [23]) be disjoint. That is, the scattering wave front set of the kernel of the the operator whose trace we intend to take must be disjoint from the conormal bundle of the diagonal – the real requirement here is that they be disjoint at infinity, i.e. at $\partial(\overline{X_0 \times X_0})$. In view of the propagation of singularities in many-body scattering, applied to the resolvent kernel, this is automatically satisfied provided that the kernel of the operator combination that we consider is essentially a generalized eigenfunction of some many-body Hamiltonian microlocally near the conormal bundle of the diagonal.

To make these statements more digestible, consider two-body scattering by a Schwartz potential V on $X_0 = \mathbb{R}^n$: $H = \Delta + V$, $H_0 = \Delta$. Then for $\lambda > 0$ the Schwartz kernel $K_{\lambda+i0} = K = K(w, w')$ of

$$\psi(H)(H-(\lambda+i0))^{-1} - \psi(H_0)(H_0-(\lambda+i0))^{-1},$$

which is a priori a tempered distribution on $(X_0)_w \times (X_0)_{w'}$, has the form

$$K(w,w') = e^{i\sqrt{\lambda}\langle w\rangle} e^{i\sqrt{\lambda}\langle w'\rangle} \langle w\rangle^{-\frac{n-1}{2}} \langle w'\rangle^{-\frac{n-1}{2}} a(w,w'),\ \langle w\rangle = (1+|w|^2)^{1/2},$$

where a is a non-classical product-type symbol on $X_0 \times X_0$ which in fact lies in $\mathcal{C}^\infty([\bar{X}_0 \times \bar{X}_0; \partial\bar{X}_0 \times \partial\bar{X}_0])$ – in particular, it *is* a classical symbol of order 0 in a conic neighborhood of diag in $X_0 \times X_0$. Thus, K is not trace class, but it is $\mathcal{C}^\infty$ on $X_0 \times X_0$, and its restriction to the diagonal $w = w'$ takes the form

$$K(w,w) = e^{2i\sqrt{\lambda}\langle w\rangle} \langle w\rangle^{-(n-1)} a(w,w),$$

and now $b(w) = a(w,w)$ is a classical symbol of order 0 on X_0, i.e. lies in $\mathcal{C}^\infty(\bar{X}_0)$ from the compactified point of view. In particular, $K(w,w)$ does *not* lie in $L^1(X_0)$ (except in trivial cases), but $\int_{X_0} K_{\lambda+i0}(w,w)\,dw$ makes sense as an oscillatory integral. It is easy to see then that the spectral shift function is given by

$$\sigma(\lambda) = (2\pi i)^{-1} \left(\int_{X_0} K_{\lambda+i0}(w,w)\,dw - \int_{X_0} K_{\lambda-i0}(w,w)\,dw \right),$$

with both integrals understood as oscillatory integrals, showing the continuity of σ. Since derivatives of the resolvent can also be analyzed similarly, this argument in fact shows that σ is $\mathcal{C}^\infty$ on $(0, +\infty)$.

In the many-body setting we do not have access to such a precise description of the resolvent kernel, except in the three-body setting [32], but we do not need it in any case: rather than considering various integrals such as $\int_{X_0} K_{\lambda+i0}(w,w)\,dw$ above as oscillatory integrals, we treat them as a pairing of the delta distribution associated to the diagonal and K, and the pairing makes sense by wave front set considerations, i.e. because the distributions K and δ_{diag} are non-trivial only in disjoint regions of phase space.

Our methods are thus an adaptation of traditional microlocal analysis to many-body scattering. In fact, we do not need the whole program initiated by Melrose [23], see [35], since the trace is a rather simple object. Thus, a moderate strengthening of propagation results in the dual of the radial variable essentially suffices. These have their origins in the Mourre estimate [26], and became partially microlocal estimates in the work of Gérard, Isozaki, Skibsted [11, 12] and the work of the second author [36]; see also [15] for a discussion of these in the geometric setting.

The weak high energy asymptotics, i.e. that of

$$\mathrm{tr}(\phi(H/\lambda) - \phi(H_0/\lambda) - \sum_{\#a=2} (\phi(H_a/\lambda) - \phi(H_0/\lambda))),$$

$\phi \in \mathcal{C}_c^\infty(\mathbb{R})$ fixed, can be derived from the semiclassical functional calculus of Helffer-Robert [29, 16]. Symbol estimates for σ follow from combining microlocal versions of high energy estimates for $R(\lambda+i0)$, [19], with our method of proving smoothness of σ (see also [37]). The perturbation series expansion for $R(\lambda+i0)$ then gives the full asymptotics.

The assumption that the V_a are Schwartz is not optimal. The distributional trace, σ, is defined if the V_a are symbols of order $< -n$ (on X^a). Below we also obtain partial results for these potentials and explain the finer tools one needs to extend the Theorem to this setting. Specifically, this would entail obtaining, at least microlocally near the conormal bundle of the diagonal at infinity, oscillatory integral estimates in place of the wave front set estimates.

We also mention that under stronger assumptions as in [10], such as analyticity of the pair potentials in a cone near infinity, one can use complex scaling, or distortion analyticity, to continue $(H-\lambda)^{-1}$ across the spectrum. Since the trace is invariant under the scaling, and the scaled operators are elliptic near the real axis, we deduce that the trace is real analytic, much like in the recent work of Bruneau and Petkov [1].

While there is quite a bit of machinery in the microlocal analysis of this paper, due to the complexities of many-body scattering, given the microlocal estimates, the arguments proving the Theorem are essentially the same as in two-body scattering. Hence we invite the reader who is familiar with the scattering microlocal analysis introduced by Melrose [23] to read Section 4 pretending that one works in the two-body setting. Moreover, in the appendix we sketch the proof of a propagation theorem that is weaker than the results of [35], but suffices for the purposes of this paper. The sketch is intended to stand on its own, given the notation of Sections 2-3, and to explain the basic ideas in microlocalizing propagation estimates.

The structure of the paper is as follows. In Section 2 we recall the standard many-body notation and make some preliminary remarks. In the following section we remind the reader of the microlocal structure of many-body scattering. In Section 4 we prove the smoothness of σ in the three-body setting, and in Section 5 we obtain the high energy expansion of σ. In the final section we state and prove the corresponding results in many-body scattering, and in the appendix we outline the proof of the simplified positive commutator estimate described above.

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2. Notation and preliminaries

Before we can state the precise definitions, we need to introduce some basic (and mostly standard) notation. We refer to [8] 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.

There is a natural partial ordering on I induced by the ordering of X^a by inclusion, i.e. $b \leq a$ means that $X^b \subset X^a$, hence $X_b \supset X_a$. A three-body Hamiltonian is a many-body Hamiltonian with $I \neq \{0, 1\}$ such that for all $a, b \notin \{0, 1\}$ with $a \neq b$, $X_a \cap X_b = \{0\}$ holds.

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

$$H^a = \Delta_{X^a} + \sum_{b\leq a} V_b, \tag{2.2}$$

Δ_{X^a} being the Laplacian of the induced metric on X^a. With

$$\mathcal{X}^a = \{X_b \cap X^a :\ b \leq a\}, \tag{2.3}$$

H^a is a many-body Hamiltonian with collision planes $\mathcal{X}^a$. We write

$$H_a = H^a \otimes \mathrm{Id}_{X_a} + \mathrm{Id}_{X^a} \otimes \Delta_{X_a} = \Delta_{X_0} + \sum_{b\leq a} V_a. \tag{2.4}$$

The L^2 eigenfunctions of H^a, also called bound states, can be used to define the set of thresholds of H^b. Namely, we let

$$\Lambda_a = \cup_{b<a} \operatorname{spec}_{pp}(H^b) \tag{2.5}$$

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

$$\Lambda'_a = \Lambda_a \cup \operatorname{spec}_{pp}(H^a) = \cup_{b\leq a} \operatorname{spec}_{pp}(H^b). \tag{2.6}$$

Thus, $0 \in \Lambda_a$ for $a \neq 0$ and $\Lambda_a \subset (-\infty, 0]$. It follows from the Mourre theory (see e.g. [9, 27]) that Λ_a is compact, countable, and $\operatorname{spec}_{pp}(H^a)$ can only accumulate at Λ_a. We also let

$$\Lambda = \Lambda_1 \cup \operatorname{spec}_{pp}(H). \tag{2.7}$$

For future reference we also define the intercluster interactions as

$$I_a = H - H_a = \sum_{b\not\leq a} V_b. \tag{2.8}$$

One of the properties of many-body operators that we exploit below is that if H_L and H_R are many-body Hamiltonians on $(X_0)_L, (X_0)_R$ respectively, then

$$P = P_\alpha = \alpha H_L \otimes \mathrm{Id} + (1-\alpha)\,\mathrm{Id} \otimes H_R, \qquad 0 < \alpha < 1, \tag{2.9}$$

is a many-body Hamiltonian on $M_0 = (X_0)_L \times (X_0)_R$. (We name the new space M_0 and the operator P to avoid confusing notation.) The collision planes are given by $(X_a)_L \times (X_b)_R$, $a, b \in I$, though they have a rather special structure generated by $(X_a)_L \times (X_0)_R$ and $(X_0)_L \times (X_a)_R$, $a \in I$, by taking intersections of these. The thresholds $\Lambda = \Lambda_\alpha$ of P are of the form $\alpha\lambda_L + (1-\alpha)\lambda_R$, where λ_L and λ_R are thresholds of H_L and H_R respectively.

Since we want to study the Schwartz kernel of the resolvent on a space, for us the relevant case is $X_0 = (X_0)_L = (X_0)_R$ (this is the space), and $H_L = H_R$, so the kernel of $(H_L - \lambda)^{-1}$ is a distribution on $M_0 = (X_0)_L \times (X_0)_R$. The thresholds of P_α vary with α, except that $\lambda \in \Lambda_R = \Lambda_L$ implies that $\lambda \in \Lambda_\alpha$ for all α. On the other hand, given $\lambda \notin \Lambda_L$, there is a countable subset C of $(0,1)$ such that $\alpha \notin C$ implies $\lambda \notin \Lambda_\alpha$. Indeed, for any pair $(\lambda_L, \lambda_R) \in \Lambda_L \times \Lambda_R$ with $\lambda_L \neq \lambda_R$, there is a unique $\alpha \in \mathbb{R}$ such that $\lambda = \alpha\lambda_L + (1-\alpha)\lambda_R$, and then we can take C to be the intersection of the set of such α's with $(0,1)$.

In the next section we explain the full microlocal propagation picture proved in [35]. However, we would like to emphasize here that apart from mild technical issues we only need an estimate of Gérard, Isozaki, Skibsted [11, 12] and the second author [36], and its slightly strengthened version. Namely, let $B = \frac{w}{2\langle w\rangle} \cdot D_w + D_w \cdot \frac{w}{2\langle w\rangle}$, and suppose that $F_1, F_2 \in \mathcal{C}_c^\infty(\mathbb{R})$, $\operatorname{supp} F_1 \subset (c, c')$, $\operatorname{supp} F_2 \subset (c', c'')$, $c < c' < c''$, $|c|, |c''|$ sufficiently small, and $\psi \in \mathcal{C}_c^\infty(\mathbb{R})$. The aforementioned papers show that $F_1(B)\psi(H)(H - (\lambda + i0))^{-1}F_2(B)$ maps $H^{0,s}$ to $H^{0,s'}$ for all s, s' when $\lambda \notin \Lambda$. In the terminology of the next section, this holds because the principal symbol of B at infinity, which is denoted by $-\tau$ there, is increasing along generalized broken bicharacteristics, and singularities propagate in the forward direction under $(H - (\lambda + i0))^{-1}$.

We only need the following strengthening of this statement (as well as its high energy version). Suppose that $\chi_1, \chi_2 \in S^0(X_0)$ are conic cutoff functions (outside a compact subset of X_0) with $\operatorname{supp}\chi_1 \cap \operatorname{supp}\chi_2 = \emptyset$. Then there exists $\epsilon > 0$ (depending on the supports and on $\lambda \notin \Lambda$) such that for $F_1, F_2 \in \mathcal{C}_c^\infty(\mathbb{R})$, $\operatorname{supp} F_1 \subset (c, c' + \epsilon)$, $\operatorname{supp} F_2 \subset (c', c'')$, $c < c' < c''$, $|c|, |c''|$ sufficiently small, and $\psi \in \mathcal{C}_c^\infty(\mathbb{R})$, $\chi_1 F_1(B)\psi(H)(H - (\lambda + i0))^{-1}F_2(B)\chi_2$ maps $H^{0,s}$ to $H^{0,s'}$ for all s, s' when $\lambda \notin \Lambda$. In the microlocal terminology, this means that the principal symbol of B at infinity has to increase by at least $\epsilon > 0$ along generalized broken bicharacteristics leaving $\operatorname{supp}\chi_2$ (near infinity) and ending in $\operatorname{supp}\chi_1$. We remark that the smoothness order r of the Sobolev space $H^{r,s}$ is left as 0 only due to the non-ellipticity (in the usual sense) of B. Slightly different pseudo-differential cutoffs, such as those described in the next section, yield maps from $H^{r,s}$ to $H^{r',s'}$ for all r, r', s, s'.

We also need the high energy version of both of these estimates, which can be proved similarly. Namely, first, that for all r, s, r', s',

$$\|F_1(B)\psi(H)(H - (\lambda + i0))^{-1}F_2(B)\|_{\mathcal{B}(H^{0,s}, H^{0,s'})} \leq C\lambda^{-1/2}, \quad \lambda \geq 1, \tag{2.10}$$

if $F_1, F_2 \in \mathcal{C}_c^\infty(\mathbb{R})$, $\operatorname{supp} F_1 \subset (c, c')$, $\operatorname{supp} F_2 \subset (c', c'')$, $c < c' < c''$, $|c|, |c''|$ sufficiently small, and $\psi \in \mathcal{C}_c^\infty(\mathbb{R})$. Next, there exists $\epsilon > 0$ (depending on the supports of χ_1 and χ_2 as above), but not on $\lambda \geq 1$) such that for $F_1, F_2 \in \mathcal{C}_c^\infty(\mathbb{R})$,

$\operatorname{supp} F_1 \subset (c, c'+\epsilon)$, $\operatorname{supp} F_2 \subset (c', c'')$, $c < c' < c''$, $|c|, |c''|$ sufficiently small, and $\psi \in \mathcal{C}_c^\infty(\mathbb{R})$, and

$$\|\chi_1 F_1(B)\psi(H)(H-(\lambda+i0))^{-1}F_2(B)\chi_2\|_{\mathcal{B}(H^{0,s},H^{0,s'})} \leq C\lambda^{-1/2}, \quad \lambda \geq 1. \tag{2.11}$$

3. Microlocal analysis in many-body scattering

We recall the microlocal tools introduced in the many-body setting in [34]. Thus, we compactify X_0 as in [23] by letting

$$\bar{X} = \bar{X}_0 = \mathbb{S}^n_+ \tag{3.1}$$

to be the radial compactification of X_0 (also called the geodesic compactification) to a closed hemisphere, i.e. a ball. Identifying X_0 with $\mathbb{R}^n$ (and using g) we write the compactification map $\mathrm{RC} : \mathbb{R}^n \to \mathbb{S}^n_+$ given by

$$\mathrm{RC}(w) = (1/(1+|w|^2)^{1/2}, w/(1+|w|^2)^{1/2}) \in \mathbb{S}^n_+ \subset \mathbb{R}^{n+1}, \quad w \in \mathbb{R}^n. \tag{3.2}$$

One can view the use of the compactification as using inverted polar coordinates $(r^{-1}, \omega) \in [0,1) \times \mathbb{S}^{n-1}$ near infinity, i.e. working near '$r^{-1} = 0$', where $w = r\omega$ in usual polar coordinates.

The reader might be curious *why* we compactify X_0. The answer is that there are two approaches: one can either work on a compact space, or work uniformly in an appropriate sense near infinity. The former approach automatically includes the appropriate notion of uniformity, and is hence very convenient, especially when additional geometry, such as collision planes, are added to the problem. To make the connection clearer, here we briefly mention the following natural identifications:

$$\mathcal{S}(X_0) = \dot{\mathcal{C}}^\infty(\bar{X}_0), \ S^{-k}_{\mathrm{cl}}(X_0) = x^k \mathcal{C}^\infty(\bar{X}_0),$$

where $\mathcal{S}(X_0)$ is the space if Schwartz functions, $\dot{\mathcal{C}}^\infty(\bar{X}_0)$ the space of $\mathcal{C}^\infty$ functions on $\bar{X}_0$ which vanish to infinite order at $\partial\bar{X}_0$, while $S^{-k}_{\mathrm{cl}}(X_0)$ is the space of classical (one-step) symbols of order $-k$ on X_0, i.e. the space of symbols of order $-k$ with a full asymptotic expansion of step size one; the asymptotic expansion corresponds to the Taylor series at the boundary under the identification with $x^k\mathcal{C}^\infty(\bar{X}_0)$. We refer to [23] for a thorough discussion of this compactification.

We write the coordinates on $\mathbb{R}^n = X_a \oplus X^a$ as (w_a, w^a). We let

$$\bar{X}_a = \mathrm{cl}(\mathrm{RC}(X_a)), \quad C_a = \bar{X}_a \cap \partial\mathbb{S}^n_+. \tag{3.3}$$

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

$$\mathcal{C} = \{C_a : \ a \in I\}. \tag{3.4}$$

Thus, $C_0 = \partial\mathbb{S}^n_+ = \mathbb{S}^{n-1}$, and $a \leq b$ if and only if $C_b \subset C_a$. We also define the regular part of C_a as

$$C_{a,\mathrm{reg}} = C_a \setminus \cup_{b \not\leq a} C_b = C_a \setminus \bigcup\{C_b : \ C_b \subsetneq C_a\} \tag{3.5}$$

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. We write H^r for the standard Sobolev space, and $H^{r,s}$ for the weighted Sobolev space $\langle w\rangle^{-s}H^r$.

In [34, Section 3] a pseudo-differential operator calculus was constructed on many-body spaces as above $(\mathbb{R}^n, \mathcal{X})$; indeed, it was defined for appropriate geometric generalizations of these spaces. The rough idea of its origins is that it should include both the inverses of elliptic translation invariant differential operators on

X_0 (elliptic both in the usual sense, and at infinity in the sense of [23], which in this case amounts to requiring that as Fourier multipliers, they never vanish), and also the potentials V_a. The latter are $\mathcal{C}^\infty$ on the blow-up $[\bar{X}_0;\mathcal{C}]$ of $\bar{X}_0$ at $\mathcal{C}$, as discussed in [34, Section 2]. The (real) blow-up is an invariant way of introducing polar coordinates around a submanifold of a $\mathcal{C}^\infty$ manifold, and its effect in this case is that it 'stretches' to compactification $\bar{X}_0$ so that the components of w^a become coordinates on it in the region where $|w^a|$ is finite, which leads to the smoothness of V_a on $[\bar{X}_0;\mathcal{C}]$, see [34, Corollary 2.6, Figure 3] for details. In particular, the closure of (distinct) translates of X_a becomes *disjoint* on $[\bar{X}_0;\mathcal{C}]$. Note that the interior of $[\bar{X}_0;\mathcal{C}]$ is diffeomorphic to that of $\bar{X}_0$, i.e. to $X_0=\mathbb{R}^n$, and there is a smooth blow-down map $\beta:[\bar{X}_0;\mathcal{C}]\to\bar{X}_0$, so every $\mathcal{C}^\infty$ function on $\bar{X}_0$ is $\mathcal{C}^\infty$ on $[\bar{X}_0;\mathcal{C}]$.

Operators of multi-order (k,l) are denoted by $\Psi^{k,l}_{\mathrm{Sc}}(\bar{X}_0;\mathcal{C})$; the notation only refers to $\mathcal{C}$ rather than $\mathcal{X}$ since this is the only pertinent information in the geometric setting. We briefly recall the definition of the many-body pseudo-differential calculus via the quantization of symbols. Thus, the polyhomogeneous space $\Psi^{m,l}_{\mathrm{Sc}}(\bar{X}_0,\mathcal{C})$ is the following. We identify $\mathrm{int}(\bar{X}_0)$ and $\mathrm{int}([\bar{X}_0;\mathcal{C}])$ with $\mathbb{R}^n$ as usual (via RC^{-1}), suppose that $a\in\mathcal{C}^\infty(\mathbb{R}^n_w\times\mathbb{R}^n_\xi)$ is in fact of the form

$$a\in\rho_\infty^{-m}\rho_\partial^{l}\mathcal{C}^\infty([\bar{X}_0;\mathcal{C}]\times\bar{X}_0^*), \tag{3.6}$$

where ρ_∂ and ρ_∞ are total boundary defining functions of the first and second factors, $[\bar{X}_0;\mathcal{C}]$ and $\bar{X}_0^*$, respectively, so they can be taken as $\langle w\rangle^{-1}$ and $\langle\xi\rangle^{-1}$ respectively. As spelled out in detail in [34, Section 3], this simply means that a is a classical symbol of order m in ξ, and its dependence on w corresponds to the form of many-body potentials V_a, so in the two-body setting, a would be a symbol in w and ξ separately (i.e. a product-type symbol). Let $A=q_L(a)$ denote the left quantization of a:

$$Au(w)=(2\pi)^{-n}\int e^{i(w-w')\cdot\xi}a(w,\xi)u(w')\,dw'\,d\xi, \tag{3.7}$$

understood as an oscillatory integral. Then $A\in\Psi^{m,l}_{\mathrm{Sc}}(\bar{X}_0,\mathcal{C})$. We could have equally well used other (right, Weyl, etc.) quantizations as well, and we could have also allowed a to depend on w' as well (with w' regarded as a smooth variable on $[\bar{X}_0;\mathcal{C}]$).

As observed in [33, Section 13] and [34, Section 9], an advantage of using symbols

$$a\in\mathcal{C}^\infty([\bar{X}_0;\mathcal{C}]_w\times[\bar{X}_0;\mathcal{C}]_{w'}\times(\bar{X}_0^*)_\xi) \tag{3.8}$$

is that certain operators with amplitudes $a=q(w,\xi)p(w',\xi)$, which can be considered the operator product $A=QP$ of the left quantization $Q:\mathcal{S}(X_0)\to\mathcal{S}(X_0)$ of q and the right quantization $P:\mathcal{S}(X_0)\to\mathcal{S}(X_0)$ of p, lie in the class $\Psi^{m,l}_{\mathrm{Sc}}(\bar{X}_0,\mathcal{C})$ even though the left quantization of q does not (see [34, Lemma 9.1]). As an example, for $\psi_0\in\mathcal{C}^\infty_c(\mathbb{R})$, we can write $\psi_0(H)$ as the right quantization of a symbol p as above that is in fact Schwartz in ξ. Then q does not have to lie $\mathcal{C}^\infty([\bar{X}_0;\mathcal{C}]\times\bar{X}_0^*)$ to make (3.8) hold, since due to the rapid decay of p in ξ, the $\xi\to\infty$ behavior of q is (mostly) irrelevant. For example, we can allow $q=f(w\cdot\xi/|w|)$, $f\in\mathcal{C}^\infty_c(\mathbb{R})$; then $a=qp$ satisfies (3.8). Thus, $A=A(f)$ defined by

$$Au(w)=(2\pi)^{-n}\int e^{i(w-w')\cdot\xi}a(w,w',\xi)u(w')\,dw'\,d\xi,\quad a(w,w',\xi)=q(w,\xi)p(w',\xi), \tag{3.9}$$

yields an element of $\Psi_{\mathrm{Sc}}^{-\infty,l}(\bar{X}_0,\mathcal{C})$. The operator $A(f)$ has very similar properties to $f(B)\psi_0(H)$, B as in the previous section, and can be considered as a pseudo-differential replacement for $f(B)\psi_0(H)$, for $f(B)\psi_0(H)$ is not a ps.d.o. (due to the lack of ellipticity of B). (Note though that it follows from the arguments of [15] that $\psi_1(H)f(B)\psi_2(H) \in \Psi_{\mathrm{Sc}}^{-\infty,0}(\bar{X}_0,\mathcal{C})$ for $\psi_1,\psi_2 \in \mathcal{C}_c^\infty(\mathbb{R})$.)

By [34, Theorem 2], elements of $\Psi_{\mathrm{Sc}}^{k,l}(\bar{X}_0;\mathcal{C})$ are bounded operators from $H^{r,s}$ to $H^{r-k,s+l}$; in fact, this follows directly from $\Psi_{\mathrm{Sc}}^{k,0}(\bar{X};\mathcal{C}) \subset \Psi_\infty^k(X_0)$, where the calculus on the right hand side is Hörmander's calculus from [18, Section 18.1]. (The different signs are due to the index convention introduced in the geometric scattering setting in [23].) It was also shown in [34, Section 4] that for $\lambda \notin \operatorname{spec}(H)$, $R(\lambda) = (H-\lambda)^{-1} \in \Psi_{\mathrm{Sc}}^{-2,0}(\bar{X}_0,\mathcal{C})$, and the Helffer-Sjöstrand argument was adopted to show that for $\phi \in \mathcal{C}_c^\infty(\mathbb{R})$, $\phi(H) \in \Psi_{\mathrm{Sc}}^{-\infty,0}(\bar{X}_0,\mathcal{C})$, so it is smoothing in the standard sense, but does not give any decay at infinity (see Section 5 for a sketch of this argument in the semiclassical setting). The construction of $R(\lambda)$ is local at $\partial\bar{X}_0$ (in fact, it is microlocal in a sense discussed below). Thus, if $H = \Delta + V$, $H' = \Delta + V'$ are many-body operators such that in a neighborhood of $p \in \partial\bar{X}_0$, $H - H' = V - V'$ is in $x^k\mathcal{C}^\infty(\bar{X}_0)$, $k \geq 1$, i.e. $\chi(V-V') \in x^k\mathcal{C}^\infty(\bar{X}_0)$ for some $\chi \in \mathcal{C}^\infty(\bar{X}_0)$, $\chi(p) \neq 0$, then $R_H(\lambda) - R_{H'}(\lambda)$ is in $\Psi_{\mathrm{Sc}}^{-2,k}(\bar{X}_0,\mathcal{C})$ near p, so $(R_H(\lambda) - R_{H'}(\lambda))\chi \in \Psi_{\mathrm{Sc}}^{-2,k}(\bar{X}_0,\mathcal{C})$. This in turn implies, via the Helffer-Sjöstrand construction, that for $\phi \in \mathcal{C}_c^\infty(\mathbb{R})$, $\phi(H) - \phi(H')$ is in $\Psi_{\mathrm{Sc}}^{-\infty,k}(\bar{X}_0,\mathcal{C})$ near p.

Applying this in our setting, i.e. for 3-body Hamiltonians H with potential $\sum_{\#a=2} V_a$, we deduce the following result.

Proposition 3.1. *For three-body Hamiltonians H with pair interactions V_b that are classical symbols of order $-k$ on X^b, and for $\phi \in \mathcal{C}_c^\infty(\mathbb{R})$,*

$$\phi(H) - \phi(H_0) - \sum_{\#a=2} (\phi(H_a) - \phi(H_0)) \in \Psi_{Sc}^{-\infty,k}(\bar{X}_0,\mathcal{C}). \tag{3.10}$$

Remark 3.2. If V_b are symbols, but not classical (do not have full asymptotic expansions), the conclusion holds with $\Psi_{\mathrm{Sc}}^{-\infty,k}(\bar{X}_0,\mathcal{C})$ replaced by the corresponding non-classical calculus.

Proof. For any a, $H - H_a$ is in $x^k\mathcal{C}^\infty(\bar{X}_0)$ away from $\cup_{\#b=2,\ b\neq a} C_b$, and $H_a - H_0$ is in $x^k\mathcal{C}^\infty(\bar{X}_0)$ away from C_a. Hence $\phi(H) - \phi(H_a)$ is in $\Psi_{\mathrm{Sc}}^{-\infty,k}(\bar{X}_0,\mathcal{C})$ away from $\cup_{\#b=2,\ b\neq a} C_b$, and $\phi(H_a) - \phi(H_0)$ is in the same class away from C_a. Now consider the expression $\phi(H) - \phi(H_0) - \sum_{\#a=2}(\phi(H_a) - \phi(H_0))$ near C_b. Rewriting it as $\phi(H) - \phi(H_b) - \sum_{\#a=2,\ a\neq b}(\phi(H_a) - \phi(H_0))$ shows that it is in $\Psi_{\mathrm{Sc}}^{-\infty,k}(\bar{X}_0,\mathcal{C})$ away from $\cup_{\#a=2,\ a\neq b} C_a$, hence in particular near C_b. Since b is arbitrary, this proves the proposition. $\square$

Since pseudo-differential operators of order (m,l), $m < -n$, $l > n$, are easily seen to be of trace class (the kernel is in particular continuous and integrable along the diagonal), we conclude:

Corollary 3.3. *(cf. Buslaev and Merkurev* [3]*) Under the assumptions of Proposition 3.1, the left hand side of* (3.10) *is trace class.*

This corollary allows us to define σ by taking its trace, i.e. by (1.1).

We need more refined tools to analyze the smoothness of σ. Namely, we need to analyze the Schwartz kernels of operators that do not lie in $\Psi_{\mathrm{Sc}}^{m,l}(\bar{X}_0,\mathcal{C})$, e.g.

of $(H-(\lambda+i0))^{-1}$. This requires the use of some microlocal analysis, which we briefly recall below.

The phase space in scattering theory is the cotangent bundle T^*X_0 which can be identified with $X_0\times(X_0)^*$. Again, following Melrose [23], it is convenient to consider its appropriate partial compactification, i.e. to consider it as a trivial vector bundle over $\bar X_0$ by compactifying the base. Hence, one defines the scattering cotangent bundle of $\bar X_0$ by

$$^{\mathrm{sc}}T^*\bar X_0=\bar X_0\times X_0^*.$$

We remark that the construction of $^{\mathrm{sc}}T^*\bar X_0$ is completely natural and geometric, just like the following ones, see [23]. Note that $(X_0)^*$ can be identified with X_0 via the metric g as we often do below.

Recall from [34] that in many-body scattering $^{\mathrm{sc}}T^*\bar X_0$ 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; see the works of Melrose, Sjöstrand [24] and Lebeau [21] on the wave equation in domains with smooth boundaries or corners, respectively. 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. Hence, one cannot expect to localize in arbitrary open subsets of $^{\mathrm{sc}}T^*_{\partial\bar X_0}\bar X_0$, i.e. to microlocalize fully. To rectify this, we replace the full bundle $^{\mathrm{sc}}T^*_{C_{a,\mathrm{reg}}}\bar X_0=C_{a,\mathrm{reg}}\times(X_0)^*\simeq C_{a,\mathrm{reg}}\times X_0$ over $C_{a,\mathrm{reg}}\subset\partial\bar X_0$ by $^{\mathrm{sc}}T^*_{C_{a,\mathrm{reg}}}\bar X_a=C_{a,\mathrm{reg}}\times X_a$, i.e. we consider

$$^{\mathrm{sc}}\dot T^*\bar X_0=\cup_a{}^{\mathrm{sc}}T^*_{C_{a,\mathrm{reg}}}\bar X_a=\cup_a(C_{a,\mathrm{reg}}\times X_a^*)=\cup_a(C_{a,\mathrm{reg}}\times X_a). \tag{3.11}$$

Over $C_{a,\mathrm{reg}}$, there is a natural projection $\pi_a:{}^{\mathrm{sc}}T^*_{C_{a,\mathrm{reg}}}\bar X_0\to{}^{\mathrm{sc}}T^*_{C_{a,\mathrm{reg}}}\bar X_a$, i.e. $\pi_a: C_{a,\mathrm{reg}}\times X_0^*\to C_{a,\mathrm{reg}}\times X_a^*$, 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 $\pi:{}^{\mathrm{sc}}T^*_{\partial\bar X_0}\bar X_0\to{}^{\mathrm{sc}}\dot T^*\bar X_0$. We put the topology induced by π on $^{\mathrm{sc}}\dot T^*\bar X_0$. As mentioned above, this definition is analogous to that of the compressed cotangent bundle in the study of the wave equation in domains with smooth boundaries or corners. Moreover, one has the following sequence of projections:

$$\partial[\bar X_0;\mathcal C]\times X_0^*\to{}^{\mathrm{sc}}T^*_{\partial\bar X_0}\bar X_0=\partial\bar X_0\times X_0^*\to{}^{\mathrm{sc}}\dot T^*\bar X_0. \tag{3.12}$$

Thus, $\partial[\bar X_0;\mathcal C]\times X_0^*$ and $^{\mathrm{sc}}\dot T^*\bar X_0$ play a symmetric role with respect to $^{\mathrm{sc}}T^*_{\partial\bar X_0}\bar X_0$: it is the non-commutativity of operators arising by symbols on the former that only allows partial microlocalization, i.e. microlocalization only on $^{\mathrm{sc}}\dot T^*\bar X_0$, not $^{\mathrm{sc}}T^*_{\partial\bar X_0}\bar X_0$.

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 [34], and which describes u modulo Schwartz functions, similarly to how the usual wave front set describes distributions modulo smooth functions. Now $^{\mathrm{sc}}\dot T^*\bar X_0$ provides the natural setting in which $\mathrm{WF}_{\mathrm{Sc}}$ is defined: $\mathrm{WF}_{\mathrm{Sc}}(u)$ is a closed subset of $^{\mathrm{sc}}\dot T^*\bar X_0$. The definition of $\mathrm{WF}_{\mathrm{Sc}}(u)$ relies on the algebra of many-body scattering pseudo-differential operators, $\Psi^{k,l}_{\mathrm{Sc}}(\bar X_0,\mathcal C)$. There are several possible definitions of $\mathrm{WF}_{\mathrm{Sc}}$, all of which agree for generalized eigenfunctions of H, but the one given in [34, Definition 5.2] that is modelled on the fibred-cusp wave front set of Mazzeo and Melrose [22] enjoys many properties of the usual wave front set.

We remark that in the two-body setting, when ${}^{\mathrm{sc}}\dot{T}^*\bar{X}_0 = {}^{\mathrm{sc}}T^*_{\partial\bar{X}_0}\bar{X}_0$, $\mathrm{WF}_{\mathrm{Sc}}$ 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 $(\omega,\xi) \in {}^{\mathrm{sc}}T^*_{\partial\bar{X}_0}\bar{X}_0$, considered as $\partial\bar{X}_0 \times \mathbb{R}^n = \partial\bar{X}_0 \times \mathbb{R}^n$, $(\omega,\xi) \notin \mathrm{WF}_{\mathrm{sc}}(u)$ means that there exists $\phi \in \mathcal{C}^\infty(\bar{X}_0)$ 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, and we could think of $\mathrm{WF}_{\mathrm{sc}}$ as a conic set *in* w. Thus, $\mathrm{WF}_{\mathrm{sc}}$ at infinity is analogous to WF with the role of position and momentum reversed. One can also talk about the wave front set $\mathrm{WF}^{k,l}_{\mathrm{sc}}(u)$ relative to the Sobolev space $H^{k,l}$; then we would require that $\mathcal{F}(\phi u)$ is in H^l locally near ξ. Thus, k only plays a role for the standard part of the wave front set, which we are not discussing here, hence we often write $\mathrm{WF}^{*,l}_{\mathrm{sc}}(u)$ to indicate that k is irrelevant.

The definition of $\mathrm{WF}_{\mathrm{Sc}}(u)$ is more complicated, but if $u = \psi(H)v$ for some $\psi \in \mathcal{C}^\infty_c(\mathbb{R})$ (the crucial point being that $\psi(H) \in \Psi^{-\infty,0}_{\mathrm{Sc}}(\bar{X},\mathcal{C})$), then the following is a sufficient condition for $(\omega,\xi_a) \in {}^{\mathrm{sc}}T^*_{C_{a,\mathrm{reg}}}\bar{X}_a$, considered as $C_{a,\mathrm{reg}} \times X_a$, *not to be* in $\mathrm{WF}_{\mathrm{Sc}}(u)$. Suppose that there exists $\phi \in \mathcal{C}^\infty(\bar{X}_0)$, $\phi(\omega) \neq 0$, 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 $(\omega,\xi_a) \notin \mathrm{WF}_{\mathrm{Sc}}(u)$. This wave front set also has complete analogues for the relative wave front set $\mathrm{WF}^{k,l}_{\mathrm{Sc}}(u)$, i.e. when one is working modulo weighted Sobolev spaces $H^{k,l}$. Again, k is irrelevant for u as above since $u \in H^{\infty,l}$ automatically as $\psi(H) \in \Psi^{-\infty,0}_{\mathrm{Sc}}(\bar{X}_0,\mathcal{C})$. In addition, although the definition of ${}^{\mathrm{sc}}\dot{T}^*\bar{X}_0$ depends on the metric g, there is a natural identification of the compressed spaces corresponding to different metrics g, and the wave front set is defined independently of the choice of g then.

As an example, consider $M_0 = X_0 \times X_0$ as the space, and let $u \in \mathcal{S}'(M_0)$ be the Schwartz kernel of $\psi(H)$, H a many-body Hamiltonian on X_0, $\psi \in \mathcal{C}^\infty_c(\mathbb{R})$. As discussed above M_0 is naturally a many-body space with collision planes $X_a \times X_b$, $a, b \in I$. However, to accommodate the diagonal singularity, we introduce additional collision planes by adding the diagonal

$$\mathrm{diag} = \{(w,w) :\ w \in X_0\} \tag{3.13}$$

to this set, as well as the diagonals of X_a:

$$\mathrm{diag}_a = \mathrm{diag} \cap (X_a \times X_a) = \{(w_a,0,w_a,0) :\ w_a \in X_a\} \subset M_0,\ a \in I;$$

the resulting set is denoted by $\mathcal{M}$:

$$\mathcal{M} = \{X_a \times X_b :\ a,b \in I\} \cup \{\mathrm{diag}_a :\ a \in I\}.$$

Recall that $\overline{\mathrm{diag}}$ is the closure of diag in $\bar{M}_0$, hence it is the b-diagonal as discussed in [23, 34].

Now the kernel K of $\psi(H)$ is conormal to $\partial\overline{\mathrm{diag}_a}$ in the strong sense that it becomes $\mathcal{C}^\infty$ upon the blow-up of these (in the appropriate order); indeed, this is essentially the definition of $\Psi^{-\infty,0}_{\mathrm{Sc}}(\bar{X}_0;\mathcal{C})$. Note that if $\psi_0 \in \mathcal{C}^\infty_c(\mathbb{R})$ is identically 1 on $[\inf\operatorname{supp}\psi, \sup\operatorname{supp}\psi]$, then $\psi_0(P_\alpha)K = K$, as follows directly from the functional calculus since $H\otimes\mathrm{Id}$, $\mathrm{Id}\otimes H$ commute, so the Fourier transform description of the wave front set given above is applicable. We now prove:

Lemma 3.4. *The kernel K of $\psi(H)$, $\psi\in\mathcal{C}_c^\infty(\mathbb{R})$, satisfies that $\mathrm{WF}_{Sc}(K)$ is a subset of the zero section $o_{\mathrm{diag},a}$ of ${}^{sc}T^*_{\partial\overline{\mathrm{diag}}_{a,reg}}\overline{\mathrm{diag}_a}$. The same holds for δ_{diag}. In particular, with $-\tau$ denoting the dual of the radial Euclidean variable, so*

$$\tau = -\frac{w\cdot\xi}{|w|}, \tag{3.14}$$

$\tau = 0$ on $\mathrm{WF}_{Sc}(K)$ and on $\mathrm{WF}_{Sc}(\delta_{\mathrm{diag}})$.

Remark 3.5. The orthocomplement of diag_a, with respect to $g_L + g_R$, is

$$\mathrm{diag}_{X^a\times X^a}\oplus\{(w,-w):\ w\in X_0\},$$

and the corresponding orthogonal projections give coordinates

$$\frac{1}{\sqrt{2}}(w_a + w'_a, w^a + (w')^a, w - w').$$

The corresponding dual variables are

$$\frac{1}{\sqrt{2}}(\xi_a + \xi'_a, \xi^a + (\xi')^a, \xi - \xi').$$

Thus, at ${}^{\mathrm{sc}}T^*_{\partial\overline{\mathrm{diag}}_{a,\mathrm{reg}}}\overline{\mathrm{diag}_a}$, the only momentum variable is $\xi_a + \xi'_a$, and the lemma states that

$$w_a = w'_a,\ w^a = 0 = (w')^a,\ \xi_a + \xi'_a = 0 \text{ on } \mathrm{WF}_{\mathrm{Sc}}(K)\cap{}^{\mathrm{sc}}T^*_{\partial\overline{\mathrm{diag}}_{a,\mathrm{reg}}}\overline{\mathrm{diag}_a}.$$

In particular,

$$\tau = -\frac{\xi\cdot w + \xi'\cdot w'}{|(w,w')|} = 0$$

there.

Note that the orthogonal projection of the conormal bundle of diag to $T^*\,\overline{\mathrm{diag}_a}$ is the zero section, and for this reason we call the zero section of ${}^{\mathrm{sc}}T^*_{\partial\overline{\mathrm{diag}}_{a,\mathrm{reg}}}\overline{\mathrm{diag}_a}$ the compressed conormal bundle of diag at diag_a.

Proof. Since K is the kernel of a pseudo-differential operator, it is immediate that $\mathrm{WF}_{\mathrm{Sc}}(K)\subset\cup_a{}^{\mathrm{sc}}T^*_{\partial\overline{\mathrm{diag}}_{a,\mathrm{reg}}}\overline{\mathrm{diag}_a}$, i.e. it lies over the boundary of the diagonal; indeed, the kernel is rapidly decreasing elsewhere by the definition of $\Psi_{\mathrm{Sc}}^{-\infty,0}(\bar{X}_0;\mathcal{C})$. We thus need to show that for all a, $\mathrm{WF}_{\mathrm{Sc}}(K)\cap{}^{\mathrm{sc}}T^*_{\partial\overline{\mathrm{diag}}_{a,\mathrm{reg}}}\overline{\mathrm{diag}_a}$ lies in the zero section of ${}^{\mathrm{sc}}T^*_{\partial\overline{\mathrm{diag}}_{a,\mathrm{reg}}}\overline{\mathrm{diag}_a}$. To see this, let $\phi\in\mathcal{C}^\infty(\bar{M}_0)$ be such that $\operatorname{supp}\phi$ is disjoint from all collision planes other than those containing diag_a. This means that ϕ localizes near the regular, and away from the singular, part of $\partial\overline{\mathrm{diag}_a}$. Since ϕK is Schwartz in $w - w'$, and is symbolic in $w + w'$ after some blow ups, in particular symbolic in $w_a + w'_a$, the Fourier transform of ϕK is Schwartz outside $\xi_a + \xi'_a = 0$. Hence $\mathrm{WF}_{\mathrm{Sc}}(K)$ lies in $\xi_a + \xi'_a = 0$, i.e. in the zero section of ${}^{\mathrm{sc}}T^*_{\partial\overline{\mathrm{diag}}_{a,\mathrm{reg}}}\overline{\mathrm{diag}_a}$ as claimed.

A similar argument proves that the part of $\mathrm{WF}_{\mathrm{Sc}}(\delta_{\mathrm{diag}})$ over $\partial\overline{\mathrm{diag}}_{a,\mathrm{reg}}$ lies in the zero section of ${}^{\mathrm{sc}}T^*_{\partial\overline{\mathrm{diag}}_{a,\mathrm{reg}}}\overline{\mathrm{diag}_a}$. Indeed, one can see this directly from the definition, for any vector field tangent to diag annihilates δ_{diag}. $\square$

Remark 3.6. Let $A(F) \in \Psi_{\mathrm{Sc}}^{-\infty,0}(\bar{M}_0, \partial\mathcal{M})$ defined by (3.9), $F \in \mathcal{C}_c^\infty(\mathbb{R})$, and note that on its operator wave front set (a notion that we briefly recall in the Appendix; see [34, Section 5] for a detailed discussion) $-\tau \in \operatorname{supp} F$. The lemma immediately implies that for $F \in \mathcal{C}_c^\infty(\mathbb{R})$ with $0 \notin \operatorname{supp} F$, $A(F)K \in \mathcal{S}$.

The main property of wave front sets that we use is the following. If $u, v \in \mathcal{S}'$, $\mathrm{WF}_{\mathrm{Sc}}(u)$ is a compact subset of ${}^{\mathrm{sc}}\dot{T}^*\bar{X}_0$, and $\mathrm{WF}_{\mathrm{Sc}}(u) \cap \mathrm{WF}_{\mathrm{Sc}}(v) = \emptyset$, then the L^2 pairing extends by continuity to define $\langle u, v\rangle$. For the relative wave front set one has stronger results. In particular, it suffices that $\mathrm{WF}_{\mathrm{Sc}}^{*,l}(u) \cap \mathrm{WF}_{\mathrm{Sc}}^{*,-l}(v) = \emptyset$; the smoothness order k is irrelevant since $\mathrm{WF}_{\mathrm{Sc}}(u)$ is assumed to be compact. This property follows immediately from [34, Proposition 5.4] and the definition of $\mathrm{WF}_{\mathrm{Sc}}$.

We also recall from [23] that the characteristic variety $\Sigma_0(\lambda)$ of $\Delta - \lambda$ is simply the subset of ${}^{\mathrm{sc}}T^*_{\partial\bar{X}_0}\bar{X}_0$ where the principal symbol of $\Delta - \lambda$ at infinity, namely $g - \lambda$, vanishes; g being the metric function. Note that this principal symbol is just usual the principal symbol of the conjugate of $\Delta - \lambda$ by the Fourier transform, which is a multiplication operator by $g - \lambda$, hence is its own principal symbol.

The characteristic set of $H - \lambda$ is defined similarly, in terms of invertibility of various 'indicial operators' at C_a, and is a subset of the compressed cotangent bundle ${}^{\mathrm{sc}}\dot{T}^*\bar{X}_0$. Since we do not want to introduce further notation, we state directly what this set is. If $\Lambda_1 = \{0\}$, the compressed characteristic set of $H - \lambda$ is $\pi(\Sigma_0(\lambda)) \subset {}^{\mathrm{sc}}\dot{T}^*\bar{X}_0$. In general, all the bound states contribute to the characteristic variety. Thus, we let

$$\Sigma_b(\lambda) = \{\zeta = (y_b, \xi_b) \in {}^{\mathrm{sc}}T^*_{C_b}\bar{X}_b : \ \lambda - |\xi_b|^2 \in \operatorname{spec}_{pp} H^b\} \subset {}^{\mathrm{sc}}T^*_{C_b}\bar{X}_b; \tag{3.15}$$

note that $|\xi_b|^2$ is the kinetic energy of a particle in a bound state of H^b. The *characteristic set* of $H - \lambda$, i.e. the 'energy shell', is the union of $\Sigma_b(\lambda)$ over all b, with the proviso that the components of the momentum in which one cannot microlocalize have to be projected out, i.e. over $C_{a,\mathrm{reg}}$ we should get a subset of ${}^{\mathrm{sc}}T^*\bar{X}_a$. To make this precise, note that if $C_a \subset C_b$, there is also a natural projection

$$\pi_{ba} : {}^{\mathrm{sc}}T^*_{C_{a,\mathrm{reg}}}\bar{X}_b = C_{a,\mathrm{reg}} \times X_b^* \to C_{a,\mathrm{reg}} \times X_a^* = {}^{\mathrm{sc}}T^*_{C_{a,\mathrm{reg}}}\bar{X}_a$$

(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

$$\dot{\Sigma}(\lambda) = \cup_a \dot{\Sigma}_a(\lambda), \qquad \dot{\Sigma}_a(\lambda) = \cup_{C_b \supset C_a} \pi_{ba}(\Sigma_b(\lambda)) \cap {}^{\mathrm{sc}}T^*_{C_{a,\mathrm{reg}}}\bar{X}_a, \tag{3.16}$$

so $\dot{\Sigma}(\lambda) \subset {}^{\mathrm{sc}}\dot{T}^*\bar{X}_0$.

The *radial subset* $R_+(\lambda) \cup R_-(\lambda)$ of $\dot{\Sigma}(\lambda)$ plays a special role in many-body scattering, for points in this form stationary generalized broken bicharacteristics. Namely, that at points $(w/|w|, \xi) \in R_\pm(\lambda)$, the Hamilton vector field of Δ_{X_b} is radial (so there is no propagation tangentially to T^*X_b as discussed below), and simultaneously the particles may be in a bound state of H^b, hence there is no propagation in normal directions either. Then

$$\begin{aligned} R_\pm(\lambda) = \{\xi = (\omega, \xi_a) \in {}^{\mathrm{sc}}T^*_{C_{a,\mathrm{reg}}}\bar{X}_a :& \\ &\exists b,\ C_a \subset C_b,\ \lambda - \tau(\xi)^2 \in \operatorname{spec}_{pp}(H^b),\ \pm\tau(\xi) = |\xi_a|\} \end{aligned} \tag{3.17}$$

are the incoming $(+)$ and outgoing $(-)$ radial sets respectively. Note that if λ is not a threshold of H, then $\tau \neq 0$ on $R_+(\lambda) \cup R_-(\lambda)$. The set $R_+(\lambda) \cup R_-(\lambda)$ is the propagation set of Sigal and Soffer [31]; this is the set where there is no real principal type propagation.

Generalized broken bicharacteristics of a many-body Hamiltonian $H-\lambda$ were defined in [35, Definition 2.1]. Here we do not recall the full definition here, but remind the reader that these are continuous maps $\gamma : I \to \dot{\Sigma}(\lambda)$, where $I \subset \mathbb{R}$ is an interval, that enjoy certain estimates with regard to Hamilton vector fields in the various subsystems. The main property for us is that the function $\tau = -\frac{w\cdot\xi}{|w|}$ on ${}^{\mathrm{sc}}\dot{T}^*\bar{X}_0$, is strictly decreasing along generalized broken bicharacteristics except at the radial points. Note that $-\tau$ is the dual of the radial variable, and as mentioned in the introduction, it played a major role in previous works on many-body scattering.

The theorem on the propagation of singularities is the following.

Theorem. *(*[35, Theorem 2.2]*) Let $u \in \mathcal{S}'(\mathbb{R}^n)$, $\lambda \in \mathbb{R}$. Then*

$$\mathrm{WF}_{Sc}(u) \setminus \mathrm{WF}_{Sc}((H-\lambda)u) \tag{3.18}$$

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

A stronger version of this is valid for $u = (H-(\lambda+i0))^{-1}f$, defined if $\mathrm{WF}_{\mathrm{Sc}}(f)$ satisfies appropriate non-incoming conditions (see [35, Section 2] for a full discussion). Namely $\mathrm{WF}_{\mathrm{Sc}}(f)$ only propagates forward along generalized broken bicharacteristics. The non-incoming conditions are satisfied, for example, if $\tau \leq 0$ on $\mathrm{WF}_{\mathrm{Sc}}(f)$, and then we conclude that $\tau \leq 0$ on $\mathrm{WF}_{\mathrm{Sc}}(u)$. These statements are also proved by positive commutator estimates, and consequences can be easily restated as operator estimates. For example, consider $A(F) \in \Psi_{\mathrm{Sc}}^{-\infty,0}(\bar{X}_0, \mathcal{C})$ defined by (3.9). The fact that $-\tau$ is increasing along generalized broken bicharacteristics then converts into the estimate of [11, 36]. Indeed, mapping properties of the wave front set, [34, Proposition 5.4], imply that for λ in a compact subset of $\mathbb{R} \setminus \Lambda$, r, s, r', s' arbitrary,

$$\|A(F)R(\lambda+i0)A(\tilde{F})\|_{\mathcal{B}(H^{r,s},H^{r',s'})} \leq C, \tag{3.19}$$

where $\tilde{F} \in \mathcal{C}_c^\infty(\mathbb{R})$, and in addition $\operatorname{supp} F \subset (c,c')$, $\operatorname{supp}\tilde{F} \subset (c',c'')$, $c < c' < c''$. $|c|, |c'|$ sufficiently small. The fact that in addition $-\tau$ is strictly increasing on any non-stationary generalized broken bicharacteristic implies the strengthened estimate that for all $\chi, \tilde{\chi} \in \mathcal{C}^\infty(\bar{X}_0)$ with $\operatorname{supp}\chi \cap \operatorname{supp}\tilde{\chi} \cap \partial\bar{X}_0 = \emptyset$, and for λ in a compact subset of $\mathbb{R} \setminus \Lambda$, r, s, r', s' arbitrary, there exists $\epsilon > 0$ such that

$$\|\chi A(F)R(\lambda+i0)A(\tilde{F})\tilde{\chi}\|_{\mathcal{B}(H^{r,s},H^{r',s'})} \leq C, \tag{3.20}$$

where $\tilde{F} \in \mathcal{C}_c^\infty(\mathbb{R})$, and in addition $\operatorname{supp} F \subset (c, c'+\epsilon)$, $\operatorname{supp}\tilde{F} \subset (c',c'')$, $c < c' < c''$. $|c|, |c'|$ sufficiently small. These are very similar to the estimates mentioned at the end of Section 2. Of course, these estimates can be simplified, but here we explicitly wanted to emphasize the connection between $\mathrm{WF}_{\mathrm{Sc}}$ and the estimates. We outline the proof of (3.20) in the appendix, so that the reader can avoid the more complicated arguments leading to the stronger results of [35].

4. Smoothness of the trace

Let $K = K_\lambda, K_a = (K_a)_\lambda$ denote the kernels of $R(\lambda+i0) = (H-(\lambda+i0))^{-1}$, and $R_a(\lambda+i0) = (H_a-(\lambda+i0))^{-1}$ respectively, in $\operatorname{Im}\lambda \geq 0$ (of course $+i0$ can be dropped if $\operatorname{Im}\lambda > 0$). Hence they are tempered distributions on $\bar{X}_0 \times \bar{X}_0$. Then K solves $(H_L-\lambda)K = \delta_{\mathrm{diag}}$, $(H_R-\lambda)K = \delta_{\mathrm{diag}}$, where H_L, H_R act on the left and right factors of $X_0 \times X_0$ respectively, and δ_{diag} is the kernel of the identity operator, hence is the natural Dirac delta distribution associated to the diagonal. (The second equation really contains the transpose of $H_R - \lambda$, but since H_R is self-adjoint and real, this is just H_R.) Thus, for example,

$$(\alpha H_L + (1-\alpha)H_R - \lambda)K_\lambda = \delta_{\mathrm{diag}}, \quad 0 < \alpha < 1, \tag{4.1}$$

for $\operatorname{Im}\lambda \geq 0$. Hence, for $\operatorname{Im}\lambda > 0$,

$$K_\lambda = (\alpha H_L + (1-\alpha)H_R - \lambda)^{-1}\delta_{\mathrm{diag}}. \tag{4.2}$$

As remarked in Section 2, $P_\alpha = \alpha H_L + (1-\alpha)H_R$ is a many-body Hamiltonian, so all the usual results on many-body Hamiltonians, such as propagation of singularities, are applicable. In particular, if $\lambda \notin \Lambda$, we can arrange that $\lambda \notin \Lambda_\alpha$ by an appropriate choice of α. We let $\tau = -(w \cdot \xi + w' \cdot \xi')/\langle (w, w')\rangle$ as usual, with (w, w') denoting coordinates on $X_0 \times X_0$, and (ξ, ξ') the dual coordinates. Thus, $-\tau$ is the dual of the radial variable $r = |(w, w')|$ with respect to the metric $g_L + g_R$. We thus deduce that $(\alpha H_L + (1-\alpha)H_R - (\lambda + i0))^{-1}\delta_{\mathrm{diag}}$ makes sense since $\tau = 0$ on $\mathrm{WF}_{\mathrm{Sc}}(\delta_{\mathrm{diag}})$ by Lemma 3.4. Thus,

$$K_\lambda = (\alpha H_L + (1-\alpha)H_R - (\lambda + i0))^{-1}\delta_{\mathrm{diag}} \equiv (P_\alpha - (\lambda + i0))^{-1}\delta_{\mathrm{diag}}. \tag{4.3}$$

For technical reasons it is convenient to eliminate the diagonal singularity (which cancels from the spectral measure anyway). This can be done by considering

$$\psi(H)(H - (\lambda + i0))^{-1} = \tilde{\psi}(H) \tag{4.4}$$

instead of $R(\lambda + i0)$, where $\psi \in \mathcal{C}_c^\infty(\mathbb{R})$ is identically 1 near λ. This has similar properties to $R(\lambda + i0)$, except that it does not have a diagonal singularity in the interior. In particular, its kernel, which we denote by $\tilde{K} = \tilde{K}_\lambda$, satisfies $(H_L - \lambda)\tilde{K} = (H_R - \lambda)\tilde{K} = K_{\psi(H)}$, $K_{\psi(H)}$ denoting the kernel of $\psi(H)$. Hence, again using Lemma 3.4,

$$\tilde{K} = \tilde{K}_\lambda = (\alpha H_L + (1-\alpha)H_R - (\lambda + i0))^{-1}K_{\psi(H)} \equiv (P_\alpha - (\lambda + i0))^{-1}K_{\psi(H)}. \tag{4.5}$$

Similarly, we write $\tilde{K}_a = (\tilde{K}_a)_\lambda$ for the Schwartz kernel of $\tilde{\psi}(H_a)$.

Lemma 4.1. *For all $a \in I$, $\tau \leq 0$ on $\mathrm{WF}_{Sc}(\tilde{K}_a)$. In fact, $\mathrm{WF}_{Sc}(\tilde{K}_a)$ lies in the image of $\mathrm{WF}_{Sc}(\delta_{\mathrm{diag}})$ under the forward generalized broken bicharacteristic relation of $P_\alpha - \lambda$.*

Proof. This follows from $\tilde{K}_a = ((P_a)_\alpha - (\lambda + i0))^{-1}K_{\psi(H_a)}$ and our theorem on the propagation of singularities, namely that they only propagate in the forward direction under $((P_a)_\alpha - (\lambda + i0))^{-1}$. P_a can be replaced by P in the statement since the relation of $P_\alpha - \lambda$ is larger than that of $(P_a)_\alpha - \lambda$. As recalled in the previous section, τ is decreasing under the forward generalized broken bicharacteristic relation, so $\tau = 0$ on $\mathrm{WF}_{\mathrm{Sc}}(\delta_{\mathrm{diag}})$ implies that $\tau \leq 0$ on $\mathrm{WF}_{\mathrm{Sc}}(\tilde{K}_a)$. □

Remark 4.2. We emphasize here that the weaker conclusion, $\tau \leq 0$, follows from [11], and that is the only part of the lemma we use in this paper. The additional microlocal estimates needed will be used in the proof of the next lemma.

In particular, the weaker conclusion can be stated explicitly as follows. If $F \in \mathcal{C}_c^\infty(\mathbb{R})$, supported in $(-\infty, 0)$, then $A(F)\tilde{K} \in \mathcal{S}$, where now $A(F)$ is an operator on $M_0 = X_0 \times X_0$, with principal symbol at infinity the 'same' as that of $F(B)\tilde{\psi}(H)$ (though the latter is not quite a ps.d.o.), B the radial vector field on $X_0 \times X_0$, with principal symbol $-\tau$.

The stronger conclusion of the lemma shows also that τ is strictly negative everywhere on this wave front set except possibly at the compressed conormal bundle of the diagonal, i.e. at the zero section of ${}^{\mathrm{sc}}T^*_{\partial\overline{\mathrm{diag}}_{a,\mathrm{reg}}}\overline{\mathrm{diag}_a}$.

We remark that while microlocally on $\mathrm{WF}_{\mathrm{Sc}}(\tilde{K})$, $\tilde{K}$ is not Schwartz, it is of course still in a weighted Sobolev space, namely in $H^{r,s-1}$ for any $s<-n/2$ and for any r. This holds because $K_{\psi(H)}$ is in $H^{r,s}$ for any $s<-n/2$ and for any r, and $(P_\alpha-(\lambda+i0))^{-1}$ loses one order of decay. (This is the standard propagation phenomenon as for the wave equation, and the factor h^{-1} appears in (5.27) for the same reason.)

Combining Lemma 4.1 for the various clusters a, we thus deduce that $\tau\leq 0$ on $\mathrm{WF}_{\mathrm{Sc}}(\tilde{K}')$,

$$\tilde{K}'=\tilde{K}-\tilde{K}_0-\sum_{\#a=2}(\tilde{K}_a-\tilde{K}_0). \tag{4.6}$$

We claim that in fact $\tau\leq\tau_0<0$ everywhere, hence in particular the compressed conormal bundle of the diagonal is disjoint from it. The key step is the following lemma.

Lemma 4.3. *Let b be a 2-cluster. Then at $\partial\overline{\mathrm{diag}}_{b,reg}$ and at $\partial\overline{\mathrm{diag}}_{0,reg}$, $\tau<0$ on $\mathrm{WF}_{Sc}(\tilde{K}-\tilde{K}_b)$ and $\mathrm{WF}_{Sc}(\tilde{K}_c-\tilde{K}_0)$, $c\neq b$, $\#c=2$. Equivalently, these wave front sets are disjoint from the zero section of ${}^{sc}T^*_{\partial\overline{\mathrm{diag}}_{b,reg}}\overline{\mathrm{diag}_b}$ and of ${}^{sc}T^*_{\partial\overline{\mathrm{diag}}_{0,reg}}\overline{\mathrm{diag}_0}$.*

Proof. To see this, we first compute $(P_\alpha-\lambda)u$, $u=\tilde{K}-\tilde{K}_b$. Thus,

$$(P_\alpha-\lambda)u=K_{\psi(H)}-K_{\psi(H_b)}+[\alpha(I_b)_L+(1-\alpha)(I_b)_R]\tilde{K}_b. \tag{4.7}$$

Thus, near $\partial\overline{\mathrm{diag}_b}$ and $\partial\overline{\mathrm{diag}}_{0,\mathrm{reg}}$, the result is rapidly decreasing since the inter-cluster interactions $(I_b)_L$, $(I_b)_R$ are such, and the same holds for the difference $K_{\psi(H)}-K_{\psi(H_b)}$. *It is only here that we use $V_a\in\mathcal{S}(X^a)$*; see the comments of the following paragraphs for potentials that do not decay rapidly.

We now have two options to proceed. In order to prove that $\tau<0$ on $\mathrm{WF}_{\mathrm{Sc}}(u)$, we can use Proposition A.1 with cluster a of the proposition being either diag or diag_b, $\bar{\tau}=0$, $\bar{y}_a$ any point in $\partial\overline{\mathrm{diag}}_{a,\mathrm{reg}}$ to deduce that for any $\bar{\xi}_a\in X_a^*$ with $\tau(\bar{y}_a,\bar{\xi}_a)=\bar{\xi}_a\cdot\bar{y}_a=\bar{\tau}=0$, $(\bar{y}_a,\bar{\xi}_a)\notin\mathrm{WF}_{\mathrm{Sc}}(u)$, since the assumption (A.6) is automatically satisfied as $\bar{\tau}+\delta_0/3>\bar{\tau}=0$ and $\tau\leq 0$ on $\mathrm{WF}_{\mathrm{Sc}}(u)$ by Lemma 4.1.

Alternatively, we can use the full power of the theorem on the propagation of singularities. Namely, near $\partial\overline{\mathrm{diag}_b}$, $\mathrm{WF}_{\mathrm{Sc}}(u)$ is a union of maximally extended generalized broken bicharacteristics of $P_\alpha-\lambda$. That is, if ζ is in ${}^{\mathrm{sc}}T^*_{\partial\overline{\mathrm{diag}}_{b,\mathrm{reg}}}\overline{\mathrm{diag}_b}\cup{}^{\mathrm{sc}}T^*_{\partial\overline{\mathrm{diag}}_{0,\mathrm{reg}}}\overline{\mathrm{diag}_0}$, and $\zeta\in\mathrm{WF}_{\mathrm{sc}}(u)$, then there exists $T>0$ and a generalized broken bicharacteristic $\gamma:[-T,T]\to\dot{\Sigma}(\lambda)$ such that $\gamma(0)=\zeta$ and $\gamma(t)\in\mathrm{WF}_{\mathrm{Sc}}(u)$ for all $t\in[-T,T]$. (The constant T depends on ζ, namely on how long it takes for bicharacteristics to leave ${}^{\mathrm{sc}}T^*_{\partial\overline{\mathrm{diag}}_{b,\mathrm{reg}}}\overline{\mathrm{diag}_b}\cup{}^{\mathrm{sc}}T^*_{\partial\overline{\mathrm{diag}}_{0,\mathrm{reg}}}\overline{\mathrm{diag}_0}$.) But if ζ is in addition in the zero section of ${}^{\mathrm{sc}}T^*_{\partial\overline{\mathrm{diag}}_{b,\mathrm{reg}}}\overline{\mathrm{diag}_b}$ or of ${}^{\mathrm{sc}}T^*_{\partial\overline{\mathrm{diag}}_{0,\mathrm{reg}}}\overline{\mathrm{diag}_0}$, then $\tau(\gamma(0))=0$, and $\tau(\gamma(t))>0$ for $t<0$, so $\gamma(t)\notin\mathrm{WF}_{\mathrm{Sc}}(u)$ (as $\tau\leq 0$ on $\mathrm{WF}_{\mathrm{Sc}}(u)$) contradicting that $\gamma(t)\in\mathrm{WF}_{\mathrm{Sc}}(u)$ for all $t\in[-T,T]$. Here we use again that λ is not a threshold, for this assumption ensures that there are no stationary bicharacteristics at $\tau=0$. Thus, the zero section of ${}^{\mathrm{sc}}T^*_{\partial\overline{\mathrm{diag}}_{b,\mathrm{reg}}}\overline{\mathrm{diag}_b}$ and of ${}^{\mathrm{sc}}T^*_{\partial\overline{\mathrm{diag}}_{0,\mathrm{reg}}}\overline{\mathrm{diag}_0}$, i.e. the compressed conormal bundle of the diagonal, is disjoint from $\mathrm{WF}_{\mathrm{Sc}}(u)$. A similar argument shows that for $b \neq c$, $\mathrm{WF}_{\mathrm{Sc}}(\tilde{K}_c - \tilde{K}_0)$ is disjoint from the compressed conormal bundle of the diagonal in the same region. Since $\tau < 0$ on $\mathrm{WF}_{\mathrm{Sc}}(\tilde{K})$, etc., over $\partial\overline{\mathrm{diag}}_{b,\mathrm{reg}}$ and $\partial\overline{\mathrm{diag}}_{0,\mathrm{reg}}$ *except* at the zero sections, the first conclusion also follows. □

Combining the statements of the lemma shows that $\mathrm{WF}_{\mathrm{Sc}}(\tilde{K}')$ has the same property for every b. Since b is arbitrary, this means that $\mathrm{WF}_{\mathrm{Sc}}(\tilde{K}')$ is (globally) disjoint from the compressed conormal bundle of the diagonal, and τ is negative on the former. The existence of a strictly negative constant τ_0 such that $\tau \leq \tau_0$ on $\mathrm{WF}_{\mathrm{Sc}}(\tilde{K}')$ follows by compactness. We have thus proved:

Proposition 4.4. *There exists $\tau_0 < 0$ such that $\tau \leq \tau_0$ on $\mathrm{WF}_{Sc}(\tilde{K}')$.*

Remark 4.5. In explicit terms, this means that there exists $\epsilon > 0$ such that if $F \in \mathcal{C}_c^\infty(\mathbb{R})$, supported in $(-\infty, \epsilon)$, then $A(F)\tilde{K}' \in \mathcal{S}$.

Corollary 4.6. *The trace of $\tilde{K}' = \tilde{K}'_\lambda$, for $\lambda \in \mathbb{C}$ with $\operatorname{Im}\lambda > 0$, extends to a continuous function up to $\mathbb{R} \setminus \Lambda$, denoted by $\operatorname{tr}\tilde{K}'_{\lambda+i0}$.*

Proof. By the preceeding Proposition and Lemma 3.4,

$$\mathrm{WF}_{\mathrm{Sc}}(\delta_{\mathrm{diag}}) \cap \mathrm{WF}_{\mathrm{Sc}}(\tilde{K}'_{\lambda+i0}) = \emptyset,$$

$\operatorname{Im}\lambda \geq 0$. Thus, by [34, Proposition 5.4], the L^2 pairing extends to these, and the pairing depends continuously on λ. This pairing is the push-forward of the restriction of $\tilde{K}'$ to the diagonal, hence agrees with $\operatorname{tr}\tilde{K}'_\lambda$ for $\operatorname{Im}\lambda > 0$.

Indeed, explicitly it is easiest to write this down by introducing a partition of unity $1 = \sum_b \chi_b + \chi'$ given by conic cutoffs, χ_b supported away from $\cup_{a\neq b}\overline{\mathrm{diag}_a}$, but near $\overline{\mathrm{diag}}$, χ' supported away from diag, so we need to consider pairing $\langle \chi_b\delta_{\mathrm{diag}}, \tilde{K}'\rangle$. As in the proof of the preceeding lemma, we divide $\tilde{K}'$ up, and consider $\langle \tilde{K} - \tilde{K}_b, \chi_b\delta_{\mathrm{diag}}\rangle$, and the similar pairing for $\tilde{K}_a - \tilde{K}_0$. Now

$$\begin{aligned}\langle \tilde{K} - \tilde{K}_b, \chi_b\delta_{\mathrm{diag}}\rangle =& \langle \chi_b(\mathrm{Id} - \psi_0(P_\alpha))(\tilde{K} - \tilde{K}_b), \delta_{\mathrm{diag}}\rangle + \langle \chi_b A(F)(\tilde{K} - \tilde{K}_b), \delta_{\mathrm{diag}}\rangle \\ &+ \langle \tilde{K} - \tilde{K}_b, (\psi_0(P_\alpha) - A(F)^*)\chi_b\delta_{\mathrm{diag}}\rangle,\end{aligned} \tag{4.8}$$

F as in the preceeding remark, with in addition $F \equiv 1$ near 0. Note that all terms on the right hand side are defined and are bounded functions of λ in compact subsets of $\{\lambda :\ \operatorname{Im}\lambda \geq 0\} \setminus \Lambda$, for in each term one of the two distributions paired is bounded in $H^{r,s}$ for some r, s, the other is bounded in $H^{r',s'}$ for every r', s'. Moreover, both distributions paired are continuous in λ with values in $H^{r'',s''}$ for some r'', s''.

Now, if v_n is a sequence of distributions bounded in $H^{r,s}$, then for every $\delta > 0$, v_n has a convergent subsequence in $H^{r-\delta,s-\delta}$. If in addition $v_n \to v_0$ in $H^{r'',s''}$ for some r'', s'', then the subsequence must converge to v_0 *in* $H^{r-\delta,s-\delta}$. In particular, $v_n \to v_0$ in $H^{r-\delta,s-\delta}$, for otherwise it would have a subsequence $\{v_{n_k}\}_{k=1}^\infty$ and an $\epsilon > 0$ with $\|v_{n_k} - v_0\|_{H^{r-\delta,s-\delta}} \geq \epsilon$, which thus could not have a subsequence converging to v_0 in $H^{r-\delta,s-\delta}$.

Let $\{\lambda_n\}_{n=1}^\infty$ be any sequence with $\operatorname{Im}\lambda_n \geq 0$, $\lim_{n\to\infty}\lambda_n = \lambda_0$. We apply this argument with v_n being either term in any of the pairings, e.g. $v_n = \chi_b A(F)((\tilde{K})_{\lambda_n} - (\tilde{K}_b)_{\lambda_n})$, and deduce that (4.8) is indeed continuous in λ, proving the corollary. □

This argument also shows that the trace of $\chi_b(\psi(H)R(\lambda+i0)-\psi(H_b)R_b(\lambda+i0))$ is already defined as an oscillatory integral, or rather by wave front considerations.

Applying the arguments of the corollary to $R(\lambda-i0)$, we deduce the corresponding conclusion pointwise for the corresponding expressions involving the spectral measure, i.e. for

$$\mathrm{sp}(\lambda)-\mathrm{sp}_0(\lambda)-\sum_a(\mathrm{sp}_a(\lambda)-\mathrm{sp}_0(\lambda)), \tag{4.9}$$

where

$$\mathrm{sp}(\lambda)=(2\pi i)^{-1}((H-(\lambda+i0))^{-1}-(H-(\lambda-i0))^{-1}), \tag{4.10}$$

and similarly with the other spectral measures. Since $\phi(H)=\int_{\mathbb{R}}\phi(\lambda)\ \mathrm{sp}(\lambda)\,d\lambda$, we conclude that the distribution σ is given by the continuous function

$$\sigma(\lambda)=\mathrm{tr}(\mathrm{sp}(\lambda)-\mathrm{sp}_0(\lambda)-\sum_a(\mathrm{sp}_a(\lambda)-\mathrm{sp}_0(\lambda))). \tag{4.11}$$

The smoothness of this function follows directly by taking derivatives of the resolvents with respect to λ. Indeed the derivative of $\tilde{K}$ with respect to λ is given by

$$\frac{d}{d\lambda}\tilde{K}_\lambda=(P_\alpha-(\lambda+i0))^{-2}K_{\psi(H)}=(P_\alpha-(\lambda+i0))^{-1}\tilde{K}_\lambda. \tag{4.12}$$

Then $\tau\leq 0$ still holds on $\mathrm{WF}_{\mathrm{Sc}}(\frac{d}{d\lambda}\tilde{K}_\lambda)$, $\mathrm{WF}_{\mathrm{Sc}}(\tilde{K}_\lambda)$. In addition,

$$(P_\alpha-\lambda)\frac{d}{d\lambda}\tilde{K}_\lambda=\tilde{K}_\lambda \tag{4.13}$$

shows that

$$(P_\alpha-\lambda)\frac{d}{d\lambda}(\tilde{K}_\lambda-(\tilde{K}_b)_\lambda)=\tilde{K}_\lambda-(\tilde{K}_b)_\lambda+[\alpha(I_b)_L+(1-\alpha)(I_b)_R](\tilde{K}_b)_\lambda. \tag{4.14}$$

Since near $\partial\overline{\mathrm{diag}_b}$, $\mathrm{WF}_{\mathrm{Sc}}(\tilde{K}_\lambda-(\tilde{K}_b)_\lambda)$ is in $\tau\leq\tau_0<0$, we deduce as above that $\mathrm{WF}_{\mathrm{Sc}}(\frac{d}{d\lambda}(\tilde{K}_\lambda-(\tilde{K}_b)_\lambda))$ is also in $\tau\leq\tau_0<0$ near $\partial\overline{\mathrm{diag}_b}$, and then further that $\mathrm{WF}_{\mathrm{Sc}}(\frac{d}{d\lambda}\tilde{K}')$ is in $\tau\leq\tau_0<0$ everywhere. This shows that $\frac{d\sigma}{d\lambda}$ is continuous, and an iterative argument yields that σ is $\mathcal{C}^\infty$. We have thus proved the following proposition, which forms the first part of the Theorem stated in the introduction.

Proposition 4.7. *Suppose that H is a three-body Hamiltonian, and the pair potentials V_a are Schwartz (on X^a). Then the spectral shift function σ, defined by (1.1), is $\mathcal{C}^\infty$ on $\mathbb{R}\setminus\Lambda$.*

If the potentials V_a are not Schwartz on X^a, rather they are symbols in $S^{-\rho}(X^a)$, the first part of (5.27), namely $K_{\psi(H)}-K_{\psi(H_b)}$, is in $H^{r,s+\rho}$ for any $s<-n/2$ (and any r) near $\partial\overline{\mathrm{diag}_b}$, while $[\alpha(I_b)_L+(1-\alpha)(I_b)_R]\tilde{K}_b$ is in $H^{r,s-1+\rho}$ in the same region. This yields that $u=\tilde{K}-\tilde{K}_b$ is in $H^{r,s-2+\rho}$ near the compressed conormal bundle of $\overline{\mathrm{diag}_b}$ (rather than Schwartz). The pairing with δ_{diag} thus makes sense if $(s-2+\rho)+s\geq 0$, i.e. $\rho\geq -2s+2$. Since $s>-n/2$ is arbitrary, this means $\rho>n+2$ suffices. This result is non-optimal, $\rho>n$ should be sufficient, but the improvement should correspond to more delicate (oscillatory integral type) behavior that we do not consider here since proving the better estimates is more complicated, especially if the set of thresholds is large! In addition, each derivative causes an additional order of decay to be lost, so to conclude that σ is $\mathcal{C}^k$ by this argument we need $\rho>n+2+k$.

We explain briefly in terms of the two-body setting why more precise, oscillatory integral type, control is needed on the resolvent kernel near the conormal bundle of the diagonal to obtain optimal results. In two-body scattering, the high-energy cut-off resolvent kernel $\tilde{K}$ is of the form $e^{i\sqrt{\lambda}\langle w-w'\rangle}\langle w-w'\rangle^{-(n-1)/2}a$, a smooth on the blown up space $[\bar{M}_0;\partial\overline{\mathrm{diag}}]$ microlocally near the conormal bundle of the diagonal, and is also a smooth function of $\lambda>0$. Differentiating the kernel, in particular the exponential, with respect to λ, gives an extra factor of growth $\langle w-w'\rangle$. However, this factor is bounded near the diagonal, so the pairing with δ_{diag} makes sense without imposing extra vanishing conditions on V. This argument shows that $\rho>n$ suffices in the two-body setting to conclude that σ is $\mathcal{C}^\infty$; indeed, it immediately generalizes to the geometric setting of [23], where it was proved by the use of trace formulae in [6], since one also knows the similar oscillatory behavior there [14]. (This FIO-type analysis originated with [25] in the geometric setting.) Such a detailed analysis is much harder in the many-body setting.

Returning to the setting of Schwartz pair interactions, we remark that a perhaps better approach, which we do not pursue here, for proving smoothness, is to include λ as a variable, i.e. to work with, say, the Schrödinger equation directly. Then the result of the pull-back to the diagonal in the spatial variables followed by the push-forward can be seen to be smooth by the wave front set calculus.

We also emphasize that apart from technical issues, the whole argument can be rewritten in terms estimates involving operators such as $F(B)$, B as in the previous sections.

5. High energy asymptotics

Below we change high energy problems into semiclassical problems, so we start by recalling some notation. First, $H_h^{r,s}=H_h^{r,s}(\mathbb{R}^n)$ is the semiclassical weighted Sobolev space, $\langle w\rangle^{-s}H_h^r(\mathbb{R}^n)$, where the norm on H_h^r is defined by

$$\|u\|_{H_h^r}=(2\pi h)^{-n/2}\|\langle\xi\rangle^r\mathcal{F}_h u\|_{L^2(\mathbb{R}^n)}, \tag{5.1}$$

$\mathcal{F}_h$ being the h-Fourier transform,

$$(\mathcal{F}_h u)(\xi)=\int e^{-iw\cdot\xi/h}u(w)\,dw. \tag{5.2}$$

For $r=0$, the norm in $H_h^r(\mathbb{R}^n)$ is the standard $L^2(\mathbb{R}^n)$ norm; the norm on $H_h^1(\mathbb{R}^n)$ is $\|(1+h^2\Delta)u\|_{L^2(\mathbb{R}^n)}$, etc. Semiclassical many-body pseudo-differential operators $A=A(h)\in\Psi^{m,l}_{\mathrm{Sc},h}(\bar{X}_0,\mathcal{C})$ are defined by the following analogue of (3.7):

$$(2\pi h)^{-n}\int e^{i(w-w')\cdot\xi/h}a(w,\xi;h)\,d\xi \tag{5.3}$$

where $a\in\rho_\infty^{-m}\rho_\partial^l\mathcal{C}^\infty([\bar{X}_0;\mathcal{C}]\times X_0^*\times[0,1))$, rapidly decreasing in the second factor. One can similarly modify (3.9), to define $A=A(F;h)$ by

$$A(F;h)u(w)=(2\pi h)^{-n}\int e^{i(w-w')\cdot\xi/h}a(w,w',\xi;h)u(w')\,dw'\,d\xi, \tag{5.4}$$

$a(w,w',\xi;h)=q(w,\xi;h)p(w',\xi;h)$, this yields an element of $\Psi^{-\infty,l}_{\mathrm{Sc},h}(\bar{X}_0,\mathcal{C})$. One can also interpret these spaces as high energy spaces by letting $h=\lambda^{-1/2}$; then $\lambda\to\infty$ corresponds to $h\to 0$.

As an example, we compute the norm of kernel $K_{A(h)}$ of

$$A = A(h) \in \Psi^{-\infty,0}_{\mathrm{Sc},h}(\bar{X}_0, \mathcal{C})$$

in $H^{0,s}_h((X_0)_w \times (X_0)_{w'})$ for $s < -n/2$. Namely, (5.3) takes the form

$$h^{-n} A(w, (w-w')/h; h),\ A \in \mathcal{C}^\infty([\bar{X}_0; \mathcal{C}] \times X_0 \times [0,1)), \tag{5.5}$$

A rapidly decreasing in the second factor. Thus, for $s < -n/2$

$$\begin{aligned} \|K_{A(h))}\|^2_{H^{0,s}_h} &= h^{-2n} \int_{X_0 \times X_0} \langle (w,w') \rangle^{2s} |A(w,(w-w')/h;h)|^2 \, dw \, dw' \\ &= h^{-n} \int_{X_0 \times X_0} \langle w \rangle^{2s} |A(w,W;h)|^2 \, dw \, dW \le C' h^{-n}, \end{aligned} \tag{5.6}$$

hence $\|K_{A(h)}\|_{H^{0,s}_h} \le C h^{-n/2}$. In fact, a similar calculation, after inserting

$$(\mathrm{Id} + h^2 \Delta_{(w,w')})^r$$

in front of A, gives that $\|K_{A(h)}\|_{H^{r,s}_h} \le C h^{-n/2}$ for all r (and for all $s < -n/2$). A similar calculation also applies to δ_{diag}, and gives for $s < -n/2$ that

$$\|\delta_{\mathrm{diag}}\|_{H^{s,s}_h} \le C h^{-n/2}. \tag{5.7}$$

We start our study of high energy asymptotics of σ by stating an averaged version.

Proposition 5.1. *Suppose that H is a three-body Hamiltonian, V_a are symbols of order $-k$ on X^a, $k > n$. Then for $\phi \in \mathcal{C}^\infty_c(\mathbb{R})$,*

(5.8)

$$\mathrm{tr}(\phi(H/\lambda) - \phi(H_0/\lambda) - \sum_a (\phi(H_a/\lambda) - \phi(H_0/\lambda))) \sim \sum_{j=0}^{\infty} \lambda^{\frac{n}{2}-2-j} d_j, \qquad \lambda \to +\infty.$$

Proof. We change the notation slightly and compute

$$\mathrm{tr}(\phi(H/\lambda') - \phi(H_0/\lambda') - \sum_a (\phi(H_a/\lambda') - \phi(H_0/\lambda'))) \tag{5.9}$$

as $\lambda' \to +\infty$. As usual, we convert the high energy problem into a semiclassical one by letting $h^2 = (\lambda')^{-1}$, and let

$$H(h) = h^2 H, \tag{5.10}$$

so $\phi(H/\lambda') = \phi(H(h))$, i.e. we are interested in the intersection of the spectrum of $H(h)$ with a compact interval (namely $\mathrm{supp}\,\phi$). Note that the high energy asymptotics $\lambda' \to +\infty$ corresponds to the semiclassical problem $h \to 0$. Note also that $h^2 H = h^2\Delta + h^2 V$, so semiclassically the potential vanishes two orders higher than the semiclassical Laplacian $h^2\Delta$. Let $\tilde{\phi} \in \mathcal{C}^\infty_c(\mathbb{C})$ be an almost analytic extension of ϕ (so $|\bar{\partial}_\lambda \tilde{\phi}(\lambda)| \le C_N |\mathrm{Im}\,\lambda|^N$ for all N), and let $R(\lambda; h) = (H(h) - \lambda)^{-1}$. Via the Cauchy formula,

$$\phi(H(h)) = -\frac{1}{2\pi i} \int \bar{\partial}_\lambda \tilde{\phi}(\lambda) R(\lambda; h) \, d\lambda \wedge d\bar{\lambda}, \tag{5.11}$$

the study of the functional calculus in a semiclassical setting reduces to that of the behavior of the resolvents away from the real axis, and the uniformity in h, up to the real axis in λ. The main fact that makes the calculations uniform in h is that by self-adjointness, the L^2 operator norm of $R(\lambda; h)$ is bounded by $|\mathrm{Im}\,\lambda|^{-1}$, for this implies (via the parametrix construction) that all seminorms of $R(\lambda; h)$ in the semiclassical version of $\Psi_{\mathrm{Sc}}^{-2,0}(\bar{X}_0, \mathcal{C})$ (cf. (5.3)) are bounded by $C|\operatorname{Im}\lambda|^{-k}$ for $\operatorname{Re}\lambda$ in a compact set, $|\operatorname{Im}\lambda|$ bounded from above, and for some C and k depending on the seminorm. Hence it follows immediately that for $\phi \in \mathcal{C}_c^\infty(\mathbb{R})$,

$$
\begin{aligned}
&\operatorname{tr}(\phi(H(h)) - \phi(H_0(h)) - \sum_a (\phi(H_a(h)) - \phi(H_0(h)))) \\
&= \operatorname{tr}\left(-\frac{1}{2\pi i}\int \bar{\partial}_\lambda \tilde{\phi}(\lambda)(R(\lambda; h) - R_0(\lambda; h) - \sum_a (R_a(\lambda; h) - R_0(\lambda; h)))\, d\lambda \wedge d\bar{\lambda}\right) \\
&\quad \sim \sum_{j=0}^\infty h^{-n+j} a_j.
\end{aligned}
\tag{5.12}
$$

While the integral is trace class, this may not be apparent since the integrand, which is in $\Psi_{\mathrm{Sc}}^{-2,k}(\bar{X}_0, \mathcal{C})$, is not such due to the diagonal singularity of the resolvents. However, it is easy to rewrite the integral so that the integrand becomes trace class as well. Namely, let $\psi(\lambda) = (\lambda - \lambda_0)^m \phi(\lambda)$, $m > (\dim X_0 - 2)/2$, $\lambda_0 \notin \mathbb{R}$, so $\phi(H(h)) = R(\lambda_0; h)^m \psi(H(h))$, and write out the Cauchy integral representation of $\psi(H(h))$ using an almost analytic continuation $\tilde{\psi}$ of ψ. Thus,

$$
\begin{aligned}
&\phi(H(h)) - \phi(H_0(h)) - \sum_a (\phi(H_a(h)) - \phi(H_0(h))) \\
&= -\frac{1}{2\pi i}\int \bar{\partial}_\lambda \tilde{\psi}(\lambda)(R(\lambda_0; h)^m R(\lambda; h) - R_0(\lambda_0; h)^m R_0(\lambda; h) \\
&\qquad - \sum_a (R_a(\lambda_0; h)^m R_a(\lambda; h) - R_0(\lambda_0; h)^m R_0(\lambda; h)))\, d\lambda \wedge d\bar{\lambda}.
\end{aligned}
\tag{5.13}
$$

The integrand is now clearly trace class, in fact it is a semiclassical many-body scattering pseudo-differential operator of order $(-2m-2, \rho)$, and the asymptotics as $h \to 0$ follows from the construction of $R(\lambda; h)$, etc.

Our first remark is that since H is a differential operator (rather than a more general pseudo-differential operator), for all odd j, $a_j = 0$, as in [28]. This follows from the fact that these terms are given by integrals of odd functions of the momentum ξ, hence these integrals vanish. Indeed, due to the additional h^2 vanishing in V, which implies similar vanishing for the difference of the various resolvents, the leading term is at least two orders higher, i.e. $a_0 = 0$ (and we have already mentioned that $a_1 = 0$). This is exactly the same order of vanishing as for two-body scattering. In fact, more is true.

To see this, we perform local calculations near C_b, i.e. we replace the full trace by the trace of χ_b times (5.13) where $\chi_b \in \mathcal{C}^\infty(\bar{X}_0)$ is supported away from the C_a for $a \neq b$. Making sure that the χ_b form a partition of unity, (5.12) becomes the sum of the local traces, so it suffices to show that the a_2 term of each local trace vanishes. Thus, $\chi_b(R(\lambda_0; h)^m R(\lambda; h) - R_b(\lambda_0; h)^m R_b(\lambda; h))$, $\chi_b(R_a(\lambda_0; h)^m R_a(\lambda; h) - R_0(\lambda_0; h)^m R_0(\lambda; h))$, $a \neq b$, are already trace class. Using $R(\lambda; h) - R_b(\lambda; h) = R(\lambda; h) h^2 I_b R_b(\lambda; h)$, a similar formula for $R_a(\lambda; h) - R_0(\lambda; h)$, that $R(\lambda; h)$, $R_b(\lambda; h)$ can be replaced by $R_0(\lambda; h)$ up to an error of h^2, and the various operators can be commuted up to an error with an additional power of h, it is easy to see that the a_2 term vanishes, where we also take into account that

$I_b = \sum_{a \neq b} V_a$. (In addition, $a_3 = 0$ since the odd coefficients vanish.) Changing back to the h-independent notation finishes the proof.

An alternative, but somewhat formal calculation (in the sense that it does not use the regularization procedure) proceeds as follows. Note first that the resolvents can be rewritten as

$$\begin{aligned} R(\lambda;h) &= R_0(\lambda;h) - \sum_a R_a(\lambda;h)h^2 V_a R_0(\lambda;h) \\ &\quad + \sum_a \sum_{b \neq a} R(\lambda;h)h^2 V_b R_a(\lambda;h)h^2 V_a R_0(\lambda;h), \\ R_a(\lambda;h) &= R_0(\lambda;h) - R_a(\lambda;h)h^2 V_a R_0(\lambda;h). \end{aligned} \tag{5.14}$$

Hence,

$$\begin{aligned} R(\lambda;h) - R_0(\lambda;h) &- \sum_a (R_a(\lambda;h) - R_0(\lambda;h)) \\ &= \sum_a \sum_{b \neq a} R(\lambda;h)h^2 V_b R_a(\lambda;h)h^2 V_a R_0(\lambda;h). \end{aligned} \tag{5.15}$$

Thus, the combination of (5.15) and a regularization argument as in (5.13), though it is rather cumbersome to keep track of the regularizing factors, shows that there is an additional h^2 vanishing here, i.e. $a_2 = 0$. Note that (5.15) is trace class when $n = \dim X_0 < 6$, hence for two-dimensional particles, so in this case we do not need the regularization procedure. □

We proceed to find the leading coefficient, $d_0 = a_4$, without using the regularization procedure, which would complicate the calculation. This is justified directly for two-dimensional particles as mentioned above (the integrand of (5.12) is trace class); in general, we need to be more careful. To avoid cumbersome notation, we emphasize the case of $\dim X_0 = 6$, i.e. the particles are three-dimensional. First, one can write $R(\lambda;h)$ in a (finite) perturbation series:

$$R(\lambda;h) = R_0(\lambda;h) - R_0(\lambda;h)h^2 V R_0(\lambda_0;h) + R(\lambda;h)h^2 V R_0(\lambda;h)h^2 V R_0(\lambda_0;h); \tag{5.16}$$

of course the last term can be expanded even further. Similarly, $R_a(\lambda;h)$ can be expanded in a finite series. The sufficiently high order terms of the series (e.g. from the second term on if $n = 6$, i.e. if the particles are three-dimensional), when $R(\lambda;h)$, etc., are substituted into the right hand side (5.15), give trace class terms which also have at least additional vanishing in h compared to the leading term, so they do not contribute to $d_0 = a_4$. So for $n = 6$,

$$(5.12) \sim \operatorname{tr}\Big(-\frac{h^4}{2\pi i} \int \bar{\partial}_\lambda \tilde{\phi}(\lambda) \sum_a \sum_{b \neq a} R_0(\lambda;h) V_b R_0(\lambda;h) V_a R_0(\lambda;h)\, d\lambda \wedge d\bar{\lambda}\Big), \tag{5.17}$$

where $\sim$ means equality of the leading terms. Here we a priori know that the integral is trace class since it is the difference of trace class operators. In addition, the factors of V_a, V_b, can be commuted to the front, and each commutator gives an extra h vanishing, and lowers the differential order of the pseudo-differential operator. In fact, the commutators take the form $[R_0(\lambda;h), h^2 V_a] = -R_0(\lambda;h)[h^2\Delta, h^2 V_a]R_0(\lambda;h)$, so for $n = 6$ the corresponding terms are trace class with extra vanishing in h, so they do not contribute to d_0 either. Thus,

$$(5.18)\qquad (5.12) \sim \operatorname{tr}\Big(-\frac{h^4}{2\pi i}\int \bar\partial_\lambda \tilde\phi(\lambda)\sum_a\sum_{b\neq a} V_bV_aR_0(\lambda;h)^3\,d\lambda\wedge d\bar\lambda\Big).$$

As before, the integrand of (5.18) is not trace class, though the integral is. Now using the Cauchy-Stokes formula, the integral can be written as

$$(5.19)\quad (5.12) \sim \operatorname{tr}\Big(\frac{h^4}{2\pi i}\int \phi(\lambda)\big(\sum_a\sum_{b\neq a} V_bV_a\big)\big(R_0(\lambda+i0;h)^3 - R_0(\lambda-i0;h)^3\big)\,d\lambda\Big),$$

Now the integrand is not trace class, but its trace is well-defined as a pairing of its kernel with the delta distribution associated to the diagonal. We write out this pairing explicitly as the integral of the restriction of the kernel to the diagonal by writing $R_0(\lambda+i0;h)^3 - R_0(\lambda-i0;h)^3$ as multiplication by a differentiated delta distribution associated to $|\xi|^2=\lambda$, conjugated by the h-Fourier transform. More specifically, we need to calculate

$$(5.20)\qquad (2\pi h)^{-n}h^4\Big(\int_{\bar X_0}(V_aV_b)\,dg\Big)\,\big((|\xi|^2-(\lambda+i0))^{-3}-(|\xi|^2-(\lambda-i0))^{-3},1\big),$$

where $(.,1)$ is the distributional pairing of a compactly supported distribution on $\mathbb{R}^n_\xi$ with 1. The latter is, in modified polar coordinates $\xi=\rho^{1/2}\omega$, $|\omega|=1$,

$$(5.21)\qquad \frac12\operatorname{vol}(\mathbb{S}^{n-1})\big((\rho-(\lambda+i0))^{-3}-(\rho-(\lambda-i0))^{-3},\rho^{(n-2)/2}\big)_{\mathbb{R}}.$$

Since $(\rho-(\lambda+i0))^{-3}-(\rho-(\lambda-i0))^{-3} = 2\pi i\,2^{-1}\delta^{(2)}_\lambda$ as a distribution in ρ, we deduce that

$$(5.22)\qquad (5.21) = \frac12\operatorname{vol}(\mathbb{S}^{n-1})2\pi i\,2^{-1}\frac{(n-2)(n-4)}{4}\lambda^{\frac n2-3}.$$

Hence,

$$(5.23)\qquad \begin{gathered}(5.12)\sim h^{4-n}c\Big(\sum_a\sum_{b\neq a}\int_{\bar X_0}(V_aV_b)\,dg\Big)\int\phi(\lambda)\lambda^{\frac n2-3}\,d\lambda,\\ c=(2\pi)^{-n}\frac{(n-2)(n-4)}{16}\operatorname{vol}(\mathbb{S}^{n-1}).\end{gathered}$$

In the general, higher dimensional ($n\geq 8$), case one simply has to keep more terms, one obtains more commutators, and arranges the factors similarly to how it was done above. Then one still needs to compute the asymptotics of all the a priori non-trivial terms, but at this point the only resolvent involved is the free one, and it is easy to see explicitly that none of the terms except the first one, namely the one kept in (5.19), contribute to d_0, so the formal calculation that would lead to (5.20) is indeed valid.

So far we have only dealt with the 'averaged asymptotics', i.e. those involving $\phi(H/\lambda)$, etc., rather than with the asymptotic behavior of the $\mathcal{C}^\infty$ function σ as $\lambda\to+\infty$. To analyze the latter, recall that $\|R(\lambda+i0;h)\|_{\mathcal{B}(H^{r,s}_h,H^{r+2,-s}_h)}\leq C/h$ for all r and for all $s>1/2$ on any appropriate weighted spaces, λ in a compact subset of $(0,+\infty)$. Now,

$$(5.24)\qquad R(\lambda)=(H-\lambda)^{-1}=h^2(h^2H-\lambda/h^2)^{-1}=h^2R(\lambda/h^2;h),$$

so taking $h=\lambda^{-1/2}$, we deduce that

$$\|R(\lambda+i0)\|_{\mathcal{B}(H^{r,s}_{\lambda^{-1/2}},H^{r+2,-s}_{\lambda^{-1/2}})}\leq C\lambda^{-1/2},\quad \lambda\geq 1. \tag{5.25}$$

Such estimates follow from positive commutator estimates (such as the Mourre estimate) [19], and require a non-trapping assumption for the semiclassical principal symbol [13] – but this is just $h^2\Delta$ since the potential is higher order, so the assumption is automatically satisfied. Microlocal versions of these estimates remain true. For example, (3.19) is replaced, for $\operatorname{supp} F\subset (c,c')$ $\operatorname{supp}\tilde F\subset (c',c'')$, $c<c'<c''$, $|c|$, $|c''|$ small, by

$$\|A(F;h)R(\lambda+i0;h)A(\tilde F;h)\|_{\mathcal{B}(H^{r,s}_h,H^{r',s'}_h)}\leq C/h, \tag{5.26}$$

and (3.20) is replaced, for $\operatorname{supp}\chi\cap\operatorname{supp}\tilde\chi=\emptyset$, $\operatorname{supp}F\subset (c,c'+\epsilon)$ $\operatorname{supp}\tilde F\subset (c',c'')$, by

$$\|\chi A(F;h)R(\lambda+i0;h)A(\tilde F;h)\tilde\chi\|_{\mathcal{B}(H^{r,s}_h,H^{r',s'}_h)}\leq C/h. \tag{5.27}$$

In the high-energy version the right hand sides are replaced by $C\lambda^{-1/2}$. The loss h^{-1} corresponds to the fact that semiclassically the commutator of two pseudodifferential operators vanishes to one order higher than the product, see the remarks following the proof of Proposition A.1 in the appendix. Similarly we can apply $R(\lambda+i0)$ iteratively and gain further decay in λ, e.g. $\|R(\lambda+i0)^2\|\leq C\lambda^{-1}$ on appropriate spaces. As in the preceeding section, below we apply these results to the resolvent $(P_\alpha-(\lambda+i0))^{-1}$ of the many-body Hamiltonian $P_\alpha=\alpha H_L+(1-\alpha H_R)$ on $X_0\times X_0$.

The remark after (5.6) shows that for $s>n/2$, and for all $r\in\mathbb{R}$,

$$\|K_{\psi(H/\lambda)}\|_{H^{r,-s}_{\lambda^{-1/2}}}\leq C\lambda^{n/4},\quad \lambda\geq 1, \tag{5.28}$$

and the same estimate holds for δ_{diag} with $H^{r,-s}_{\lambda^{-1/2}}$ replaced by $H^{-s,-s}_{\lambda^{-1/2}}$. Similar calculations also yield estimates corresponding to the wave front set, for example that for $\tilde F$ with $0\notin\operatorname{supp}(1-\tilde F)$, $A(1-\tilde F)=A(1-\tilde F;\lambda^{-1/2})$ as in (5.4), and for any $r',s'\in\mathbb{R}$

$$\|A(1-\tilde F)K_{\psi(H/\lambda)}\|_{H^{r',s'}_{\lambda^{-1/2}}}\leq C\lambda^{n/4},\quad \lambda\geq 1, \tag{5.29}$$

and the same estimate holds for δ_{diag}. Let

$$\operatorname{supp}\tilde F\subset (c',\infty),\ c'<0,\ |c'|\text{small}, \tag{5.30}$$

(we can take, for example, $c'=-1/2$), $\tilde F$ identically 1 on a slightly smaller set, in particular on a neighborhood of $[0,+\infty)$. Write

$$\mathrm{Id}=A(\tilde F)+A(1-\tilde F)+(\mathrm{Id}-\tilde\psi_0(P_\alpha/\lambda)), \tag{5.31}$$

where $\tilde\psi_0(P_\alpha/\lambda)$ is the operator with amplitude p in the quantization map (5.4). Since

(5.32)

$$\begin{aligned}
&\|(P_\alpha-(\lambda+i0))^{-1}A(\tilde F)K_{\psi(H/\lambda)}\|\leq\|(P_\alpha-(\lambda+i0))^{-1}A(\tilde F)\|\|K_{\psi(H/\lambda)}\|\\
&\|(P_\alpha-(\lambda+i0))^{-1}A(1-\tilde F)K_{\psi(H/\lambda)}\|\leq\|(P_\alpha-(\lambda+i0))^{-1}\|\|A(1-\tilde F)K_{\psi(H/\lambda)}\|,\\
&\|(P_\alpha-(\lambda+i0))^{-1}(\mathrm{Id}-\tilde\psi_0(P_\alpha/\lambda))K_{\psi(H/\lambda)}\|\\
&\qquad\leq\|(P_\alpha-(\lambda+i0))^{-1}(\mathrm{Id}-\tilde\psi_0(P_\alpha/\lambda))\|\|K_{\psi(H/\lambda)}\|,
\end{aligned}$$

we deduce that for $s > n/2+1$, and for all r,

$$\|\tilde{K}_\lambda\|_{H^{r,-s}_{\lambda^{-1/2}}} = \|(P_\alpha - (\lambda + i0))^{-1} K_{\psi(H/\lambda)}\|_{H^{r,-s}_{\lambda^{-1/2}}} \le C\lambda^{n/4-1/2}, \quad \lambda > 1. \tag{5.33}$$

Now let F be such that $\operatorname{supp} F \subset (-\infty, c')$. The estimates (5.32), with a factor of $A(F)$ in front of $(P_\alpha - (\lambda + i0))^{-1}$, yield similar results, but in $H^{r',s'}_{\lambda^{-1/2}}$ for all r', s', so we deduce that

$$\|A(F)\tilde{K}_\lambda\|_{H^{r',s'}_{\lambda^{-1/2}}} \le C\lambda^{n/4-1/2}, \quad \lambda > 1. \tag{5.34}$$

Let b be a 2-cluster, and let $\chi = \chi_b$ be a conic cut-off supported away from $\cup_{a \ne b} \overline{\mathrm{diag}_a}$, but near $\overline{\mathrm{diag}}$. Let $\tilde{\chi}$ be a similar conic cutoff, $\tilde{\chi}$ identically 1 on $\operatorname{supp}\chi$. Then for all s',

$$\|\tilde{\chi}(K_{\psi(H/\lambda)} - K_{\psi(H_b/\lambda)})\|_{H^{r',s'}_{\lambda^{-1/2}}} \le C\lambda^{n/4}, \quad \lambda \ge 1. \tag{5.35}$$

Moreover, from (5.33) and since $\tilde{\chi}(\alpha(I_b)_L + (1-\alpha)(I_b)_R)$ is Schwartz, we deduce that for all s',

$$\|\tilde{\chi}(\alpha(I_b)_L + (1-\alpha)(I_b)_R)\tilde{K}_b\|_{H^{r',s'}_{\lambda^{-1/2}}} \le C\lambda^{n/4-1/2}, \quad \lambda \ge 1. \tag{5.36}$$

Let v denote the right hand side of (4.7). Thus,

$$\|\tilde{\chi}v\|_{H^{r',s'}_{\lambda^{-1/2}}} \le C\lambda^{n/4}, \quad \|A(F)(1-\tilde{\chi})v\|_{H^{r',s'}_{\lambda^{-1/2}}} \le C\lambda^{n/4}, \quad \lambda \ge 1. \tag{5.37}$$

But

$$\begin{aligned} \tilde{K}_\lambda - (\tilde{K}_b)_\lambda &= (P_\alpha - (\lambda + i0))^{-1} v \\ &= (P_\alpha - (\lambda + i0))^{-1}\tilde{\chi}v + (P_\alpha - (\lambda + i0))^{-1}\tilde{\psi}_0(P_\alpha/\lambda)(1-\tilde{\chi})v \\ &\quad + (P_\alpha - (\lambda + i0))^{-1}A(F)(1-\tilde{\chi})v \\ &\quad + (P_\alpha - (\lambda + i0))^{-1}A(1-F)(1-\tilde{\chi})v. \end{aligned} \tag{5.38}$$

Let F_0 satisfy $\operatorname{supp} F_0 \subset (-\infty, \epsilon)$, $\epsilon > 0$ sufficiently small, and apply $\chi A(F_0)$ to the previous equation. We can then estimate each resulting term on the right hand side in $H^{r',s'}_{\lambda^{-1/2}}$ for all s' by $C\lambda^{n/4-1/2}$. Namely the first three terms can be estimated by using the operator estimates of $A(F_0)(P_\alpha - (\lambda+i0))^{-1}$, since it is applied to functions bounded in $H^{r',s'}_{\lambda^{-1/2}}$ by $C\lambda^{n/4}$ for all s'. On the other hand, the last term can be estimated by using the operator estimate of $\chi A(F_0)(P_\alpha - (\lambda+i0))^{-1}A(1-F)(1-\tilde{\chi})$. We therefore deduce that for all r', s',

$$\|\chi A(F_0)(\tilde{K}_\lambda - (\tilde{K}_b)_\lambda))\|_{H^{r',s'}_{\lambda^{-1/2}}} \le C\lambda^{n/4-1/2}, \quad \lambda \ge 1. \tag{5.39}$$

Combined with a similar result for $(\tilde{K}_a)_\lambda - (\tilde{K}_0)_\lambda$, $a \ne b$, and summing over a partition of unity χ_b of a neighborhood of $\overline{\mathrm{diag}}$, we deduce a bound for $\chi' A(F_0)\tilde{K}'_\lambda$ if χ' is supported near the diagonal. Since the corresponding bound is automatic away from the diagonal even for $A(F_0)\tilde{K}_\lambda$ by (5.27), we conclude that

$$\|A(F_0)\tilde{K}'_\lambda\|_{H^{r',s'}_{\lambda^{-1/2}}} \le C\lambda^{n/4-1/2}, \quad \lambda \ge 1. \tag{5.40}$$

Our proof of the smoothness of $\sigma = \langle \tilde{K}'_\lambda, \delta_{\mathrm{diag}} \rangle$ then first yields that

$$|\sigma(\lambda)| \le C\lambda^{(n-1)/2},$$

since the appropriate microlocal norms of $\tilde{K}'_\lambda$ are bounded by $C'\lambda^{n/4-1/2}$, while those of δ_{diag} are bounded by $C''\lambda^{n/4}$. Indeed, in (4.8), for $F \in \mathcal{C}_c^\infty(\mathbb{R})$ supported in $(-\infty, \epsilon)$, identically 1 near 0, and for $s > n/2$ and $\lambda > 1$,

(5.41)
$$\begin{aligned}
&|\langle(\mathrm{Id} - \psi_0(P_\alpha/\lambda))\tilde{K}'_\lambda, \delta_{\mathrm{diag}}\rangle| \leq \|(\mathrm{Id} - \psi_0(P_\alpha/\lambda))\tilde{K}'_\lambda\|_{H^{s,s}} \|\delta_{\mathrm{diag}}\|_{H^{-s,-s}} \leq C\lambda^{n/2-1/2},\\
&|\langle A(F_0)\tilde{K}'_\lambda, \delta_{\mathrm{diag}}\rangle| \leq \|A(F_0)\tilde{K}'_\lambda\|_{H^{s,s}} \|\delta_{\mathrm{diag}}\|_{H^{-s,-s}} \leq C\lambda^{n/2-1/2},\\
&|\langle \tilde{K}'_\lambda, (\psi_0(P_\alpha/\lambda) - A(F_0)^*)\delta_{\mathrm{diag}}\rangle|\\
&\qquad \leq \|\tilde{K}'_\lambda\|_{H^{-s,-s}} \|(\psi_0(P_\alpha/\lambda) - A(F_0)^*)\delta_{\mathrm{diag}}\|_{H^{s,s}} \leq C\lambda^{n/2-1/2}.
\end{aligned}$$

The identity $\lambda dR(\lambda)/d\lambda = HR^2(\lambda) - R(\lambda)$ also allows us to deduce that

$$|(\lambda\partial_\lambda)^k \sigma(\lambda)| \leq C_k \lambda^{(n-1)/2}, \tag{5.42}$$

hence σ is a symbol (outside a compact set). Applying a perturbation series argument, as for the 'averaged asymptotics' above with λ replaced by $\lambda + i0$, then shows that for all $k \geq 0$, σ has an asymptotic expansion, up to $\lambda^{(n-k)/2}$, modulo symbols of order $(n-k)/2$. (Note that a priori there is only a gain of $\lambda^{-1/2}$, rather than λ^{-1}, between consecutive terms of the perturbation series, due to (5.25); this does not appear in the trace due to the special behavior of the kernel near the diagonal: sharper (subconic) localization near the diagonal would give, even a priori, a better result.) Hence σ is indeed a classical symbol, i.e. has an asymptotic expansion, with the top coefficient calculated above. In view of (5.23), we have thus proved the theorem from the introduction, which we now restate.

Theorem 5.2. *Suppose that the pair potentials V_a are Schwartz (on X^a). Then the spectral shift function σ is $\mathcal{C}^\infty$ on $\mathbb{R} \setminus \Lambda$. Moreover, σ is a symbol outside a compact set, and it has a full asymptotic expansion as $\lambda \to +\infty$:*

$$\sigma(\lambda) \sim \sum_{j=0}^\infty \lambda^{\frac{n}{2}-3-j} c_j, \quad c_0 = C_0 \sum_a \sum_{b \neq a} \int_{X_0} V_a V_b \, dg,$$

where $C_0 = \frac{1}{16}(n-2)(n-4)(2\pi)^{-n} \operatorname{vol}(\mathbb{S}^{n-1})$ depends only on $n = \dim X_0$.

6. Many-body spectral shift functions

We now define a modified spectral shift function in the general N-body setting. Essentially the same proofs as above show its smoothness away from the thresholds and yield its high energy asymptotics, though now the combinatorial part becomes a little more complicated. We define these recursively for subsystems, starting with the free (i.e. N-) cluster. So, for $\phi \in \mathcal{C}_c^\infty(\mathbb{R})$, let

$$\begin{aligned}
&T(X_0, X^0, \mathcal{X}^0)(\phi) = \phi(H_0),\\
&T(X_0, X^a, \mathcal{X}^a)(\phi) = \phi(H_a) - \sum_{c \leq a,\ c \neq a} T(X_0, X^c, \mathcal{X}^c)(\phi).
\end{aligned} \tag{6.1}$$

The second equation can be rewritten as

$$\phi(H_a) = \sum_{c \leq a} T(X_0, X^c, \mathcal{X}^c)(\phi), \tag{6.2}$$

and it defines $T(X_0, X^a, \mathcal{X}^a)(\phi)$ recursively. Note that $T(X_0, X^a, \mathcal{X}^a)(\phi)$ is an operator on X_0; more precisely, it is in $\Psi_{\mathrm{Sc}}^{-\infty,0}(\bar{X}_0; \mathcal{C})$, though some of the elements of $\mathcal{C}$ can be dropped. We write

$$T(\phi) = T(X_0, X^1, \mathcal{X}^1)(\phi). \tag{6.3}$$

For example, if H is a two-body Hamiltonian, we get $T(\phi) = \phi(H) - \phi(H_0)$, and if H is a three-body Hamiltonian we obtain the Buslaev-Merkurev expression, $T(\phi) = \phi(H) - \phi(H_0) - \sum_{\#a=2}(\phi(H_a) - \phi(H_0))$. We continue with a lemma.

Lemma 6.1. *Suppose that $V_a \in x^k\mathcal{C}^\infty(\bar{X}^a)$. Then for all a, $T(X_0, X^a, \mathcal{X}^a)(\phi)$ is in $\Psi_{Sc}^{-\infty,k}(\bar{X}_0, \mathcal{C})$ away from C_a, i.e. on $C_0 \setminus C_a$. In particular, if all V_a are Schwartz, then for all a, $T(X_0, X^a, \mathcal{X}^a)(\phi)$ is in $\Psi_{Sc}^{-\infty,\infty}(\bar{X}_0, \mathcal{C})$ away from C_a.*

Proof. This statement is empty for $T(X_0, X^0, \mathcal{X}^0)(\phi)$, since $C_0 \setminus C_0 = \emptyset$. We proceed by induction, assuming that we have shown that for all $c \leq a$, $c \neq a$, $T(X_0, X^c, \mathcal{X}^c)(\phi)$ is in $\Psi_{\mathrm{Sc}}^{-\infty,\infty}(\bar{X}_0, \mathcal{C})$ away from C_c. Suppose that $p \in C_{b,\mathrm{reg}}$, $p \notin C_a$; in particular, $b \not\geq a$ (for then $C_a \supset C_b$ would hold). Then $T(X_0, X^c, \mathcal{X}^c)(\phi)$ is in $\Psi_{\mathrm{Sc}}^{-\infty,\infty}(\bar{X}_0, \mathcal{C})$ near p unless $p \in C_c$, i.e. unless $C_b \subset C_c$, i.e. $b \geq c$. Now,

$$\begin{aligned} T(X_0, X^a, \mathcal{X}^a)(\phi) = \phi(H_a) &- \sum_{c\leq a,\ c\neq a\ c\leq b} T(X_0, X^c, \mathcal{X}^c)(\phi) \\ &- \sum_{c\leq a,\ c\neq a\ c\not\leq b} T(X_0, X^c, \mathcal{X}^c)(\phi), \end{aligned} \tag{6.4}$$

and we have just seen that each term in the last sum is in $\Psi_{\mathrm{Sc}}^{-\infty,\infty}(\bar{X}_0, \mathcal{C})$ near p. On the other hand, let d be the maximal element with the property $d \leq a$ and $d \leq b$. Note that this maximal element is unique, namely it is given by $X^d = \mathrm{span}\{X^c : c \leq a,\ c \leq b\} \subset X^a \cap X^b$, i.e. $X_d = \bigcap\{X_c :\ c \leq a,\ c \leq b\} \supset X_a + X_b$, which is a collision plane since $\mathcal{X}$ is closed under intersections. In particular, $d \neq a$ since $a \not\leq b$, hence the first sum in (6.4) is $\sum_{c\leq d} T(X_0, X^c, \mathcal{X}^c)(\phi) = \phi(H_d)$, so

$$T(X_0, X^a, \mathcal{X}^a)(\phi) = \phi(H_a) - \phi(H_d) - \sum_{c\leq a,\ c\neq a,\ c\not\leq b} T(X_0, X^c, \mathcal{X}^c)(\phi). \tag{6.5}$$

Since $H_a - H_d = \sum_{c\leq a,\ c\not\leq b} V_c$, it is in $x^k\mathcal{C}^\infty(\bar{X}_0)$ (resp. Schwartz) near p if the potentials V_c are in $x^k\mathcal{C}^\infty(\bar{X}^c)$ (resp. Schwartz on X^c), hence the local nature of the construction of $\phi(H_a)$ and $\phi(H_d)$ (functional calculus and resolvent construction) yields that $\phi(H_a) - \phi(H_d)$ is in $\Psi_{\mathrm{Sc}}^{-\infty,\infty}(\bar{X}_0, \mathcal{C})$ near p, hence providing the inductive step. $\square$

This shows, in particular, that $T(\phi) \in \Psi_{\mathrm{Sc}}^{-\infty,k}(\bar{X}_0, \mathcal{C})$, and is hence trace class if $k > n$. Moreover, the map $\mathcal{C}_c^\infty(\mathbb{R}) \ni \phi \mapsto \mathrm{tr}(T(\phi)) \in \mathbb{C}$ is linear and continuous. We thus make the following definition.

Definition 6.2. Let H be a many-body Hamiltonian, and define T by (6.1)-(6.3). Suppose that the potentials V_a are symbols of order $k > n$ on X^a: $V_a \in S^{-k}(X^a)$. The modified spectral shift function σ is defined, as a distribution on $\mathbb{R}$, by

$$\sigma(\phi) = \mathrm{tr}(T(\phi)),\ \phi \in \mathcal{C}_c^\infty(\mathbb{R}). \tag{6.6}$$

For Schwartz potentials V_c (on X^c), the arguments presented in the previous sections apply, with the result that σ is $\mathcal{C}^\infty$ on $\mathbb{R} \setminus \Lambda$. Indeed, note first that the wave front set of kernel of $T(X_0, X^a, \mathcal{X}^a)(\phi)$ is in the compressed conormal bundle of the diagonal (since the operator is a linear combination of the $\phi(H_c)$), hence $\tau = 0$ on it. Let $\psi \in \mathcal{C}_c^\infty(\mathbb{R})$, and let $\tilde{\psi}(t) = \psi(t)(t - (\lambda + i0))^{-1}$. We will write

$T(X_0, X^a, \mathcal{X}^a)(\tilde{\psi})$ even though $\tilde{\psi}$ is not smooth. We claim that near any $p \notin C_a$, $T(X_0, X^a, \mathcal{X}^a)(\tilde{\psi})$ is a sum of terms T_j, each of which satisfies that for some $a_j \leq a$, $(H_{a_j} - \lambda)T_j, T_j(H_{a_j} - \lambda)$ are in $\Psi_{\mathrm{Sc}}^{-\infty,\infty}(\bar{X}_0, \mathcal{C})$ near p. The proof again proceeds by induction, the statement being empty for $a = 0$. So suppose that for all $c \leq a$, $c \neq a$, we have shown the claim, and suppose that $p \in C_{b,\mathrm{reg}}$. Now (6.5) becomes

$$T(X_0, X^a, \mathcal{X}^a)(\tilde{\psi}) = \tilde{\psi}(H_a) - \tilde{\psi}(H_d) - \sum_{c \leq a,\ c \neq a,\ c \not\leq b} T(X_0, X^c, \mathcal{X}^c)(\tilde{\psi}). \tag{6.7}$$

Each term in the sum on the right hand side can be written as a sum of operators $T_{c,j}$ with the desired properties by the induction hypothesis. On the other hand,

$$(H_a - \lambda)(\tilde{\psi}(H_a) - \tilde{\psi}(H_d)) = \psi(H_a) - \psi(H_d) + (\sum_{c \leq a,\ c \not\leq d} V_c)\psi(H_d). \tag{6.8}$$

Since $c \leq b$, together with $c \leq a$, would imply $c \leq d$, we deduce that each V_c is Schwartz near p, hence the last term is in $\Psi_{\mathrm{Sc}}^{-\infty,\infty}(\bar{X}_0, \mathcal{C})$ near p, while the same statement for $\psi(H_a) - \psi(H_d)$ has already been demonstrated above. Proceeding in the three-body setting, i.e. using the propagation of singularities, shows that the wave front set of the kernel of $T(\tilde{\psi})$ is in $\tau \leq \tau_0 < 0$, and then we deduce that σ is continuous. Iterating the argument gives that σ is $\mathcal{C}^\infty$.

The pseudodifferential functional calculus shows, as in the previous section, that for $\phi \in \mathcal{C}_c^\infty(\lambda)$,

$$\sigma(\phi(./\lambda)) \sim \sum_{j=0}^{\infty} \lambda^{(n-j)/2} a_j, \tag{6.9}$$

with $a_j = 0$ for all odd j. The symbol estimates for the $\mathcal{C}^\infty$ function σ itself also proceed as before, so $|(\lambda\partial_\lambda)^k \sigma(\lambda)| \leq C_k \lambda^{(n-1)/2}$. A perturbation series argument again yields a full asymptotic expansion. Since $R_a(\lambda) - R_0(\lambda) = R_a(\lambda)(\sum_{c \leq a} V_c)R_0(\lambda)$, $\lambda \notin \mathbb{R}$, we deduce that the leading terms a_0 and a_1 vanish. If all potentials are pair potentials, i.e. if $V_c = 0$ for all clusters c that are not $N-1$-clusters, one can show that $a_j = 0$ for $j \leq 2N - 1$ and $a_{2N} = c_{n,N} C(V)$ where $C(V) = \sum_\sigma \int V_{\sigma_1} \cdots V_{\sigma_{N-1}} dx$, the sum is taken over all sequences $\sigma = (\sigma_1, \sigma_2, \cdots, \sigma_{N-1})$ of $(N-1)$ -cluster decompositions σ_j such that $\cup_{j=1}^{N-1} \sigma_j = a_{\max}$ and $c_{n,N}$ is a contant depending only on n and N which can be calculated by the method of Section 5.

We have thus proved the following result.

Theorem 6.3. *Suppose that for all a, V_a is a Schwartz function on X^a. The modified spectral shift function, σ, defined as a distribution by* (6.6)*, is $\mathcal{C}^\infty$ on $\mathbb{R} \setminus \Lambda$. In addition, σ is a symbol outside a compact set, and it has a full asymptotic expansion:*

$$\sigma(\lambda) \sim \sum_{j=0}^{\infty} \lambda^{\frac{n}{2}-2-j} c_j, \quad \lambda \to +\infty.$$

Here we do not assume that all potentials are pair potentials.

Appendix A. Sketch of relevant positive commutator estimates

To illustrate the proof of the propagation of singularities by positive commutator estimates in [35], we sketch the proof of a simpler version here which still suffices for the purposes of the present paper. We state it both as a wave front set estimate and as a microlocal energy estimate to emphasize the very direct connection between these. We assume that the reader is familiar with the notation and concepts of Section 2 and Section 3, up to the statement of the Theorem on the propagation of singularities, though the part from (3.13) to Remark 3.6 can be skipped as it does not play a role below.

First we introduce some notation. For a cluster a (possibly $a = 0!$) let

$$x_a = |w_a|^{-1},\ y_a = w_a/|w_a|,\ z^a = w^a/|w_a|; \tag{A.1}$$

these are local coordinates on the radial compactification $\bar{X}_0$ near $\bar{X}_a$. Let

$$\tau = -\frac{w \cdot \xi}{|w|},\ \tau_a = -\frac{w_a \cdot \xi_a}{|w_a|}, \tag{A.2}$$

so $\tau = \tau_a$ at $\bar{X}_a$. We also write $x = |w|^{-1}$. In addition, it is sometimes convenient, for $X_b \supset X_a$, i.e. $X^b \subset X^a$, to decompose $w^a \in X^a$ as $(w^{ab}, w^a_b) \in X^b \oplus (X^a \ominus X^b)$, and write (z^{ab}, z^a_b) accordingly.

Below we work in a neighborhood of an energy $\lambda \notin \Lambda_1$, and a point $\bar{y}_a \in C_{a,\mathrm{reg}}$, as well as in a neighborhood of a radial momentum $\bar{\tau}$ such that $\lambda - \bar{\tau}^2 \notin \Lambda_1$. Our positive commutator estimates at energy $\lambda \notin \Lambda_1$ will arise by considering

$$\phi = \bar{\tau} - \tau + \frac{\beta}{\epsilon}(|z^a|^2 + |y_a - \bar{y}_a|^2), \tag{A.3}$$

where $\beta > 0$ will be fixed later and $\epsilon > 0$ is arbitrary as long as it is sufficiently small. Now, the quantization of $\bar{\tau} - \tau$ has a positive commutator with the Hamiltonian in the relevant region of phase space – it is essentially the operator $\bar{\tau} + B$ used in the works of Gérard, Isozaki and Skibsted [11, 12]. On the other hand, for (y_a, z^a) near $(\bar{y}_a, 0)$, the commutator of $|z^a|^2 + |y_a - \bar{y}_a|^2$ with the Hamiltonian is small, since the commutator involves the first derivative of this (plus terms that have extra x vanishing, hence can be neglected modulo a compact error), and these *vanish* at $(\bar{y}_a, 0)$, hence are small nearby, so can be absorbed into the positive commutator given by $\bar{\tau} - \tau$, at least *sufficiently close to* $(\bar{y}_a, 0)$. The key question then is whether we can use this ϕ to localize in a small neighborhood of $(\bar{y}_a, 0)$ at the same time. The answer is yes, and such a construction appeared first in the ground-breaking work of Melrose and Sjöstrand when they proved propagation of singularities for the wave equation for rays tangent to the boundary of a domain [24], see [18, Chapter 24] for another discussion of this construction. This is achieved by considering functions of ϕ.

More precisely, 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

$$q = \chi_0(A_0^{-1}(2 - \phi/\epsilon))\chi_1((\bar{\tau} - \tau)/\epsilon + 2). \tag{A.4}$$

Thus, at $\tau = \bar{\tau}$, $z^a = 0$, $y_a = \bar{y}_a$, $q = \chi_0(2/A_0) > 0$, and on $\operatorname{supp} q$ we have

$$\phi \leq 2\epsilon \text{ and } \bar{\tau} - \tau \geq -2\epsilon. \tag{A.5}$$

Using the positivity of $|z^a|^2 + |y_a - \bar{y}_a|^2$ it is easy to see that q can be made to be supported in an arbitrarily small neighborhood of $\tau = \bar{\tau}$, $y_a = \bar{y}_a$, $z^a = 0$ by choosing $\epsilon > 0$ small enough. (We quantize q as in (3.9); this localizes near energy λ, so we are working in a compact region of phase space, but in this preliminary discussion we ignore this point.) The crucial issue is whether the support is small enough so that the commutator of the quantization of q with H is positive, i.e.

whether the commutator arising from $\bar{\tau}-\tau$ can be used to dominate the terms arising from $\frac{\beta}{\epsilon}(|z^a|^2+|y_a-\bar{y}_a|^2)$, especially since the latter gets larger as $\epsilon\to 0$! Again, the answer is affirmative, as follows from an explicit calculation which we perform below in the proof of our central Proposition A.1. We emphasize that this proposition is merely a weaker version of the fully microlocal estimates of [35], and it is stated and its proof outlined here to make these estimates more accessible.

The main technical result is thus the following.

Proposition A.1. [35, Weaker version of Proposition 7.1] *Suppose that H is a many-body Hamiltonian. Let $u\in\mathcal{C}^{-\infty}(\bar{X})$, $\lambda\notin\Lambda_1$. Let $\bar{y}_a\in C_{a,reg}$, $\bar{\tau}$ such that $\lambda-\bar{\tau}^2\notin\Lambda_1$. Suppose that for all $\bar{\zeta}=(\bar{y}_a,\bar{\xi}_a)\in{}^{sc}T^*_{C_a}\bar{X}_a$ with $\tau(\bar{\zeta})=\bar{\tau}$, we have $\bar{\zeta}\notin\mathrm{WF}_{Sc}((H-\lambda)u)$. Then there exist $\bar{\delta}_0>0$ and $C>0$, depending only on $\bar{\tau}$, $\bar{y}_a$ and $\mathrm{WF}_{Sc}((H-\lambda)u)$, with the following property. Suppose that $\delta_0\in(0,\bar{\delta}_0)$ and*

$$\forall\zeta\ \ (|y_0(\zeta)-\bar{y}_a|<C\delta_0\ \text{and}\ \bar{\tau}+\delta_0/3<\tau(\zeta)<\bar{\tau}+\delta_0\Rightarrow\zeta\notin\mathrm{WF}_{Sc}(u))\,. \tag{A.6}$$

Then

$$\bar{\zeta}=(\bar{y}_a,\bar{\xi}_a),\ \tau(\bar{\zeta})=\bar{\tau}\Rightarrow\bar{\zeta}\notin\mathrm{WF}_{Sc}(u).$$

In fact, there exists $C'>0$ depending only on $\bar{\tau}$, $\bar{y}_a$ and $\mathrm{WF}_{Sc}((H-\lambda)u)$, so that the following holds. For any $s,s'\in\mathbb{R}$, there exists $C_1>0$ such that for all u as above,

$$\begin{aligned}\|A(\chi_{U'}(y_0)\chi_{(-\delta_0/3,\delta_0/3)}(\tau-\bar{\tau}))u\|_{H^{*,s}}&\leq C_1(\|A(\chi_U(y_0)\chi_{(\delta_0/3,\delta_0)}(\tau-\bar{\tau}))u\|_{H^{*,s}}\\&\quad+\|A(\chi_U(y_0)\chi_{(-\delta_0/3,\delta_0)}(\tau-\bar{\tau}))(H-\lambda)u\|_{H^{*,s+1}}+\|u\|_{H^{*,s'}}),\end{aligned} \tag{A.7}$$

where U is the ball $|y_0(\zeta)-\bar{y}_a|<C\delta_0$, U' the ball $|y_0(\zeta)-\bar{y}_a|<C'\delta_0$, $\chi_U(y)$, resp. $\chi_I(\tau-\bar{\tau})$ denote a smoothed characteristic function of U_y, resp. the interval $I_{\tau-\bar{\tau}}$, and A denotes quantization as in (3.9), and $H^{*,s}$ stands for the space $H^{r,s}$, r arbitrary.

Remark A.2. We emphasize that the positive commutator estimate we prove involves quantization of q given in (A.4). The operators in the estimate (A.7) are *not* given by the commutator, they are *easily estimated by* the commutator. Indeed, cutoffs as in (A.7) cannot yield positive commutator estimates – the problems arise at the boundary of $\mathrm{supp}\,\chi_{U'}$.

Remark A.3. Since $\bar{\zeta}\notin\mathrm{WF}_{\mathrm{Sc}}((H-\lambda)u)$, by elliptic regularity we deduce that $\bar{\zeta}\notin\mathrm{WF}_{\mathrm{Sc}}(u)$ for $\bar{\zeta}\notin\dot{\Sigma}(\lambda)$, i.e. for $\bar{\zeta}$ not in the λ characteristic set (energy shell).

The estimate of (A.7) implies (3.20) directly. Indeed, if $\tilde{\chi}$ is such that $\mathrm{supp}\,\chi_{U'}\cap\mathrm{supp}\,\tilde{\chi}=\emptyset$, consider $u=R(\lambda+i0)v$, $v=A(\tilde{\chi}(y_0)\chi_{(-\delta_0/4,\delta_0/4)}(\tau-\bar{\tau}))f$, $f\in H^{r',s'}$. Then the second and third terms are directly bounded in terms of v, while the first term is bounded in terms of f due to the boundedness of $A(\chi_{(\delta_0/3,\delta_0)}(\tau-\bar{\tau}))R(\lambda+i0)A(\chi_{(-\delta_0/4,\delta_0/4)}(\tau-\bar{\tau}))$ between any two weighted Sobolev spaces.

Before giving the proof, we introduce additional notation. We also let W_c be the rescaled Hamilton vector field of Δ_{X_c}, so

$$W_c=2\frac{\xi_c}{|w_c|}\cdot\partial_{w_c}; \tag{A.8}$$

this should be regarded as a vector field on T^*X_c which extends to a smooth vector field on ${}^{\mathrm{sc}}T^*\bar{X}_c$ tangent to the boundary ${}^{\mathrm{sc}}T^*_{C_c}\bar{X}_c=C_c\times X_c^*$, and hence can be considered as a vector field on ${}^{\mathrm{sc}}T^*_{C_c}\bar{X}_c$. Recall also that the part of the characteristic variety corresponding to the bound states of H^b is

$$\Sigma_b(\lambda) = \{\zeta = (y_b, \xi_b) \in {}^{\mathrm{sc}}T^*_{C_b}\bar{X}_b : \ \lambda - |\xi_b|^2 \in \mathrm{spec}_{pp} H^b\} \subset {}^{\mathrm{sc}}T^*_{C_b}\bar{X}_b. \tag{A.9}$$

For $C_a \subset C_b$, we write the projection

$$\hat{\pi}_{ba} : \Sigma_b(\lambda) \cap {}^{\mathrm{sc}}T^*_{C_{a,\mathrm{reg}}}\bar{X}_b \to {}^{\mathrm{sc}}T^*_{C_{a,\mathrm{reg}}}\bar{X}_a \subset \dot{\Sigma}(\lambda); \tag{A.10}$$

this is the restriction of $\pi_{ba} : {}^{\mathrm{sc}}T^*_{C_{a,\mathrm{reg}}}\bar{X}_b \to {}^{\mathrm{sc}}T^*_{C_{a,\mathrm{reg}}}\bar{X}_a$ to $\Sigma_b(\lambda)$. For $A \in \Psi^{-\infty,l}_{\mathrm{Sc}}(\bar{X}, \mathcal{C})$, the operator wave front set $\mathrm{WF}'_{\mathrm{Sc}}(A)$ was defined in [34] as a subset of the compressed cotangent bundle ${}^{\mathrm{sc}}\dot{T}^*\bar{X}$. Namely, let p denote the projection $[\bar{X}; \mathcal{C}] \times \bar{X}^* \to {}^{\mathrm{sc}}\dot{T}^*\bar{X}$ in (3.12), given by the composition of the blow-down map and the projection $\pi : {}^{\mathrm{sc}}T^*\bar{X} \to {}^{\mathrm{sc}}\dot{T}^*\bar{X}$. Then $\zeta \in {}^{\mathrm{sc}}\dot{T}^*\bar{X} \setminus \mathrm{WF}'_{\mathrm{Sc}}(A)$ means that in a neighborhood of $p^{-1}(\{\zeta\})$, the amplitude a defining A as in (3.6) vanishes to infinite order. This notion is independent of the choice of quantization.

Proof. (Sketch, see [35, Proof of Proposition 7.1] for complete details.) We give the full commutator construction at the symbol level, and indicate why it gives rise to a microlocally positive commutator. In fact, the commutator will be positive in part of phase space, negative (or not necessarily positive) in another part of phase space. The propagation of singularities estimates, which should be thought of as microlocal energy estimates, work by estimating u in the former region in terms of u in the latter region and $(H - \lambda)u$ in the union of both regions.

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

For points $\zeta = (y_b, \xi_b)$ in ${}^{\mathrm{sc}}T^*_{C_b}\bar{X}_b$,

$$-W_b\tau(\zeta) = 2(|\xi_b|^2 - \tau(\zeta)^2) \geq 0. \tag{A.11}$$

For $\zeta \in \Sigma_b(\lambda) \subset {}^{\mathrm{sc}}T^*_{C_b}\bar{X}_b$, $\lambda - |\xi_b|^2 = \epsilon_\beta \in \mathrm{spec}_{pp}(H^b)$, so

$$-W_b\tau(\zeta) = 2(\lambda - \tau(\zeta)^2 - \epsilon_\beta). \tag{A.12}$$

We define

(A.13)

$$c_0 = \frac{1}{2}\inf\{-W_b\tau(\bar{\zeta}_b) : \exists\bar{\xi}_a \text{ such that } \tau((\bar{y}_a, \bar{\xi}_a)) = \bar{\tau}, \ \bar{\zeta}_b \in \hat{\pi}_{ba}^{-1}((\bar{y}_a, \bar{\xi}_a)), \ C_b \supset C_a\}.$$

Due to (A.12), and due to $\lambda - \bar{\tau}^2 \notin \Lambda_1$, we deduce that $c_0 > 0$. Thus, there exists $\delta_1 > 0$ such that for all clusters b with $C_b \supset C_a$, and for all $\zeta \in \Sigma_b(\lambda)$ that satisfies $|y_a(\zeta) - \bar{y}_a| < \delta_1$, $|z^a(\zeta)| < \delta_1$, $|\tau(\zeta) - \bar{\tau}| < \delta_1$, we deduce that

$$-W_b\tau(\zeta) \geq 3c_0/2. \tag{A.14}$$

As mentioned above, our positive commutator estimate arises by considering functions of

$$\phi = \bar{\tau} - \tau + \frac{\beta}{\epsilon}(|z^a|^2 + |y_a - \bar{y}_a|^2), \tag{A.15}$$

where $\beta > 0$ will be fixed later and $\epsilon > 0$ is arbitrary as long as it is sufficiently small. Note that for all b with $C_b \supset C_a$, $W_b|z^a|^2 = 4z^a_b \cdot \xi^a_b$ under the decomposition $\xi_b = (\xi_a, \xi^a_b)$, so $W_b|z^a|^2 \leq C_1|z^a|$ on $\Sigma_b(\lambda)$, and similarly, possibly by increasing C_1, $|W_b(y_a - \bar{y}_a)^2| \leq C_1|y_a - \bar{y}_a|$.

Now suppose that

$$\phi \leq 2\epsilon,\ \bar{\tau} - \tau \geq -2\epsilon. \tag{A.16}$$

Then we conclude that

$$|\bar{\tau} - \tau| \leq 2\epsilon,\ |z^a| \leq 2\epsilon/\sqrt{\beta},\ |y_a - \bar{y}_a| \leq 2\epsilon/\sqrt{\beta}. \tag{A.17}$$

Let $\beta = (c_0/4C_1)^2$. For $\epsilon > 0$ small, (A.16) thus implies that $|y_a(\zeta) - \bar{y}_a| < \delta_1$, $|z^a(\zeta)| < \delta_1$, $|\tau(\zeta) - \bar{\tau}| < \delta_1$, so we deduce from (A.14) that

$$W_b\phi \geq -W_b\tau - 2\sqrt{\beta}C_1 > c_0,\ \text{where } \beta = (c_0/4C_1)^2. \tag{A.18}$$

The positive commutator estimate then arises by considering the following symbol q and quantizing it as in (3.9). 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

$$q = \chi_0(A_0^{-1}(2 - \phi/\epsilon))\chi_1((\bar{\tau} - \tau)/\epsilon + 2). \tag{A.19}$$

Thus, $q(\tilde{\zeta}) = \chi_0(2/A_0) > 0$, and on $\operatorname{supp} q$ we have

$$\phi \leq 2\epsilon \text{ and } \bar{\tau} - \tau \geq -2\epsilon, \tag{A.20}$$

which is (A.16), so $\operatorname{supp} q$ is a subset of (A.17). 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 by reducing ϵ, we can make q supported in an arbitrary small neighborhood of $\bar{y}_a$ and $\bar{\tau}_a$.

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

$$\tilde{q} = \tilde{\psi}(x)q. \tag{A.21}$$

Let A be the operator given by (3.9) with $\tilde{q}$ in place of q. Note that this includes a spectral cutoff in the definition of A.

The commutator $i[\Delta_{X_c}, A]$ is given to top order by $W_c q$. This is the commutator that gives microlocal positivity on the L^2 eigenspace of H^c, see e.g. the Froese-Herbst proof of the Mourre estimate [9]. We proceed to esimate $W_c q$ directly.

Thus,

$$\begin{aligned} W_c q = &-A_0^{-1}\epsilon^{-1}\chi_0'(A_0^{-1}(2 - \phi/\epsilon))\chi_1((\bar{\tau} - \tau)/\epsilon + 2)W_c\phi \\ &- \epsilon^{-1}\chi_0(A_0^{-1}(2 - \phi/\epsilon))\chi_1'((\bar{\tau} - \tau)/\epsilon + 2)W_c\tau. \end{aligned} \tag{A.22}$$

Then

$$W_c q = -\tilde{b}_c^2 + e_c \tag{A.23}$$

with

$$\tilde{b}_c^2 = A_0^{-1}\epsilon^{-1}\chi_0'(A_0^{-1}(2 - \phi/\epsilon))\chi_1((\bar{\tau} - \tau)/\epsilon + 2)W_c\phi. \tag{A.24}$$

Hence, with

$$b^2 = c_0 A_0^{-1}\epsilon^{-1}\chi_0'(A_0^{-1}(2 - \phi/\epsilon))\chi_1((\bar{\tau} - \tau)/\epsilon + 2), \tag{A.25}$$

we deduce that

$$W_c q \leq -b^2 + e_c. \tag{A.26}$$

Moreover,

$$b^2 \geq (c_0 A_0/16)q \tag{A.27}$$

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

$$\begin{aligned}\chi_0'(A_0^{-1}(2-\phi/\epsilon)) &= A_0^2(2-\phi/\epsilon)^{-2}\chi_0(A_0^{-1}(2-\phi/\epsilon))\\ &\geq (A_0^2/16)\chi_0(A_0^{-1}(2-\phi/\epsilon)).\end{aligned} \tag{A.28}$$

On the other hand, e_c is supported where

$$-2\epsilon \leq \bar{\tau} - \tau \leq -\epsilon,\ |y_a - \bar{y}_a|,\ |z^a| \leq 2\epsilon/\sqrt{\beta}. \tag{A.29}$$

By our assumption, this region is disjoint from $\mathrm{WF}_{\mathrm{Sc}}(u)$, if we choose $\epsilon > 0$ sufficiently small. Moreover, by (A.20), for $\epsilon > 0$ sufficiently small, we deduce from the inductive hypothesis that $\operatorname{supp} q$ (hence $\operatorname{supp} b$) is disjoint from $\mathrm{WF}_{\mathrm{Sc}}^{*,l}(u) \cap \dot{\Sigma}(\lambda)$.

Let $B \in \Psi_{\mathrm{Sc}}^{-\infty,0}(\bar{X}, \mathcal{C})$ be a quantization of $bq^{1/2}$ as in (3.9). Suppose that $M > 0$ and $\epsilon' > 0$. By choosing A_0 large, depending on M, ϵ', (using (A.28)), one can derive a positive commutator estimate from (A.26) using the many-body pseudodifferential calculus, see [35, End of proof of Proposition 7.1] for details. Apart from technical details it essentially corresponds to using the Mourre estimate and the functional calculus microlocally, namely that when localized in phase space in the region of interest, the commutator of a quantization of ϕ is positive. We deduce that there exists $\delta' > 0$, such that for $\psi \in \mathcal{C}_c^\infty(\mathbb{R})$ is supported in $(\lambda - \delta', \lambda + \delta')$, $\psi \equiv 1$ near λ, $E \in \Psi_{\mathrm{Sc}}^{-\infty,0}(\bar{X}, \mathcal{C})$, $F \in \Psi_{\mathrm{Sc}}^{-\infty,1}(\bar{X}, \mathcal{C})$ with $\mathrm{WF}'_{\mathrm{Sc}}(E), \mathrm{WF}'_{\mathrm{Sc}}(F)$ in a small neighborhood of $\dot{\Sigma}(\lambda)$,

$$\mathrm{WF}'_{\mathrm{Sc}}(E) \subset \operatorname{supp} e,\ \mathrm{WF}'_{\mathrm{Sc}}(F) \subset \operatorname{supp} q, \tag{A.30}$$

such that

$$\begin{aligned}i\psi(H)x^{-1/2}[A^*A, H]x^{-1/2}\psi(H) &- M\psi(H)A^*A\psi(H)\\ &\geq (2-2\epsilon')\psi(H)B^*B\psi(H) + E + F.\end{aligned} \tag{A.31}$$

By $\operatorname{supp} e$ we mean the support of the function $\chi_0(A_0^{-1}(2-\phi/\epsilon))\chi_1'((\bar{\tau}-\tau)/\epsilon + 2)$, which is independent of c in (A.22). Here F is the error term, it has first order decay, hence it is 'negligible'. On the other hand, E has the same order as B^*B, and it is negative (i.e. has the opposite sign of B^*B) in part of the phase space. As mentioned above, positive commutator estimates for approximate solutions u, i.e. $(H - \lambda)u$ microlocally Schwartz, work by estimating $\|B\psi(H)u\|^2$ in terms of $\langle u, Eu\rangle$ (plus error terms), i.e. u is estimated on $\operatorname{supp} b$ by its estimate on $\operatorname{supp} e$.

One can now use M, chosen sufficiently large, to deal with arbitrary weights $x^{-l-1/2}$. A standard commutator and regularization argument then proves that $x^{-l-1/2}Bu \in L^2(X_0)$, which in turn finishes the proof. We refer to [35, Proposition 7.1] for details.

Instead of following this route, we prove the corresponding resolvent estimate. So suppose that

$$u_t^+ = (H - (\lambda + it))^{-1}f,\ t > 0, \tag{A.32}$$

and $\mathrm{WF}_{\mathrm{Sc}}(f)$ is disjoint from the region of interest, and it is, say, in $\tau < \tau_0$, $\tau_0 > 0$ sufficiently small, so that u_t^+ converges to $(H - (\lambda + i0))^{-1}f$ as $t \to 0$ in sufficiently large weighted Sobolev spaces. As above, assume that u_t^+ is uniformly bounded in the region of interest in $H^{*,l}(X_0)$; we want to prove that it is also uniformly bounded in $H^{*,l+1/2}(X_0)$. For $\psi \in \mathcal{C}_c^\infty(\mathbb{R}; [0,1])$ supported sufficiently close to λ, with $A_l = A\psi(H)x^{-l-1}$, $B_l = x^{-l-1/2}B\psi(H)$, we deduce from (A.31) that

$$ix^{l+1/2}[A_l^*A_l, H]x^{l+1/2} \geq x^{l+1/2}((2-2\epsilon')B_l^*B_l + E_l + F_l)x^{l+1/2}, \quad \epsilon' > 0, \tag{A.33}$$

$E_l \in \Psi_{\mathrm{Sc}}^{-\infty,-2l-1}(\bar{X},\mathcal{C})$, $F_l \in \Psi_{\mathrm{Sc}}^{-\infty,-2l}(\bar{X},\mathcal{C})$, with similar properties as in (A.30). Since

$$\langle u_t^+, i[A_l^* A_l, H]u_t^+\rangle = -2\,\mathrm{Im}\langle u_t^+, A_l^* A_l(H-(\lambda+it))u_t^+\rangle - 2t\|A_l u_t^+\|^2, \tag{A.34}$$

we conclude that

$$\begin{aligned} \|B_l u_t^+\|^2 + 2t\|A_l u_t^+\|^2 \leq |\langle u_t^+, E_l u_t^+\rangle| + |\langle u_t^+, F_l u_t^+\rangle| \\ + 2|\langle u_t^+, A_l^* A_l(H-(\lambda+it))u_t^+\rangle|. \end{aligned} \tag{A.35}$$

Since $t>0$, the second term on the left hand side can be dropped. Since $u_t^+ \to u_+$ in $H^{0,l'}(X_0)$ for $l' < -1/2$, we conclude that for $l \in (-1,-1/2)$ the right hand side stays bounded as $t \to 0$, for u_t^+ is uniformly bounded in $H^{0,l+1/2}(X_0)$ on $\mathrm{WF}'_{\mathrm{Sc}}(E_l)$ and it is uniformly bounded in $H^{0,l}(X_0)$ on $\mathrm{WF}'_{\mathrm{Sc}}(F_l)$. Thus, $B_l u_t^+$ is uniformly bounded in $L^2(X_0)$, and as $u_t^+ \to u_+$ in $H^{0,l'}(X_0)$, we conclude that $B_l u_+ \in L^2(X_0)$.

□

The semiclassical version of the estimate (A.7) is

(A.36)
$$\begin{aligned} \|A(\chi_{U'}(y_0)\chi_{(-\delta_0/3,\delta_0/3)}(\tau-\bar{\tau}))u\|_{H_h^{r,s}} \leq C_1(\|A(\chi_U(y_0)\chi_{(\delta_0/3,\delta_0)}(\tau-\bar{\tau}))u\|_{H_h^{r,s}} \\ + h^{-1}\|A(\chi_U(y_0)\chi_{(-\delta_0/3,\delta_0)}(\tau-\bar{\tau}))(H-\lambda)u\|_{H_h^{r,s+1}} + \|u\|_{H_h^{r',s'}}). \end{aligned}$$

The proof of this proceeds just as above. Equation (A.31) is replaced by

$$\begin{aligned} i\psi(H)x^{-1/2}[A^*A, H(h)]x^{-1/2}\psi(H) - hM\psi(H(h))A^*A\psi(H(h)) \\ \geq (2-2\epsilon')h\psi(H(h))B^*B\psi(H(h)) + hE + h^2F, \end{aligned} \tag{A.37}$$

i.e. the principal terms B^*B and E have an extra factor of h (since the semiclassical calculus is commutative to top order in h), and the error term F has a gain of h. Note that $H(h) = \Delta + h^2 V$ shows that semiclassically V is two orders lower in h that Δ, which in fact significantly simplifies the argument that turns (A.26) into (A.31) (for sufficiently small h). Then (A.35) becomes, after dropping the second term on the left hand side and multiplying through by h^{-1},

$$\|B_l u_t^+\|^2 \leq |\langle u_t^+, E_l u_t^+\rangle| + h|\langle u_t^+, F_l u_t^+\rangle| + 2h^{-1}|\langle u_t^+, A_l^* A_l(H-(\lambda+it))u_t^+\rangle|, \tag{A.38}$$

and then one can finish the proof as before, using that u_t^+ is bounded by Ch^{-1}.

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