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Quantum scattering at low energies ☆

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Abstract

For a class of negative slowly decaying potentials, including $V(x) := -\gamma|x|^{-\mu}$ with $0 < \mu < 2$, we study the quantum mechanical scattering theory in the low-energy regime. Using appropriate modifiers of the Isozaki–Kitada type we show that scattering theory is well behaved on the *whole* continuous spectrum of the Hamiltonian, including the energy 0. We show that the modified scattering matrices $S(\lambda)$ are well-defined and strongly continuous down to the zero energy threshold. Similarly, we prove that the modified wave matrices and generalized eigenfunctions are norm continuous down to the zero energy if we use appropriate weighted spaces. These results are used to derive (oscillatory) asymptotics of the standard short-range and Dollard type S-matrices for the subclasses of potentials where both kinds of S-matrices are defined. For potentials whose leading part is $-\gamma|x|^{-\mu}$ we show that the location of singularities of the kernel of $S(\lambda)$ experiences an abrupt change from passing from positive energies λ to the limiting energy $\lambda = 0$. This change corresponds to the behaviour of the classical orbits. Under stronger conditions one can extract the leading term of the asymptotics of the kernel of $S(\lambda)$ at its singularities.

Keywords: Schrödinger operators; Wave operators; Scattering operator; WKB method

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Contents

1. Introduction and results

Scattering theory of 2-body systems, both classical and quantum, both short- and long-range, is nowadays a well understood subject [4,13,15,18,19,31,32]. In particular, for large natural classes of potentials we know a lot about the properties of wave and scattering matrices at positive energies. Zero – the only threshold energy – in most works on the subject is avoided, since scattering at zero energy is much more difficult to describe and strongly depends on the choice of the potential.

In this paper we consider a class of potentials that have an especially well behaved, nontrivial and interesting low energy scattering theory. Precise conditions used in our paper are described in Section 2. Roughly speaking, the potentials that we consider have a dominant negative radial term $V_1(x)$ similar to $-\gamma|x|^{-\mu}$ with $\gamma > 0$ and $0 < \mu < 2$, plus a faster decaying perturbation.

Similar classes of potentials appeared in the literature already in [10]. A systematic study of such 2-body systems at low energies was undertaken in [8], where a complete expansion of the resolvent at the zero-energy threshold was obtained, and in [6], where classical low-energy scattering theory was developed. This paper can be viewed as a continuation of [6,8].

In this paper we show that quantum scattering theory for such potentials is well behaved down to the energy zero. In particular, we study appropriately defined modified wave and scattering matrices for a fixed energy. We show that they have limits at zero energy. Our results were partly announced in [5].

Let us mention also our recent paper [7], where some closely related results about the zero-energy scattering matrix are proven for a class of radial potentials. [7] and this paper can be viewed as companion papers, even though they can be read independently.

For positive energies most (but probably not all) of our results are contained in the literature, scattered in many sources [13,15,18,19,31,32]. Almost all our material about the zero energy case is new.

In the introduction we will first review scattering for positive energies for a rather general class of potentials. Then we will describe a simplified version of the main results of our paper, which concerns scattering at low energies for a more restrictive class of potentials.

1.1. *Classical orbits at positive energies*

For the presentation of known results about positive energies we assume that the potentials satisfy the following condition:

Condition 1.1. $V = V_1 + V_3$ is a sum of real measurable functions on $\mathbb{R}^d$ such that V_1 is smooth and for some $\mu > 0$,

$$\partial_x^\alpha V_1(x) = O\big(|x|^{-\mu-|\alpha|}\big), \quad |\alpha| \geqslant 0, \tag{1.1}$$

V_3 is compactly supported and $V_3(H_0+1)^{-1}$ is a compact operator on the Hilbert space $L^2(\mathbb{R}^d)$. Here $H_0 := 2^{-1}p^2$ with $p := -\mathrm{i}\,\nabla_x$. The Hamiltonian $H = H_0 + V$ does not have positive eigenvalues.

Let us first consider the classical Hamiltonian $h_1(x,\xi) := \frac{1}{2}\xi^2 + V_1(x)$ on the phase space $\mathbb{R}^d \times \mathbb{R}^d$, using $h_0(x,\xi) := \frac{1}{2}\xi^2$ as the free Hamiltonian. (The analysis of the classical case is needed in the quantum case.) One can prove that for any $\xi \in \mathbb{R}^d$, $\xi \neq 0$, and x in an appropriate outgoing/incoming region the following problem admits a solution (strictly speaking, meaning one solution for $t \to +\infty$ and one for $t \to -\infty$):

$$\begin{cases} \ddot{y}(t) = -\nabla V_1(y(t)), \\ y(\pm 1) = x, \\ \xi = \lim_{t\to\pm\infty} \dot{y}(t). \end{cases} \tag{1.2}$$

One obtains a family $y^\pm(t,x,\xi)$ of solutions smoothly depending on parameters. All (positive energy) scattering orbits, i.e. orbits satisfying $\lim_{t\to\pm\infty}|y(t)| = \infty$, are of this form (the energy is $\lambda = \frac{1}{2}\xi^2$). Using these solutions, in an appropriate incoming/outgoing region one can construct a solution $\phi^\pm(x,\xi)$ to the eikonal equation

$$\frac{1}{2}\big(\nabla_x\phi^\pm(x,\xi)\big)^2 + V_1(x) = \frac{1}{2}\xi^2 \tag{1.3}$$

satisfying $\nabla_x\phi^\pm(x,\xi) = \dot{y}(\pm 1, x, \xi)$.

1.2. Wave and scattering matrices at positive energies

Let us turn to the quantum case. Following Isozaki–Kitada, see [18,19,25,31], one can use the functions $\phi^\pm(x,\xi)$ in the quantum case to construct appropriate modifiers, which can be taken to be

$$J^\pm f(x) := (2\pi)^{-d}\int \mathrm{e}^{\mathrm{i}\phi^\pm(x,\xi)-\mathrm{i}\xi\cdot y} a^\pm(x,\xi) f(y)\,\mathrm{d}y\,\mathrm{d}\xi. \tag{1.4}$$

Here $a^\pm(x,\xi)$ is an appropriate cut-off supported in the domain of the definition of $\phi^\pm$, equal to one in the incoming/outgoing region. Then one constructs modified wave operators

$$W^\pm f := \lim_{t\to\pm\infty} \mathrm{e}^{\mathrm{i}tH} J^\pm \mathrm{e}^{-\mathrm{i}tH_0} f, \quad \hat{f} \in C_c\big(\mathbb{R}^d \setminus \{0\}\big), \tag{1.5}$$

and the modified scattering operator

$$S = W^{+*}W^-. \tag{1.6}$$

We remark that $W^{\pm}$ are isometric with range given by the projection onto the continuous spectrum of H

$$1_{\mathrm{c}}(H)L^2(\mathbb{R}^d) = 1_{]0,\infty[}(H)L^2(\mathbb{R}^d).$$

(Whence S is unitary.)

Throughout our paper the modified wave operators $W^{\pm}$ and the modified scattering operators S defined using certain well chosen modifiers will be the main object of study. In what follows we will call them simply *wave and scattering operators*, dropping the word *modified*.

The free Hamiltonian H_0 can be diagonalized by the direct integral

$$\mathcal{H}_0 = \int_0^\infty \oplus L^2(S^{d-1})\,\mathrm{d}\lambda, \tag{1.7}$$

$$\mathcal{F}_0(\lambda)f(\omega) = (2\lambda)^{(d-2)/4}\hat{f}(\sqrt{2\lambda}\omega), \quad f \in L^2(\mathbb{R}^d). \tag{1.8}$$

Here $\hat{f}$ refers to the d-dimensional Fourier transform. The operator $\mathcal{F}_0(\lambda)$ can be interpreted as a bounded operator from the weighted space $L^{2,s}(\mathbb{R}^d) := \langle x\rangle^{-s}L^2(\mathbb{R}^d)$, $s > \frac{1}{2}$, to $L^2(S^{d-1})$. One can ask whether the wave and scattering operators can be restricted to a fixed energy λ.

This question is conceptually simpler in the case of the scattering operator S. Due to the intertwining property, $W^{\pm}H_0 = HW^{\pm}$ it satisfies $SH_0 = H_0S$, so abstract theory guarantees the existence of a decomposition

$$S \simeq \int_{]0,\infty[} \oplus S(\lambda)\,\mathrm{d}\lambda,$$

where $S(\lambda)$ are unitary operators on $L^2(S^{d-1})$ defined for almost all λ. One can prove that, under Condition 1.1, $S(\lambda)$ can be chosen to be a strongly continuous function (which fixes uniquely $S(\lambda)$ for all $\lambda \in]0,\infty[$). $S(\lambda)$ is called the *scattering matrix at the energy* λ.

The case of wave operators is somewhat more complicated. By the intertwining property it is natural to use the direct integral decomposition (1.7) only from the right and the question is whether we can give a rigorous meaning to $W^{\pm}\mathcal{F}_0(\lambda)^*$. Again, under Condition 1.1 one can show that there exists a unique strongly continuous function $]0,\infty[\, \ni \lambda \mapsto W^{\pm}(\lambda)$ with values in the space of bounded operators from $L^2(S^{d-1})$ to $L^{2,-s}(\mathbb{R}^d)$ with $s > \frac{1}{2}$ such that for $f \in L^{2,s}(\mathbb{R}^d)$

$$W^{\pm}f = \int_{]0,\infty[} W^{\pm}(\lambda)\mathcal{F}_0(\lambda)f\,\mathrm{d}\lambda.$$

The operator $W^{\pm}(\lambda)$ is called the *wave matrix at energy* λ. One can also extend the domain of $W^{\pm}(\lambda)$ so that it can act on the delta-function at $\omega \in S^{d-1}$, denoted δ_ω. Now $w^{\pm}(\omega,\lambda) := W^{\pm}(\lambda)\delta_\omega$ is an element of $L^{2,-p}(\mathbb{R}^d)$ for $p > \frac{d}{2}$. It satisfies

$$\left(-\frac{1}{2}\Delta + V(x) - \lambda\right)w^{\pm}(\omega,\lambda) = 0. \tag{1.9}$$

It behaves in the outgoing/incoming region as a plane wave. It will be called the *generalized eigenfunction of H at energy λ and at asymptotic normalized velocity ω*; this terminology is justified in Section 1.5.

1.3. Short-range wave and scattering operators

Let us recall that in the short-range case, that is $\mu > 1$, the standard definitions of wave and scattering operators are

$$W_{\mathrm{sr}}^{\pm} f := \lim_{t\to\pm\infty} \mathrm{e}^{\mathrm{i}tH}\mathrm{e}^{-\mathrm{i}tH_0} f, \tag{1.10}$$

$$S_{\mathrm{sr}} := W_{\mathrm{sr}}^{+*} W_{\mathrm{sr}}^{-}. \tag{1.11}$$

We will call $W_{\mathrm{sr}}^{\pm}$ and S the *standard short-range wave and scattering operators*. They differ from $W^{\pm}$ and S by a momentum-dependent phase factor:

$$W^{\pm} = W_{\mathrm{sr}}^{\pm} \mathrm{e}^{\mathrm{i}\psi_{\mathrm{sr}}^{\pm}(p)}, \tag{1.12}$$

$$S = \mathrm{e}^{-\mathrm{i}\psi_{\mathrm{sr}}^{+}(p)} S_{\mathrm{sr}} \mathrm{e}^{\mathrm{i}\psi_{\mathrm{sr}}^{-}(p)}. \tag{1.13}$$

Note that $W_{\mathrm{sr}}^{\pm}$ and S_{sr} are canonically defined given the potential V, whereas $W^{\pm}$, S are not. They depend on the phase functions $\phi^{\pm}$, which are non-canonical. Nevertheless, we will see that $W^{\pm}$ and S have better properties in the low energy regime than $W_{\mathrm{sr}}^{\pm}$ and S_{sr}.

1.4. Dollard wave and scattering operators

Similarly, in the case $\mu > \frac{1}{2}$ one can use the so-called Dollard construction:

$$W_{\mathrm{dol}}^{\pm} f := \lim_{t\to\pm\infty} \mathrm{e}^{\mathrm{i}tH} U_{\mathrm{dol}}(t) f, \tag{1.14}$$

$$U_{\mathrm{dol}}(t) := \mathrm{e}^{-\mathrm{i}\int_0^t (p^2/2 + V(sp)1_{\{|sp|\geqslant R_0\}})\,\mathrm{d}s}, \quad R_0 > 0, \tag{1.15}$$

$$S_{\mathrm{dol}} := W_{\mathrm{dol}}^{+*} W_{\mathrm{dol}}^{-}. \tag{1.16}$$

Analogously, we have

$$W^{\pm} = W_{\mathrm{dol}}^{\pm} \mathrm{e}^{\mathrm{i}\psi_{\mathrm{dol}}^{\pm}(p)}, \tag{1.17}$$

$$S = \mathrm{e}^{-\mathrm{i}\psi_{\mathrm{dol}}^{+}(p)} S_{\mathrm{sr}} \mathrm{e}^{\mathrm{i}\psi_{\mathrm{dol}}^{-}(p)}. \tag{1.18}$$

Dollard wave and scattering operators are non-canonical (they depend on R_0). Again, $W^{\pm}$ and S have better properties in the low energy regime than $W_{\mathrm{dol}}^{\pm}$ and S_{dol}.

1.5. Asymptotic normalized velocity operator

We mentioned above that the main objects of our study, $W^{\pm}$ and S are non-canonical, given the potential V. This does not mean that they have no physical content. The operator $W^{\pm}$ is an element of the family of incoming/outgoing wave operators, and S is an element of the family of scattering operators, which are canonically defined. In this subsection we briefly describe a possible definition of these families, following essentially [3,4].

Suppose that V satisfies (1.1) (or even much weaker conditions). Then it can be shown that there exists the following operator:

$$v^{\pm} := \mathrm{s}-\lim_{t\to\pm\infty} \pm \mathrm{e}^{\mathrm{i}tH}\hat{x}\mathrm{e}^{-\mathrm{i}tH}1_{\mathrm{c}}(H), \quad \hat{x} = \frac{x}{|x|}. \tag{1.19}$$

$v^{\pm}$ can be called the *asymptotic normalized velocity operator*. It is a vector of commuting self-adjoint operators (on the space $1_{\mathrm{c}}(H)L^2(\mathbb{R}^d)$) satisfying

$$\left(v^{\pm}\right)^2 = 1_{\mathrm{c}}(H), \qquad \left[v^{\pm}, H\right] = 0. \tag{1.20}$$

We say that $\breve{W}^{\pm}$ is *an outgoing/incoming wave operator associated with H* if it is isometric and satisfies

$$\breve{W}^{\pm}H_0 = H\breve{W}^{\pm}, \qquad \breve{W}^{\pm}\hat{p} = v^{\pm}\breve{W}^{\pm}, \tag{1.21}$$

where $\hat{p} = \frac{p}{|p|}$. We say that $\breve{S}$ is a scattering operator iff it is of the form $\breve{W}^{+*}\breve{W}^{-}$ for some wave operators $\breve{W}^{\pm}$.

Note that if $\breve{W}_1^{\pm}$ and $\breve{W}_2^{\pm}$ are two wave operators associated with a given H, then there exists a function $\psi^{\pm}$ such that

$$\breve{W}_1^{\pm} = \breve{W}_2^{\pm}\mathrm{e}^{\mathrm{i}\psi^{\pm}(p)}. \tag{1.22}$$

Therefore, scattering cross sections $|S(\lambda)(\omega,\omega')|^2$, which are usually considered to be the only measurable quantities in scattering theory, are insensitive to the choice of a scattering operator.

It is easy to show that $W^{\pm}$, $W^{\pm}_{\mathrm{sr}}$, $W^{\pm}_{\mathrm{dol}}$ are all wave operators in the sense of the above definition. Likewise, S, S_{sr}, S_{dol} are all scattering operators in the sense of the above definition.

Clearly, the standard short-range wave and scattering operators $W^{\pm}_{\mathrm{sr}}$, S_{sr} are canonically distinguished. However their definition is possible only if $\mu > 1$. In the long-range case, $\mu \leqslant 1$, apparently there are no distinguished wave and scattering operators. Therefore in the long-range case the families of wave and scattering operators as defined above seem to be the natural basic objects of scattering theory.

Nevertheless, as we will show in our paper, the operators $W^{\pm}$, S that we consider are useful also in the short-range case, even though they are non-canonical.

Let us remark in parenthesis that in the case of scattering on $[0,\infty[$, every unitary operator commuting with H_0 is a scattering operator according to our definition. Therefore, our definition of a scattering operator is not very interesting in this case. On $\mathbb{R}^d$, however, the families of wave operators and scattering operators defined above constitute nontrivial and interesting families of operators.

1.6. Low-energy asymptotics of classical orbits

In the remaining part of the introduction we consider a more restricted class of potentials. To simplify the presentation, in this introduction let us assume that the potential takes the form

$$V(x) = -\gamma|x|^{-\mu} + O\big(|x|^{-\mu-\epsilon}\big), \tag{1.23}$$

where $\mu \in]0,2[$ and $\gamma, \epsilon > 0$. For derivatives, assume that $\partial^\beta(V(x) + \gamma|x|^{-\mu}) = O(|x|^{-\mu-\epsilon-|\beta|})$. Compactly supported singularities can be included.

Let us note in parenthesis that in all our results, even though we suppose that the dominant part of the potential is radial, we allow for a non-radial perturbation. This lack of radial symmetry requires additional technical complications as compared with the radial case in some of our arguments, especially in [6]. We are convinced, however, that our results are interesting also in the purely radial case.

For potentials satisfying (1.23) we would like to extend the results described in Section 1.1 down to the energy $\lambda = 0$. To this end we change variables to "blow up" the discontinuity at $\lambda = 0$. This amounts to looking at $\xi = \sqrt{2\lambda}\omega$ as depending on two independent variables $\lambda \geqslant 0$ and $\omega \in S^{d-1}$. It is proven in [6] that for any $\omega \in S^{d-1}$, $\lambda \in [0, \infty[$ and x from an appropriate outgoing/incoming region there exists a solution of the problem

$$\begin{cases} \ddot{y}(t) = -\nabla V(y(t)), \\ \lambda = \frac{1}{2}\dot{y}(t)^2 + V(y(t)), \\ y(\pm 1) = x, \\ \omega = \pm \lim_{t\to\pm\infty} y(t)/|y(t)|. \end{cases} \tag{1.24}$$

One obtains a family $y^\pm(t, x, \omega, \lambda)$ of solutions smoothly depending on parameters. All scattering orbits are of this form. Using these solutions one can construct a solution $\phi^\pm(x, \omega, \lambda)$ to the eikonal equation

$$\frac{1}{2}\big(\nabla_x\phi^\pm(x, \omega, \lambda)\big)^2 + V(x) = \lambda \tag{1.25}$$

satisfying $\nabla_x\phi^\pm(x, \omega, \lambda) = \dot{y}(\pm 1, x, \omega, \lambda)$.

1.7. Low-energy asymptotics of wave and scattering matrices

In the quantum case, we can use the new functions $\phi^\pm(x, \omega, \lambda)$ in the modifiers $J^\pm$, which lead to the definitions of the wave operators $W^\pm$ and the scattering operator S. We can also improve on the choice of the symbols $a^\pm(x, \xi)$ by assuming that in the incoming/outgoing region they satisfy the appropriate transport equations.

The first main new result of our paper concerns wave operators and their corresponding wave matrices and is expressed in Theorems 6.5, 6.6 and Corollary 6.7. Its simplified version can be stated as follows:

Theorem 1.2. *There exists the norm limit of wave matrices at zero energy*:

$$W^\pm(0) = \lim_{\lambda\searrow 0} W^\pm(\lambda)$$

in the sense of operators in $\mathcal{B}(L^2(S^{d-1}), L^{2,-s}(\mathbb{R}^d))$, *where* $s > \frac{1}{2} + \frac{\mu}{4}$.

The operator $W^{\pm}(0)$ can be called *the wave matrix at zero energy*. We can introduce $w^{\pm}(\omega,0) := W^{\pm}(0)\delta_\omega$, called the *generalized eigenfunction of H at zero energy and fixed asymptotic normalized velocity ω*. It belongs to the weighted space $L^{2,-p}(\mathbb{R}^d)$ where $p > \frac{d}{2} + \frac{\mu}{2} - \frac{d\mu}{4}$. We shall also show weighted L^2-bounds on its ω-derivatives.

It is interesting to note that the behaviour of the generalized eigenfunction $w^{\pm}(\omega,0)$ depends strongly on the dimension. In dimension 1 it is unbounded, in dimension 2 it is almost bounded and in dimension greater than 2 it decays at infinity (without being square integrable).

The next main result of our paper concerns scattering matrices. It is given in Theorem 7.2. Its simplified version reads:

Theorem 1.3. *There exists the strong limit of scattering matrices at zero energy*

$$S(0) = \operatorname{s-}\lim_{\lambda \searrow 0} S(\lambda)$$

in the space $\mathcal{B}(L^2(S^{d-1}))$. This limit $S(0)$ is unitary on $L^2(S^{d-1})$.

We remark that neither $W(\lambda)$ nor $S(\lambda)$ are smooth in $\lambda \geqslant 0$ at the threshold 0, which can seem somewhat surprising given the fact that the boundary value of the resolvent $R(\lambda + \mathrm{i}0) = (H - \lambda - \mathrm{i}0)^{-1}$ (interpreted as acting between appropriate weighted spaces) has this property (see [2] for explicit expansions in the purely Coulombic case).

1.8. Geometric approach to scattering theory

There exists an alternative approach to scattering theory, based on the study of generalized eigenfunctions. It allows us to characterize scattering matrices by the spatial asymptotics of generalized eigenfunctions. It was used in particular in Vasy [26] or [27, Remark 19.12]. We shall study this approach, including the case of the zero energy, in Section 8.3.

1.9. Low energy asymptotics of short-range and Dollard operators

Let us stress again that the existence of the limits of wave and scattering matrices at zero energy is made possible not only by appropriate assumptions on the potentials, but also by the use of appropriate modifiers. Wave matrices $W^{\pm}_{\mathrm{sr}}(\lambda)$ defined by the standard short-range procedure, as well as the Dollard modified wave operators $W^{\pm}_{\mathrm{dol}}(\lambda)$, *do not* have this property. They differ from our $W^{\pm}(\lambda)$ by a momentum dependent phase factor that has an oscillatory behaviour as $\lambda \searrow 0$. In particular,

$$W^{\pm}_{\mathrm{sr}}(\lambda) = W^{\pm}(\lambda)\exp\bigl(\mathrm{i}\,O\bigl(\lambda^{\frac{1}{2}-\frac{1}{\mu}}\bigr)\bigr), \quad 1 < \mu < 2; \tag{1.26a}$$

$$W^{\pm}_{\mathrm{dol}}(\lambda) = W^{\pm}(\lambda)\exp\bigl(\mathrm{i}\,O\bigl(\lambda^{-\frac{1}{2}}\ln\lambda\bigr)\bigr), \quad \mu = 1; \tag{1.26b}$$

$$W^{\pm}_{\mathrm{dol}}(\lambda) = W^{\pm}(\lambda)\exp\bigl(\mathrm{i}\,O\bigl(\lambda^{\frac{1}{2}-\frac{1}{\mu}}\bigr)\bigr), \quad \frac{1}{2} < \mu < 1. \tag{1.26c}$$

By Theorem 1.2, we can replace $W^{\pm}(\lambda)$ with $W^{\pm}(0)$ in (1.26a), (1.26b) and (1.26c). Thus study of $W^{\pm}$ gives asymptotics of more conventional kinds of wave operators: $W^{\pm}_{\mathrm{sr}}$ and $W^{\pm}_{\mathrm{dol}}$.

We remark that scattering theory for slowly decaying potentials at low energies in the 1-dimensional setting was studied in [28] (for both negative and positive potentials). In particular, an oscillatory behaviour similar to (1.26a) was proved in dimension 1 in [28]. Thus applied to radially symmetric potentials our results concerning the low energy asymptotics of wave matrices have an overlap with [28]. The asymptotics (1.26b) and (1.26c) seem to be new.

1.10. Location of singularities of the zero energy scattering matrix

A recurrent idea of scattering theory is the parallel behaviour of classical and quantum systems. One of its manifestations is the relationship between scattering orbits at a given energy and the location of singularities of the scattering matrix.

In the case of positive energies the relationship is simple and well-known. To describe it note that scattering orbits of positive energy have the deflection angle that goes to zero when the distance of the orbit to the center goes to infinity. In the quantum case this corresponds to the fact that the integral kernel of scattering matrices $S(\lambda)(\omega,\omega')$ at positive energies λ are smooth for $\omega\neq\omega'$ and has a singularity at $\omega=\omega'$.

This picture changes at the zero energy. For potentials considered in our paper, the deflection angle of zero-energy orbits does not go to zero for orbits far from the center. The angle of deflection is small for small μ and goes to infinity as μ approaches 2.

For the strictly homogeneous potential, $V(r)=-\gamma r^{-\mu}$, one can solve the equations of motion at zero energy. The (non-collision) zero-energy orbits are given by the implicit equation (in polar coordinates)

$$\sin\left(1-\frac{\mu}{2}\right)\theta(t)=\left(\frac{r(t)}{r_{\mathrm{tp}}}\right)^{-1+\frac{\mu}{2}}, \tag{1.27}$$

see [6, Example 4.3]. Whence the deflection angle of such trajectories equals $-\frac{\mu\pi}{2-\mu}$. In particular, for attractive Coulomb potentials it equals $-\pi$, which corresponds to the well-known fact that in this case zero-energy orbits are parabolas (see [23, p. 126] for example).

One of the main results of our paper is a quantum analogue of this fact:

Theorem 1.4. *The integral kernel of the zero-energy scattering matrix $S(0)(\omega,\omega')$ is smooth away from ω,ω' satisfying $\omega\cdot\omega'=\cos\frac{\mu\pi}{2-\mu}$.*

We note that for the attractive Coulomb potential this result can be proven using known formulas (which can be found e.g. in [30]). In fact, in this case one can compute that $S(0)=\mathrm{e}^{\mathrm{i}c}P$, where $(P\tau)(\omega)=\tau(-\omega)$, as well as the following asymptotics

$$S_{\mathrm{dol}}(\lambda)=\mathrm{e}^{\mathrm{i}\lambda^{-1/2}\{C_1\ln\lambda+C_2+o(\lambda^0)\}}\big(P+o\big(\lambda^0\big)\big). \tag{1.28}$$

Note that Theorem 1.4 implies that the scattering cross section at zero energy $|S(0)(\omega,\omega')|^2$ can have a singularity only at $\omega\cdot\omega'=\cos\frac{\mu\pi}{2-\mu}$.

1.11. Kernel of $S(0)$ as an explicit oscillatory integral

In the case $V=-\gamma|x|^{-\mu}+O(|x|^{-1-\frac{\mu}{2}-\epsilon})$, $\epsilon>0$, it is possible to represent the distributional kernel of the scattering matrix $S(0)$ (modulo a smoothing term) in terms of a fairly explicit oscillatory integral. This provides an alternative way to prove Theorem 1.4 on the location of singularities of the scattering matrix – given the stronger conditions on the potential (we remark that our proof of Theorem 1.4 is rather abstract, see Section 1.13).

Let us remark that in [7], which can be viewed as a companion paper to this one, we present an independent study of the zero-energy scattering matrix for the class of *radial* potentials satisfying $V = -\gamma r^{-\mu} + O(r^{-1-\frac{\mu}{2}-\epsilon})$, $\epsilon > 0$. Using the 1-dimensional WKB-method, [7] gives an explicit formula for $S(0)$, up to a compact term.

1.12. Generalized eigenfunctions

A solution of the equation

$$\bigl(-\Delta + V(x) - \lambda\bigr)u = 0 \tag{1.29}$$

in $\bigcup_s L^{2,-s}(\mathbb{R}^d)$ will be called a *generalized eigenfunction with energy* λ. One of our results says that each generalized eigenfunction with positive or zero energy is of the form $W^{\pm}(\lambda)\tau$, where τ is a distribution on the sphere S^{d-1}.

Such generalized eigenfunctions are never square-integrable. A rough method to describe their behaviour for large x is to use weighted spaces $L^{2,s}(\mathbb{R}^d)$ with appropriate s. A more precise description is provided by the so-called *Besov spaces*. One of our results says that the range of (incoming and outgoing) wave matrices can be described precisely by an appropriate Besov space. One can also describe quite precisely their spatial asymptotics. In the case of zero energy, these results are new.

1.13. Propagation of singularities for zero-energy generalized eigenfunctions

It is well known that some of the properties of solutions of PDE's of the form $P(x, D)u = 0$ can be explained by the behaviour of classical Hamiltonian dynamics given by the principal symbol of P. One of the best known expressions of this idea is Hörmander's theorem about propagation of singularities.

Similar ideas are true in the case of Schrödinger operators. This is well understood for positive energies. In the case of zero energy a similar analysis is possible. It has an especially clean formulation if we assume that the potential is $V(x) = -\gamma|x|^{-\mu}$. Under this condition, the set of orbits of the classical system given by $h(x, \xi)$ is invariant with respect to an appropriate scaling. This allows us to reduce the phase space.

In the quantum case, we introduce an appropriate concept of a *wave front set* adapted to the solutions to (1.29), different from Hörmander's. One of our main results describes a possible location of this special wave front set for solutions to (1.29) for $\lambda = 0$ – the statement is very similar to the statement of the original Hörmander's theorem; it is used in a proof of Theorem 1.4.

1.14. Sommerfeld radiation condition

Another of our main results is a version of the Sommerfeld radiation condition for zero energies. It says that given v in a certain weighted space a solution u of the equation $(H - \lambda)u = v$ satisfying appropriate outgoing/incoming phase space localization is always of the form $u = R(\lambda \pm \mathrm{i}0)v$.

This somewhat technical result has a number of interesting applications. In particular, we use it in our proof that $S(0)$ can be expressed in terms of an oscillatory integral, and also in the description of the asymptotics of generalized eigenfunctions at large distances.

1.15. Organization of the paper

The paper is organized as follows: In Section 2 we impose conditions on the potential. In the case we allow the potential to have a non-spherically symmetric term we shall need certain regularity properties of the leading spherically symmetric term. These properties are stated in Condition 2.2; they are fulfilled for the example (1.23) discussed above.

In Section 3 we describe and extend some of results from our previous papers. In particular, we recall the construction of scattering phases in [6] (given there under the same conditions). We describe and to some extend the study of the properties of these objects.

In Section 4 we recall various microlocal resolvent estimates from [8] (slightly extended). We also introduce the concept of the scattering wave front set adapted to energy zero. We give its applications, in particular a result about the Sommerfeld radiation condition at zero energy.

In Section 5 we describe the modifiers used in our paper. They are given by a WKB-type ansatz, which involves solving transport equations.

In Section 6 we introduce wave operators and wave matrices. We describe their low-energy asymptotics.

In Section 7 we introduce scattering operators and matrices. We analyse their low-energy asymptotics.

In Section 8 we study properties of generalized eigenfunctions for non-negative energies.

In Section 9 we restrict our attention to potentials of the form (1.23). We show the classical rule, $\omega \cdot \omega' = \cos \frac{\mu}{2-\mu}\pi$, for the location of zero-energy singularities (cf. Theorem 1.4). We also show a "propagation of scattering singularities result", see Proposition 9.1, on generalized zero-energy eigenfunctions. Under stronger conditions than (1.23) we represent the kernel of $S(0)$ as an explicit oscillatory integral.

In Appendix A we present, in an abstract setting, various elements of stationary scattering theory used in our paper.

2. Conditions

We shall consider a classical Hamiltonian $h = \frac{1}{2}\xi^2 + V$ on $\mathbb{R}^d \times \mathbb{R}^d$ where V satisfies Condition 2.1 (in classical mechanics we can take $V_3 = 0$) and possibly Condition 2.2 (both stated below). Throughout the paper we shall use the non-standard notation $\langle x\rangle$ for $x \in \mathbb{R}^d$ to denote a function $\langle x\rangle = f(r)$; $r = |x|$, where here $f \in C^\infty([0,\infty[)$ is taken convex, and obeys $f = \frac{1}{2}$ for $r < \frac{1}{4}$ and $f = r$ for $r > 1$. We shall often use the notation $\hat{x} = x/r$ for vectors $x \in \mathbb{R}^d \setminus \{0\}$. Let $L^{2,s} = L^{2,s}(\mathbb{R}^d_x) = \langle x\rangle^{-s} L^2(\mathbb{R}^d_x)$ for any $s \in \mathbb{R}$ (the corresponding norm will be denoted by $\|\cdot\|_s$). Introduce also $L^{2,-\infty}(= L^{2,-\infty}(\mathbb{R}^d)) = \bigcup_{s\in\mathbb{R}} L^{2,s}$ and $L^{2,\infty} = \bigcap_{s\in\mathbb{R}} L^{2,s}$. The notation $F(s > \epsilon)$ denotes a smooth increasing function $= 1$ for $s > \frac{3}{4}\epsilon$ and $= 0$ for $s < \frac{1}{2}\epsilon$; $F(\cdot < \epsilon) := 1 - F(\cdot > \epsilon)$. The symbol g will be used extensively; it stands for the function $g(r) = \sqrt{2\lambda - 2V_1(r)}$ (for V_1 obeying Condition 2.1 and $\lambda \in [0,\infty[$).

Condition 2.1. The function V can be written as a sum of three real-valued measurable functions, $V = V_1 + V_2 + V_3$, such that, for some $\mu \in]0,2[$, we have:

(1) V_1 is a smooth negative function that only depends on the radial variable r in the region $r \geqslant 1$ (that is $V_1(x) = V_1(r)$ for $r \geqslant 1$). There exists $\epsilon_1 > 0$ such that

$$V_1(r) \leqslant -\epsilon_1 r^{-\mu}, \quad r \geqslant 1.$$

(2) For all $\gamma \in (\mathbb{N} \cup \{0\})^d$ there exists $C_\gamma > 0$ such that

$$\langle x \rangle^{\mu+|\gamma|} \big|\partial^\gamma V_1(x)\big| \leqslant C_\gamma.$$

(3) There exists $\tilde{\epsilon}_1 > 0$ such that

$$r V_1'(r) \leqslant -(2 - \tilde{\epsilon}_1) V_1(r), \quad r \geqslant 1. \tag{2.1}$$

(4) $V_2 = V_2(x)$ is smooth and there exists $\epsilon_2 > 0$ such that for all $\gamma \in (\mathbb{N} \cup \{0\})^d$

$$\langle x \rangle^{\mu+\epsilon_2+|\gamma|} \big|\partial^\gamma V_2(x)\big| \leqslant C_\gamma.$$

(5) $V_3 = V_3(x)$ is compactly supported.

The following condition will be needed only in the case $V_2 \neq 0$:

Condition 2.2. Let V_1 be given as in Condition 2.1 and $\alpha := \frac{2}{2+\mu}$. There exists $\bar{\epsilon}_1 > \max(0, 1 - \alpha(\mu + 2\epsilon_2))$ such that

$$\limsup_{r\to\infty} r^{-1} V_1'(r) \left(\int_1^r \big(-2V_1(\rho)\big)^{-\frac{1}{2}} \, \mathrm{d}\rho \right)^2 < 4^{-1}\big(1 - \bar{\epsilon}_1^2\big), \tag{2.2}$$

$$\limsup_{r\to\infty} V_1''(r) \left(\int_1^r \big(-2V_1(\rho)\big)^{-\frac{1}{2}} \, \mathrm{d}\rho \right)^2 < 4^{-1}\big(1 - \bar{\epsilon}_1^2\big). \tag{2.3}$$

We notice that (2.1) and (2.2) tend to be somewhat strong conditions for $\mu \approx 2$. On the other hand Conditions 2.1 and 2.2 hold for all $\epsilon_2 > 0$ for the particular example $V_1(r) = -\gamma r^{-\mu}$ (with $\epsilon_1 = \gamma$, $\tilde{\epsilon}_1 = 2 - \mu$ and some $\bar{\epsilon}_1 < 1 - \alpha\mu$).

In quantum mechanics we consider $H = H_0 + V$, $H_0 = \frac{1}{2} p^2$, $p = -\imath\nabla$, on $\mathcal{H} = L^2(\mathbb{R}^d)$, and we need the following additional condition. Clearly Condition 2.3(1) assures that H is self-adjoint. For an elaboration of Condition 2.3(2), see [8]; it guarantees that zero is not an eigenvalue of H. Condition 2.3(3) is included here only for convenience of presentation; with the other conditions there are no small positive eigenvalues, cf. [8].

Condition 2.3. In addition to Condition 2.1

(1) $V_3(H_0 + \imath)^{-1}$ is a compact operator on $L^2(\mathbb{R}^d)$.
(2) H satisfies the unique continuation property at infinity.
(3) H does not have positive eigenvalues.

3. Classical orbits

In this section we recall and extend the results of [6] about low energy classical orbits that we will need in our paper.

3.1. Scattering orbits at positive energies

We introduce for $R \geqslant 1$ and $\sigma > 0$

$$\Gamma^+_{R,\sigma}(\omega) = \{ y \in \mathbb{R}^d \mid y \cdot \omega \geqslant (1-\sigma)|y|,\ |y| \geqslant R \}; \quad \omega \in S^{d-1},$$
$$\Gamma^+_{R,\sigma} = \{ (y,\omega) \in \mathbb{R}^d \times S^{d-1} \mid y \in \Gamma^+_{R,\sigma}(\omega) \}.$$

Lemma 3.1. *Suppose that V_1 satisfies* (1.1). *Let $\sigma \in]0,2[$. Then there exists a decreasing function $]0,\infty[\ni \lambda \mapsto R_0(\lambda)$ such that for all $|\xi| \geqslant \sqrt{2\lambda}$ and $x \in \Gamma^+_{R_0(\lambda),\sigma}(\hat{\xi})$ there exists a unique solution $y(t) = y^+(t,x,\xi)$ of the problem* (1.2) *such that $y(t) \in \Gamma^+_{R_0(\lambda),\sigma}(\hat{\xi})$ for $t > 1$. If we set*

$$F^+(x,\xi) := \dot{y}^+(1,x,\xi),$$

then $\operatorname{rot}_x F^+(x,\xi) = 0$.

For any $\xi \neq 0$ we let $\lambda = 2^{-1}\xi^2$, $\omega = \hat{\xi}$ and $R = R_0(\lambda)$. For $(x,\omega) \in \Gamma^+_{R,\sigma}$ we choose a path $[0,1] \ni l \mapsto \gamma(l) \in \Gamma^+_{R,\sigma}(\omega)$ such that $\gamma(0) = R\omega$ and $\gamma(1) = x$. We set

$$\phi^+(x,\xi) := \int_0^1 F^+\big(\gamma(l), \sqrt{2\lambda}\omega\big) \cdot \frac{\mathrm{d}\gamma(l)}{\mathrm{d}l}\,\mathrm{d}l + \sqrt{2\lambda}R.$$

Note that $\phi^+(x,\xi)$ does not depend on the choice of the path γ. For instance, we can take the interval joining these two points and then

$$\phi^+(x,\xi) = (x - R\omega) \cdot \int_0^1 F^+\big(l(x-R\omega) + R\omega, \sqrt{2\lambda}\omega\big)\,\mathrm{d}l + \sqrt{2\lambda}R. \tag{3.1}$$

Another possible choice is the radial interval from $R\omega$ to $|x|\omega$ and then the arc towards x:

$$\phi^+(x,\xi) = \int_R^{|x|} F^+\big(l\omega, \sqrt{2\lambda}\omega\big) \cdot \omega\,\mathrm{d}l + \int_0^{\arccos \omega\cdot\hat{x}} F^+\big(|x|v_\alpha, \sqrt{2\lambda}\omega\big) \cdot |x| \frac{\mathrm{d}v_\alpha}{\mathrm{d}\alpha}\,\mathrm{d}\alpha + \sqrt{2\lambda}R, \tag{3.2}$$

where $v_\alpha := \cos\alpha\,\omega + \sin\alpha \frac{\hat{x} - \omega\ \omega\cdot\hat{x}}{\sqrt{1-(\omega\cdot\hat{x})^2}}$.

The phase function constructed above essentially coincides with the Isozaki Kitada (outgoing) phase function, cf. [16], [18, Definition 2.3] or [4, Proposition 2.8.2]. In particular, for any $\xi \neq 0$, there are bounds

$$\partial_\xi^\kappa \partial_x^\gamma \big(\phi^+(x,\xi) - \xi \cdot x\big) = O\big(|x|^{\delta - |\gamma|}\big) \quad \text{for } |x| \to \infty, \qquad \delta > \max(1-\mu, 0). \tag{3.3}$$

These bounds are not uniform in $\xi \neq 0$, they are however uniform on compact subsets of $\mathbb{R}^d \setminus \{0\}$.

3.2. Scattering orbits at low energies

Let us now recall some results about scattering orbits taken from [6].

We assume Conditions 2.1 and 2.2 (only Condition 2.1 if $V_2 = 0$). The fact that our Condition 2.1 includes a possibly singular potential V_3 is irrelevant for this subsection since by assumption this term is compactly supported. More precisely we just need to make sure that the $R_0 \geqslant 1$ in Lemma 3.2 stated below is taken so large that $V_3(x) = 0$ for $|x| \geqslant R_0$, then [6] applies.

Lemma 3.2. *There exist $R_0 \geqslant 1$ and $\sigma_0 > 0$ such that for all $R \geqslant R_0$ and for all positive $\sigma \leqslant \sigma_0$ the problem* (1.24) *is solved for all data $(x,\omega) \in \Gamma^+_{R,\sigma}$ and $\lambda \geqslant 0$ by a unique function $y^+(t,x,\omega,\lambda)$, $t \geqslant 1$, such that $y^+(t,x,\omega,\lambda) \in \Gamma^+_{R,\sigma}(\omega)$ for all $t \geqslant 1$. Define a vector field $F^+(x,\omega,\lambda)$ on $\Gamma^+_{R_0,\sigma_0}(\omega)$ by*

$$F^+(x,\omega,\lambda) = \dot{y}^+(t=1; x,\omega,\lambda). \tag{3.4}$$

Then

$$\mathrm{rot}_x F^+(x,\omega,\lambda) = 0.$$

Note that under the assumptions of Lemma 3.2, we can suppose that $R_0(\lambda)$, introduced in Lemma 3.1, equals R_0 for all $\lambda > 0$. We can define $\phi^+(x,\omega,\lambda)$ on $(x,\omega,\lambda) \in \Gamma^+_{R,\sigma} \times [0,\infty[$. For further reference let us record the analogues of (3.1) and (3.2):

$$\phi^+(x,\omega,\lambda) = (x - R_0\omega) \cdot \int_0^1 F^+\big(l(x-R_0\omega) + R_0\omega, \omega, \lambda\big)\,\mathrm{d}l + \sqrt{2\lambda}R_0,$$

$$\phi^+(x,\omega,\lambda) = \int_{R_0}^{|x|} F^+(l\omega,\omega,\lambda)\cdot\omega\,\mathrm{d}l + \int_0^{\arccos \omega\cdot\hat{x}} F^+\big(|x|v_\alpha,\omega,\lambda\big)\cdot\frac{\mathrm{d}v_\alpha}{\mathrm{d}\alpha}\,\mathrm{d}\alpha + \sqrt{2\lambda}R_0.$$

We will add the subscript "sph" to all objects where V is replaced by the (spherically symmetric) potential V_1. The following result is proven in [6]:

Proposition 3.3. *There exists $\check{\epsilon} = \check{\epsilon}(\mu, \bar{\epsilon}_1, \epsilon_2) > 0$ and uniform bounds*

$$F^+(x) - F^+_{\mathrm{sph}}(x) = O\big(|x|^{-\mu/2 - \check{\epsilon}}\big). \tag{3.5a}$$

In particular, for constants $C, c > 0$ *independent of* x, ω *and* λ

$$\left|\frac{F^+(x)}{|F^+(x)|} - \frac{F^+_{\rm sph}(x)}{|F^+_{\rm sph}(x)|}\right| \leqslant C|x|^{-\breve{\epsilon}}, \tag{3.5b}$$

and

$$\frac{F^+(x)}{|F^+(x)|} \cdot \hat{x} \geqslant 1 - C(1 - \hat{x} \cdot \omega) - C|x|^{-\breve{\epsilon}}, \tag{3.5c}$$

$$\frac{F^+(x)}{|F^+(x)|} \cdot \hat{x} \leqslant 1 - c(1 - \hat{x} \cdot \omega) + C|x|^{-\breve{\epsilon}}, \tag{3.5d}$$

$$\frac{F^+(x)}{|F^+(x)|} \cdot \omega \geqslant 1 - C(1 - \hat{x} \cdot \omega) - C|x|^{-\breve{\epsilon}}. \tag{3.5e}$$

More generally (*with the same* $\breve{\epsilon} > 0$)*, for all multiindices* δ *and* γ *there are uniform bounds*

$$\partial_\omega^\delta \partial_x^\gamma F^+(x) = \langle x\rangle^{-|\gamma|} O\big(g\big(|x|\big)\big), \tag{3.5f}$$

$$\partial_\omega^\delta \partial_x^\gamma \big(F^+(x) - F^+_{\rm sph}(x)\big) = \langle x\rangle^{-\breve{\epsilon}-|\gamma|} O\big(g\big(|x|\big)\big). \tag{3.5g}$$

The vector field $F^+(x, \omega, \lambda)$*, as well as all derivatives* $\partial_\omega^\delta \partial_x^\gamma F^+$*, are jointly continuous in the variables* $(x, \omega) \in \Gamma^+_{R_0,\sigma_0}$ *and* $\lambda \geqslant 0$*.*

The problem (1.24) in the case of $t \to -\infty$ can also be solved. We introduce for $R \geqslant 1$ and $\sigma > 0$

$$\Gamma^-_{R,\sigma}(\omega) = \big\{y \in \mathbb{R}^d \;\big|\; y \cdot \omega \leqslant (\sigma - 1)|y|,\ |y| \geqslant R\big\}, \quad \omega \in S^{d-1};$$
$$\Gamma^-_{R,\sigma} = \big\{(y, \omega) \in \mathbb{R}^d \times S^{d-1} \;\big|\; y \in \Gamma^-_{R,\sigma}(\omega)\big\}.$$

Mimicking the previous procedure, starting from the mixed problem (1.24) in the case of $t \to -\infty$, we can similarly construct a solution $\phi^-(x, \omega, \lambda)$ to the eikonal equation in some $\Gamma^-_{R,\sigma}(\omega)$. This amounts to setting

$$\phi^-(x, \omega, \lambda) = -\phi^+(x, -\omega, \lambda), \quad x \in \Gamma^-_{R_0,\sigma_0}(\omega) = \Gamma^+_{R_0,\sigma_0}(-\omega). \tag{3.6}$$

3.3. Radially symmetric potentials

In this subsection we assume that $V_2 = 0$, which means that the potential is spherically symmetric. More precisely, we assume that for $r \geqslant R_0$

$$\big|\partial_r^n V(r)\big| \leqslant c_n r^{-n-\mu}, \qquad V(r) \leqslant -cr^{-\mu}, \quad c > 0, \qquad rV'(r) + 2V(r) < 0.$$

Note that motion in such a potential is confined to a 2-dimensional plane. In the case of the trajectory $y^+(t, x, \omega, \lambda)$, it is the plane spanned by ω and $\hat{x}$. It is also convenient to introduce the vectors $x^\perp := \frac{\omega - \cos\theta_1 \hat{x}}{\sin\theta_1}$ and $\omega^\perp := \frac{\hat{x} - \cos\theta_1 \omega}{\sin\theta_1}$, where $\omega \cdot \hat{x} = \cos\theta_1$. Therefore, we can restrict temporarily our attention to a 2-dimensional system. We will use the polar coordinates $(r\cos\theta, r\sin\theta)$. Note that the energy λ and the angular momentum L are preserved quantities. Therefore, the Newton equations (for outgoing orbits) can be reduced to

$$\begin{cases} \dot{\theta} = Lr^{-2}, \\ \dot{r} = \sqrt{2\lambda - 2V(r) - L^2 r^{-2}}. \end{cases} \tag{3.7}$$

Lemma 3.4. *For some $\theta_0 > 0$, for all $r_1 \geqslant R_0$, $|\theta_1| \leqslant \theta_0$ and $\lambda \geqslant 0$ we can find a solution of* (3.7) *satisfying*

$$r(1) = r_1, \qquad \dot{r}(1) > 0, \qquad \lim_{t \to \infty} \theta(t) = 0, \qquad \theta(1) = \theta_1.$$

There exists a function $(r_1, \theta_1, \lambda) \mapsto L(r_1, \theta_1, \lambda) \in \mathbb{R}$ specifying the total angular momentum of the solution $y^+(t, x, \omega, \lambda)$. This function L is an odd function in θ_1. We have the following estimates:

$$\partial_{r_1}^n \partial_{\theta_1^2}^m L^2 = O\big(r_1^{2-n} g(r_1)^2\big), \quad n, m \geqslant 0; \tag{3.8a}$$

$$\partial_{r_1}^n \partial_{\theta_1^2}^m \frac{L}{\theta_1} = O\big(r_1^{1-n} g(r_1)\big), \quad n, m \geqslant 0. \tag{3.8b}$$

This allows us to compute the initial velocity of the trajectory:

$$F^+(x, \omega, \lambda) = \sqrt{2\lambda - 2V(r) - L^2/r^2}\,\hat{x} - \frac{L}{r} x^\perp.$$

The function ϕ^+ equals, with $r = |x|$ and $\cos\theta = \hat{x} \cdot \omega$,

$$\phi^+(x, \omega, \lambda) = \sqrt{2\lambda} R_0 + \int_{R_0}^{r} \sqrt{2\lambda - 2V(r')}\, \mathrm{d}r' + \int_0^{\theta} L(r, \theta', \lambda)\, \mathrm{d}\theta'. \tag{3.9}$$

Therefore, using also that $\nabla_\omega \theta = -\omega^\perp$,

$$\nabla_\omega \phi^+ = -L(r, \theta, \lambda)\omega^\perp. \tag{3.10}$$

This gives the following estimates (in any dimension):

Lemma 3.5. *There exist constants $C, c > 0$ such that*

$$\big|\hat{x} \cdot F^+(x) - g\big(|x|\big)\big| \leqslant C(1 - \hat{x} \cdot \omega) g\big(|x|\big), \tag{3.11a}$$

$$\big|F^+(x) - \hat{x}\hat{x} \cdot F^+(x)\big| \leqslant C\sqrt{1 - \hat{x} \cdot \omega}\, g\big(|x|\big), \tag{3.11b}$$

$$\big|\nabla_\omega \phi^+\big| \geqslant c\sqrt{1 - \hat{x} \cdot \omega}\, g\big(|x|\big)|x|, \tag{3.11c}$$

$$\partial_\omega^\delta \partial_x^\gamma \phi^+ = \langle x \rangle^{1-|\gamma|} O\big(g\big(|x|\big)\big). \tag{3.11d}$$

We calculate for $\lambda > 0$:

$$\nabla_\xi F^+ = (2\lambda)^{-\frac{1}{2}} \nabla_\omega F^+ + (2\lambda)^{\frac{1}{2}} \partial_\lambda F^+ \otimes \omega,$$

$$\nabla_\omega F^+ = L\partial_\theta L\big(2\lambda - 2V(r) + L^2 r^{-2}\big)^{-\frac{1}{2}} r^{-2} \omega^\perp \otimes \hat{x} + \partial_\theta L r^{-1} \omega^\perp \otimes x^\perp - \frac{L}{r} \nabla_\omega x^\perp,$$

$$\partial_\lambda F^+ = \big(2\lambda - 2V(r) - L^2 r^{-2}\big)^{-\frac{1}{2}} \big(1 - L\partial_\lambda L r^{-2}\big)\hat{x} - \partial_\lambda L r^{-1} x^\perp.$$

Specifying to x parallel to ω and noting that $L(x, \hat{x}, \lambda) = 0$, we obtain

$$\begin{aligned}
\nabla_\xi F^+ &= (2\lambda)^{1/2} \partial_\lambda \big(2\lambda - 2V\big(|x|\big)\big)^{1/2} \hat{x} \otimes \hat{x} - (2\lambda)^{-1/2} |x|^{-1} \partial_\theta L\, x^\perp \otimes x^\perp \\
&= (2\lambda)^{1/2} \big(2\lambda - 2V\big(|x|\big)\big)^{-1/2} \hat{x} \otimes \hat{x} \\
&\quad + (2\lambda)^{-1/2} |x|^{-1} \left(\int_{|x|}^{\infty} r^{-2} \big(2\lambda - 2V(r)\big)^{-1/2} \,\mathrm{d}r \right)^{-1} x^\perp \otimes x^\perp,
\end{aligned} \tag{3.12}$$

cf. [6, (4.5)].

In an arbitrary dimension, the formula is the same except that the second term is repeated $d - 1$ times on the diagonal. Therefore,

$$\det\big(\nabla_\xi \nabla_x \phi^+\big(x, \sqrt{2\lambda}\hat{x}\big)\big)^{1/2} = (2\lambda)^{(2-d)/4} g(r)^{-1/2} \big(r^{-1} h(r)\big)^{(d-1)/2}, \tag{3.13}$$

where we have introduced the notation

$$h(r) := \left(\int_r^\infty r'^{-2} g(r')^{-1} \,\mathrm{d}r' \right)^{-1}. \tag{3.14}$$

Note the (uniform) bounds

$$crg(r) \leqslant h(r) \leqslant Crg(r). \tag{3.15}$$

Whence, combining (3.13) and (3.15),

$$\begin{aligned}
c(2\lambda)^{(2-d)/4} g(r)^{(d-2)/2} &\leqslant \det\big(\nabla_\xi \nabla_x \phi^+\big(x, \sqrt{2\lambda}\hat{x}\big)\big)^{1/2} \\
&\leqslant C(2\lambda)^{(2-d)/4} g(r)^{(d-2)/2}.
\end{aligned} \tag{3.16}$$

4. Boundary values of the resolvent

In this section we impose Conditions 2.1 and 2.3. We shall recall (and extend) some resolvent estimates of [8]. They are important tools used throughout our paper.

In Section 4.2 we will also introduce the notion of the scattering wave front set, which is well adapted to scattering theory at various energies. We will return to this concept in particular in Section 9, where we will prove a theorem about propagation of singularities for potentials with a homogeneous principal part. A somewhat cruder version of this theorem is given already in Section 4.2 (valid, however, for a more general class of potentials).

In Section 4.4 we prove a version of the Sommerfeld radiation condition for the zero energy.

4.1. Low energy resolvent estimates

Let c be a function on the phase space $\mathbb{R}^d \times \mathbb{R}^d$. The left and right Kohn–Nirenberg quantization of the symbol c are the operators $\mathrm{Op}^{\mathrm{l}}(c)$ and $\mathrm{Op}^{\mathrm{r}}(c)$ acting as

$$\big(\mathrm{Op}^{\mathrm{l}}(c)f\big)(x) = (2\pi)^{-d/2}\int \mathrm{e}^{\mathrm{i}x\cdot\xi}c(x,\xi)\hat{f}(\xi)\,\mathrm{d}\xi,$$

$$\big(\mathrm{Op}^{\mathrm{r}}(c)f\big)(x) = (2\pi)^{-d}\iint \mathrm{e}^{\mathrm{i}(x-y)\cdot\xi}c(y,\xi)f(y)\,\mathrm{d}y\,\mathrm{d}\xi,$$

respectively. Notice that $\mathrm{Op}^{\mathrm{l}}(c)^* = \mathrm{Op}^{\mathrm{r}}(\bar{c})$. In Proposition 4.1 stated below we use for convenience both of these quantizations, although they can be used interchangeably. Alternatively one can use Weyl quantization denoted by $\mathrm{Op}^{\mathrm{w}}(c)$, cf. [8]. We will often use the following (λ-dependent) symbols:

$$a(x,\xi) = \frac{\xi^2}{g(|x|)^2}, \qquad b(x,\xi) = \frac{\xi}{g(|x|)}\cdot\frac{x}{\langle x\rangle}. \tag{4.1}$$

It is convenient to introduce the following symbol class: Let $c \in S(m, g_{\mu,\lambda})$, $g_{\mu,\lambda} = \langle x\rangle^{-2}\,\mathrm{d}x^2 + g^{-2}\,\mathrm{d}\xi^2$ and $m = m_\lambda = m_\lambda(x,\xi)$ be a uniform weight function [12]. Here $\lambda \in [0,\lambda_0]$ (for an arbitrarily fixed $\lambda_0 > 0$) is considered as a parameter; the function m obeys bounds uniform in this parameter (see [8, Lemma 4.3(ii)] for details). For a uniform weight function m, the symbol class $S_{\mathrm{unif}}(m, g_{\mu,\lambda})$ is defined to be the set of parameter-dependent smooth symbols $c = c_{\omega,\lambda}$ satisfying

$$\big|\partial_\omega^\delta \partial_x^\gamma \partial_\xi^\beta c_{\omega,\lambda}(x,\xi)\big| \leqslant C_{\delta,\gamma,\beta} m_\lambda(x,\xi)\langle x\rangle^{-|\gamma|}g^{-|\beta|}. \tag{4.2}$$

We notice that the "Planck constant" for this class is $\langle x\rangle^{-1}g^{-1}$. The corresponding class of quantizations is denoted by $\Psi_{\mathrm{unif}}(m, g_{\mu,\lambda})$ (it does not depend on whether left or right quantization is used). Finally we remark that the quantizations appearing in Proposition 4.1 stated below belong to $\Psi_{\mathrm{unif}}(1, g_{\mu,\lambda})$, and hence they are bounded uniformly in λ (these symbols are independent of ω).

We can obtain the following estimates by mimicking the proof of [8, Theorem 4.1] (first for the smooth case $V_3 = 0$, and then the general case by a resolvent equation, see [8, Subsection 5.1]; here the unique continuation assumption Condition 2.3(2) comes into play). In particular, Proposition 4.1(i) follows from [8, Corollary 3.5] and a resolvent identity (cf. [8, (5.12)]). Similarly Proposition 4.1(ii) follows from [8, Lemma 4.5] and the proof of [8, Lemma 4.6] (notice that it suffices to show the bounds (4.3b) and (4.3c) for $t = 0$ due to this proof), while Proposition 4.1(iii) follows from [8, Lemma 4.9] and the same minor modification of the proof of [8, Lemma 4.6]. As for the continuity statement at the end of the proposition we refer the reader to the end of this subsection.

The notation $R(\lambda + \mathrm{i}0)$ refers to the limit of the resolvent $R(\lambda + \mathrm{i}\epsilon)$ as $\epsilon \to 0^+$ in the sense of a form on the Schwartz space $\mathcal{S}(\mathbb{R}^d)$, cf. Remark 4.2(2).

Proposition 4.1. *Fix any $\lambda_0 > 0$. The following conclusions,* (i)–(v)*, hold uniformly in $\lambda \in [0, \lambda_0]$:*

(i) *For all $\delta > \frac{1}{2}$ there exists $C > 0$ such that*

$$\left\| \langle x\rangle^{-\delta} g^{\frac{1}{2}} R(\lambda + \mathrm{i}0) g^{\frac{1}{2}} \langle x\rangle^{-\delta} \right\| \leqslant C. \tag{4.3a}$$

(ii) *There exists $C_0 \geqslant 1$ such that if $\chi_+ \in C^\infty(\mathbb{R})$,* $\operatorname{supp}(\chi_+) \subset]C_0, \infty[$ *and $\chi_+' \in C_c^\infty(\mathbb{R})$, then for all $\delta > \frac{1}{2}$ and all $s, t \geqslant 0$ there exists $C > 0$ such that*

$$\left\| \big(\langle x\rangle g\big)^{s} \langle x\rangle^{t-\delta} g^{\frac{1}{2}} \operatorname{Op}^{\mathrm{l}}\big(\chi_+(a)\big) R(\lambda + \mathrm{i}0) g^{\frac{1}{2}} \langle x\rangle^{-t-\delta} \big(\langle x\rangle g\big)^{-s} \right\| \leqslant C, \tag{4.3b}$$

$$\left\| \big(\langle x\rangle g\big)^{-s} \langle x\rangle^{-t-\delta} g^{\frac{1}{2}} R(\lambda + \mathrm{i}0) \operatorname{Op}^{\mathrm{r}}\big(\chi_+(a)\big) g^{\frac{1}{2}} \langle x\rangle^{t-\delta} \big(\langle x\rangle g\big)^{s} \right\| \leqslant C. \tag{4.3c}$$

(iii) *Let $\bar\sigma > 0$ and $\chi_- \in C_c^\infty(\mathbb{R})$. Suppose $\tilde\chi_-, \tilde\chi_+ \in C^\infty(\mathbb{R})$ satisfy*

$$\sup\operatorname{supp}\tilde\chi_- \leqslant 1 - \bar\sigma, \qquad \inf\operatorname{supp}\tilde\chi_+ \geqslant \bar\sigma - 1.$$

Then for all $\delta > \frac{1}{2}$ and all $s, t \geqslant 0$ there exists $C > 0$ such that

$$\left\| \big(\langle x\rangle g\big)^{s} \langle x\rangle^{t-\delta} g^{\frac{1}{2}} \operatorname{Op}^{\mathrm{l}}\big(\chi_-(a)\tilde\chi_-(b)\big) R(\lambda + \mathrm{i}0) g^{\frac{1}{2}} \langle x\rangle^{-t-\delta} \big(\langle x\rangle g\big)^{-s} \right\| \leqslant C, \tag{4.3d}$$

$$\left\| \big(\langle x\rangle g\big)^{-s} \langle x\rangle^{-t-\delta} g^{\frac{1}{2}} R(\lambda + \mathrm{i}0) \operatorname{Op}^{\mathrm{r}}\big(\chi_-(a)\tilde\chi_+(b)\big) g^{\frac{1}{2}} \langle x\rangle^{t-\delta} \big(\langle x\rangle g\big)^{s} \right\| \leqslant C. \tag{4.3e}$$

(iv) *Suppose $\chi_-^1, \chi_-^2 \in C_c^\infty(\mathbb{R})$, $\tilde\chi_-$ and $\tilde\chi_+$ satisfy the assumptions from* (3) *and in addition*

$$\sup\operatorname{supp}\tilde\chi_- < \inf\operatorname{supp}\tilde\chi_+.$$

Then for all $s \geqslant 0$ there exists $C > 0$ such that

$$\left\| \langle x\rangle^{s} \operatorname{Op}^{\mathrm{l}}\big(\chi_-^1(a)\tilde\chi_-(b)\big) R(\lambda + \mathrm{i}0) \operatorname{Op}^{\mathrm{r}}\big(\chi_-^2(a)\tilde\chi_+(b)\big) \langle x\rangle^{s} \right\| \leqslant C. \tag{4.3f}$$

(v) *Suppose χ_+ is given as in* (2)*, some functions $\tilde\chi_+, \tilde\chi_-, \chi_-$ are given as in* (3) *and suppose*

$$\operatorname{dist}(\operatorname{supp}\chi_-, \operatorname{supp}\chi_+) > 0.$$

Then for all $s \geqslant 0$ there exists $C > 0$ such that

$$\left\| \langle x\rangle^{s} \operatorname{Op}^{\mathrm{l}}\big(\chi_+(a)\big) R(\lambda + \mathrm{i}0) \operatorname{Op}^{\mathrm{r}}\big(\chi_-(a)\tilde\chi_+(b)\big) \langle x\rangle^{s} \right\| \leqslant C, \tag{4.3g}$$

$$\left\| \langle x\rangle^{s} \operatorname{Op}^{\mathrm{l}}\big(\chi_-(a)\tilde\chi_-(b)\big) R(\lambda + \mathrm{i}0) \operatorname{Op}^{\mathrm{r}}\big(\chi_+(a)\big) \langle x\rangle^{s} \right\| \leqslant C. \tag{4.3h}$$

All the forms appearing in (i)–(v) *are continuous in $\lambda \geqslant 0$. In fact the families of corresponding operators are continuous $\mathcal{B}(L^2(\mathbb{R}^d))$-valued functions.*

Remarks 4.2.

(1) Although this will not be needed we have in fact (2) with $C_0 = 1$; see Corollary 4.4 for a related result.

(2) The paper [8] contains a stronger version of the so-called limiting absorption principle than can be read from Proposition 4.1(i): For all $\delta > \frac{1}{2}$ there exists $C > 0$ such that

$$\sup_{\lambda+\mathrm{i}\epsilon\in M} \left\| \langle x\rangle^{-\delta} g^{\frac{1}{2}} R(\lambda+\mathrm{i}\epsilon) g^{\frac{1}{2}} \langle x\rangle^{-\delta} \right\| \leqslant C; \qquad M := [0,\lambda_0]\times \mathrm{i}\,]0,1],$$

and the $\mathcal{B}(L^2(\mathbb{R}^d)$-valued function $\langle x\rangle^{-\delta-\frac{\mu}{4}} R(\zeta)\langle x\rangle^{-\delta-\frac{\mu}{4}}$ is uniformly Hölder continuous in $\zeta \in M$. The (well-known) positive energy analogue of this assertion states that for any positive $\lambda_1 < \lambda_0$ the $\mathcal{B}(L^2(\mathbb{R}^d)$-valued function $\langle x\rangle^{-\delta} R(\zeta)\langle x\rangle^{-\delta}$ is uniformly Hölder continuous in $\zeta \in M \setminus \{\operatorname{Re}\zeta < \lambda_1\}$; see (4) for a related remark.

(3) The paper [8] also contains an extension of Proposition 4.1 to powers of the resolvent, however this will not be useful in the forthcoming sections; see Example 7.5 for a discussion. This is related to the fact that our classical constructions are not smooth in λ at zero energy, cf. [6, Remarks 4.7(1)]. The collection of all estimates in Proposition 4.1 (more precisely a collection of similar estimates with a complex spectral parameter) yields similar estimates for powers of the resolvent by a completely algebraic reasoning, cf. [8, Appendix A].

(4) Assume that the potential satisfies Condition 1.1. Then all the bounds of Proposition 4.1 remain true uniformly in $\lambda \in [\lambda_1, \lambda_0]$ for any positive $\lambda_1 < \lambda_0$ provided we replace

$$a \to a := \frac{\xi^2}{2\lambda}, \qquad b \to b := \frac{\xi}{\sqrt{2\lambda}} \cdot \frac{x}{\langle x\rangle} \quad \text{and} \quad g \to 1. \tag{4.4}$$

(Under the stronger Conditions 2.1 and 2.3 the validity of this modification is a direct consequence of the bounds of Proposition 4.1.) Also in this case the families of associated operators are norm continuous (now in $\lambda > 0$ only).

Proof of continuity statements in Proposition 4.1. Due to Remark 4.2(2) and the calculus of pseudodifferential operators all appearing forms in Proposition 4.1 are continuous in $\lambda \geqslant 0$.

Norm continuity of the corresponding operator-valued functions also follows from Remark 4.2(2). This can be seen as follows for $B_\delta(\lambda) := \langle x\rangle^{-\delta} g^{\frac{1}{2}} R(\lambda+\mathrm{i}0) g^{\frac{1}{2}} \langle x\rangle^{-\delta}$ (appearing in (i)):

Pick $\delta' \in]\frac{1}{2}, \delta[$, insert for (small) $\kappa > 0$ the identity $I = F(\kappa|x| < 1) + F(\kappa|x| > 1)$ on both sides of $B_\delta(\lambda)$ and expand (into three terms). This yields

$$\left\| B_\delta(\lambda) - F\big(\kappa|x| < 1\big) B_\delta(\lambda) F\big(\kappa|x| < 1\big) \right\| \leqslant C\kappa^{\delta-\delta'} \left\| B_{\delta'}(\lambda) \right\|.$$

Due to Proposition 4.1(i) the right-hand side is $O(\kappa^{\delta-\delta'})$ uniformly $\lambda \geqslant 0$. On the other hand due to Remark 4.2(2) (and the calculus of pseudodifferential operators) for fixed $\kappa > 0$ the $\mathcal{B}(L^2(\mathbb{R}^d))$-valued function $F(\kappa|x| < 1) B_\delta(\cdot) F(\kappa|x| < 1)$ is continuous. Hence $B_\delta(\cdot)$ is a uniform limit of continuous functions and therefore indeed continuous.

The other operator-valued functions can be dealt with in the same fashion. □

4.2. Scattering wave front set

The remaining subsections of Section 4 are devoted to a number of somewhat technical estimates on solutions to the equation $(H-\lambda)u = v$ for a fixed $\lambda \geqslant 0$. Although they are proved under Conditions 2.1 and 2.3 we remark that there are similar estimates under Condition 1.1 for a fixed $\lambda > 0$. The reader may skip this material on the first reading.

Throughout the remaining part of this section we use the notation $\langle\xi\rangle_1 = (1+|\xi|^2)^{1/2}$ and $X = (1+|x|^2)^{1/2}$ for $\xi, x \in \mathbb{R}^d$.

With reference to the symbol class $S_{\mathrm{unif}}(m, g_{\mu,\lambda})$ from Section 4.1 clearly $h_1, h_2 \in S_{\mathrm{unif}}(m, g_{\mu,\lambda})$ with $h_1 := \frac{1}{2}\xi^2 + V_1$, $h_2 := \frac{1}{2}\xi^2 + V_1 + V_2$ and $m = g^2\langle\xi/g\rangle_1^2$. In the remaining part of Section 4 we shall however only need a reminiscence of this symbol class given by disregarding the uniformity in $\lambda \geqslant 0$. Whence we shall consider symbols $c \in S(m, g_{\mu,\lambda})$ meaning, by definition, that

$$\left|\partial_x^\gamma \partial_\xi^\beta c(x,\xi)\right| \leqslant C_{\gamma,\beta} m(x,\xi)\langle x\rangle^{-|\gamma|} g^{-|\beta|}. \tag{4.5}$$

The corresponding class of standard Weyl quantizations $\mathrm{Op}^{\mathrm{w}}(c)$ is denoted by $\Psi(m, g_{\mu,\lambda})$.

It is convenient to introduce the following constants:

$$s_0 = \begin{cases} \left(1+\frac{\mu}{2}\right)/2, \\ 1/2, \end{cases} \qquad s_1 = \begin{cases} 1-\frac{\mu}{2}, \\ 1, \end{cases} \qquad s_2 = \begin{cases} \mu, & \text{for } \lambda = 0, \\ 0, & \text{for } \lambda > 0. \end{cases} \tag{4.6}$$

If $\epsilon > 0$, then $\langle x\rangle^{-s_0-\epsilon}$ will be a typical weight that appears in resolvent estimates. (Notice that in the uniform estimates of Proposition 4.1 the corresponding weight is $g^{\frac{1}{2}}\langle x\rangle^{-\frac{1}{2}-\epsilon}$.) The weight $\langle x\rangle^{-s_1}$ plays the role of the "Planck constant" for the class $\Psi(m, g_{\mu,\lambda})$. Finally, $\langle x\rangle^{-s_2}$ will appear in the "elliptic regularity estimate" of Proposition 4.3. Clearly $s_0 > s_2$ and $s_1 > 0$.

Let us decompose the normalized momentum ξ/g as follows:

$$\frac{\xi}{g} = b\frac{x}{\langle x\rangle} + \bar{c}, \qquad b := \frac{x}{\langle x\rangle}\cdot\frac{\xi}{g} \quad \text{and} \quad \bar{c} := \left(I - \left|\frac{x}{\langle x\rangle}\right\rangle\left\langle\frac{x}{\langle x\rangle}\right|\right)\frac{\xi}{g}. \tag{4.7}$$

Notice that b was already defined in Section 4.1, besides for $r = |x| \geqslant 1$, $b^2 + \bar{c}^2 = a$ with a also defined in Section 4.1. Moreover for $r \geqslant 1$ we have the identification $b = \hat{x}\cdot\frac{\xi}{g} \in \mathbb{R}$ and $\bar{c} = (I - |\hat{x}\rangle\langle\hat{x}|)\frac{\xi}{g} \in T_{\hat{x}}^*(S^{d-1})$ with $\hat{x} = x/r \in S^{d-1}$, which obviously constitute canonical coordinates for "the phase space" $\mathbb{T}^* := T^*(S^{d-1}) \times \mathbb{R} = S^{d-1} \times \mathbb{R}^d$. This partly motivates the following definition:

The wave front set $WF_{\mathrm{sc}}^s(u)$ of a distribution $u \in L^{2,-\infty}$ is the subset of $\mathbb{T}^*$ given by the condition

$$\begin{aligned} &z_1 = (\omega_1, \bar{c}_1, b_1) = (\omega_1, b_1\omega_1 + \bar{c}_1) = (\omega_1, \eta_1) \notin WF_{\mathrm{sc}}^s(u) \quad \Leftrightarrow \\ &\quad \exists \text{ neighbourhoods } \mathcal{N}_{\omega_1} \ni \omega_1,\ \mathcal{N}_{\eta_1} \ni \eta_1\ \forall \chi_{\omega_1} \in C_c^\infty(\mathcal{N}_{\omega_1}),\ \chi_{\eta_1} \in C_c^\infty(\mathcal{N}_{\eta_1}): \\ &\quad \mathrm{Op}^{\mathrm{w}}\big(\chi_{z_1} F(r>2)\big)u \in L^{2,s} \quad \text{where } \chi_{z_1}(x,\xi) = \chi_{\omega_1}(\hat{x})\chi_{\eta_1}(b\hat{x} + \bar{c}). \end{aligned} \tag{4.8}$$

Notice that this quantization is defined by the substitution $b\hat{x} + \bar{c} \to \xi/g$, cf. (4.7). Keep in mind that the whole concept depends on the given energy $\lambda \in [0,\infty[$ in consideration (through g, which enters in the definition of b and $\bar{c}$).

The above notion of wave front set is of course adapted to the problem in hand. The classical definition is taylored to measure decay in momentum space; see for example [14, Chapter VIII]. Our definition concerns decay in position space, and thus it is more related to the wave front set introduced in [21, Section 7] (dubbed there as "the scattering wave front set").

Obviously

$$u \in L^{2,s} \quad \Rightarrow \quad WF^s_{\mathrm{sc}}(u) = \emptyset.$$

Conversely (by a compactness argument), if for some $\chi \in C_c^\infty(\mathbb{R}^d)$

$$u - \mathrm{Op}^{\mathrm{w}}\big(\chi(\xi/g)\big)u \in L^{2,s}, \tag{4.9}$$

then

$$WF^s_{\mathrm{sc}}(u) = \emptyset \quad \Rightarrow \quad u \in L^{2,s}.$$

Proposition 4.3. *Let $\lambda \geqslant 0$ and s_2 be defined in* (4.6)*. Let $u \in L^{2,-\infty}$, $v \in L^{2,s+s_2}$ and $(H-\lambda)u = v$. Then the estimates* (4.9) *and*

$$WF^s_{\mathrm{sc}}(u) \subseteq \big\{z \in \mathbb{T}^* \,\big|\, b^2 + \bar{c}^2 = 1\big\} \tag{4.10}$$

hold.

More generally, suppose $u \in L^{2,-\infty}$, $g^{-1}v \in L^{2,s}$ and $(H-\lambda)u = v$. Then the following estimates hold:

$$\text{For all } \epsilon > 0\text{:} \quad g\,\mathrm{Op}^{\mathrm{w}}\big(F\big(b^2 + \bar{c}^2 - 1 > \epsilon\big)\big)u \in L^{2,s}, \tag{4.11a}$$

$$\text{For all } \epsilon > 0, \quad g\,\mathrm{Op}^{\mathrm{w}}\big(\langle \xi/g\rangle_1^2 F\big(b^2 + \bar{c}^2 - 1 > \epsilon\big)\big)u \in L^{2,s}, \tag{4.11b}$$

$$\text{For all } \epsilon > 0\text{:} \quad g\,\mathrm{Op}^{\mathrm{w}}\big(F\big(1 - b^2 - \bar{c}^2 > \epsilon\big)\big)u \in L^{2,s}, \tag{4.11c}$$

$$WF^s_{\mathrm{sc}}(gu) \subseteq \big\{z \in \mathbb{T}^* \,\big|\, b^2 + \bar{c}^2 = 1\big\}. \tag{4.11d}$$

Proof. Obviously (4.11b) is stronger than (4.11a). Notice also that (4.11a) in some sense is stronger than Proposition 4.1(ii) (involves weaker weights). It is also obvious that (4.11d) is a consequence of (4.11b) and (4.11c).

The proof of (4.11b) given below is somewhat similar to the proof of the analogue of Proposition 4.1(ii) given in [8]. For convenience we have divided the proof into four steps. For the calculus of pseudodifferential operators, used tacitly below, we refer to [14, Theorems 18.5.4, 18.6.3, 18.6.8] (the reader might find it more convenient to consult [8] for an elaboration).

The bounds (4.11c) can be proved by mimicking Steps III and IV below. We note that the complication due to high energies, cf. Step II below, is absent. For this reason (4.11c) is somewhat easier to establish than (4.11b) and we shall leave the details of proof to the reader.

Step I. At various points in the proof of (4.11b) we need to control the possibly existing local singularities of the potential V_3. This is done in terms of the following elementary bounds:

$$T_1 := \langle x\rangle^{t'} g^{-1} V_3 (H - \mathrm{i})^{-1} g^{-1} \langle x\rangle^{-t} \in \mathcal{B}\big(L^2\big), \quad t, t' \in \mathbb{R}; \tag{4.12a}$$

$$\widetilde{T}_1 := \langle x\rangle^{t'} g^{-1} V_3 \big(1 + p^2\big)^{-1} g^{-1} \langle x\rangle^{-t} \in \mathcal{B}\big(L^2\big), \quad t, t' \in \mathbb{R}; \tag{4.12b}$$

$$T_2 := \langle x\rangle^{t} \big(1 + p^2\big) g (H - \mathrm{i})^{-1} g^{-1} \langle x\rangle^{-t} \in \mathcal{B}\big(L^2\big), \quad t \in \mathbb{R}. \tag{4.12c}$$

Step II. Suppose $gu \in L^{2,t}$ for some fixed $t \leqslant s$. We shall prove that then $Agu \in L^{2,t}$ for all $A \in \Psi(\langle \xi/g\rangle_1^2, g_{\mu,\lambda})$, more precisely, that

$$\text{for all } A \in \Psi\big(\langle \xi/g\rangle_1^2, g_{\mu,\lambda}\big): \quad \|Agu\|_t \leqslant C\big(\|gu\|_t + \big\|g^{-1}v\big\|_s\big). \tag{4.13}$$

For any such an operator A and any $m \in \mathbb{R}$, we decompose

$$\langle x\rangle^t A = B_m \langle x\rangle^t \operatorname{Op}^{\mathrm{w}}\big(\langle \xi/g\rangle_1^2\big) + R_m, \tag{4.14}$$

where $B_m \in \Psi(1, g_{\mu,\lambda})$ and $R_m \in \Psi(\langle \xi/g\rangle_1^2 \langle x\rangle^{-m}, g_{\mu,\lambda})$.

Now, cf. [8, proof of Lemma 4.5],

$$\operatorname{Op}^{\mathrm{w}}\big(\langle \xi/g\rangle_1^2\big) = g^{-1}p^2g^{-1} + \operatorname{Op}^{\mathrm{w}}(a_1) = 2g^{-1}(H-\lambda)g^{-1} + \operatorname{Op}^{\mathrm{w}}(a_2) - 2g^{-2}V_3;$$
$$a_1 = 1 - \big|\nabla g^{-1}\big|^2 + 4^{-1}\Delta g^{-2}, \qquad a_2 = a_1 + 1 - 2g^{-2}V_2 \in S(1, g_{\mu,\lambda}). \tag{4.15}$$

We substitute (4.15) in (4.14), expand into altogether four terms and apply the resulting sum to the state gu. The contribution from the first term of (4.15) is estimated as

$$\big\|B_m\langle x\rangle^t 2g^{-1}(H-\lambda)g^{-1}(gu)\big\| \leqslant C_1\big\|g^{-1}v\big\|_t \leqslant C_2\big\|g^{-1}v\big\|_s.$$

Similarly, the contribution from the second term of (4.15) is estimated as

$$\big\|B_m\langle x\rangle^t \operatorname{Op}^{\mathrm{w}}(a_2)gu\big\| \leqslant C\|gu\|_t.$$

As for the third term of (4.15) we use (4.12a) with $t = t'$ to bound

$$2\big\|B_m\langle x\rangle^t g^{-2}V_3 gu\big\| \leqslant 2\|B_m\|\big\|T_1\langle x\rangle^t g(H-\mathrm{i})u\big\|$$
$$\leqslant C_1\big(\|gv\|_t + \big\|(\lambda-\mathrm{i})gu\big\|_t\big) \leqslant C_2\big(\|gu\|_t + \big\|g^{-1}v\big\|_s\big).$$

To treat the contribution from the second term of (4.14) we note that

$$\Psi\big(\langle \xi/g\rangle_1^2\langle x\rangle^{-m}, g_{\mu,\lambda}\big) \subseteq \Psi\big(\langle \xi\rangle_1^2\langle x\rangle^{2-m}, g_{\mu,\lambda}\big).$$

Whence, using (4.12c) and choosing $m = 2 - t$,

$$\|R_m gu\| \leqslant C_1\big\|T_2\langle x\rangle^t g(H-\mathrm{i})u\big\| \leqslant C_2\big(\|gu\|_t + \big\|g^{-1}v\big\|_s\big).$$

We conclude (4.13).

Step III. Suppose $gu \in L^{2,t}$ for some fixed $t < s$. Fix $s' \in \,]t, t+1-\mu/2]$ with $s' \leqslant s$. We shall show that (4.11a) holds with s replaced by s'. We set $F_\epsilon := F(b^2 + \bar{c}^2 - 1 > \epsilon)$.

We need a regularization in x-space given in terms of $\iota_\kappa = X_\kappa^{-\frac{2-\mu}{2}}$, where for $\kappa \in \,]0,1]$ we let

$$X_\kappa := \big(1 + \kappa|x|^2\big)^{1/2}. \tag{4.16}$$

Mimicking [8, proof of Lemma 4.5], for $R > 1$ large enough we clearly have

$$F_\epsilon^2 F(r > R)^2 \leqslant \frac{3}{\epsilon} \operatorname{Re}\left(\frac{2h_2 - 2\lambda}{g^2}\right) F_\epsilon^2 F(r > R)^2.$$

Let

$$D = \operatorname{Op}^{\mathrm{w}}(d), \qquad d = \langle \xi/g \rangle_1^{-1} \langle x \rangle^{1-s'} = \hbar^{-1} \langle \xi/g \rangle_1^{-1} g^{-1} \langle x \rangle^{-s'};$$
$$P_\kappa = \operatorname{Op}^{\mathrm{w}}(p_\kappa), \qquad p_\kappa = q_\kappa^2 \left(\frac{6}{\epsilon} \operatorname{Re}(h_2 - \lambda) - g^2\right), \qquad q_\kappa = \langle x \rangle^{s'} F_\epsilon \iota_\kappa F(r > R).$$

Since $0 \leqslant p_\kappa \in S(\hbar^{-2} d^{-2}, g_{\mu,\lambda})$,

$$D^* P_\kappa D \geqslant -C$$

uniformly in κ. Since $0 < d \in S(d, g_{\mu,\lambda})$, we can for any $m \in \mathbb{R}$ find $e_m \in S(d^{-1}, g_{\mu,\lambda})$ such that

$$D E_m - I \in \Psi\big(\langle x \rangle^{-2m}, g_{\mu,\lambda}\big); \qquad E_m = \operatorname{Op}^{\mathrm{w}}(e_m).$$

Consequently, we have the uniform bound

$$P_\kappa \geqslant -C E_m^* E_m + R_m, \qquad R_m \in \Psi\big(\langle \xi/g \rangle_1^2 g^2 \langle x \rangle^{2s'-2m}, g_{\mu,\lambda}\big),$$

and therefore by choosing $m = s' - t$ and by using (4.13) that the expectation

$$\langle P_\kappa \rangle_u \geqslant -C\big(\|gu\|_t + \big\|g^{-1} v\big\|_s\big)^2. \tag{4.17}$$

On the other hand, for any $\delta \in]0, 1[$

$$\langle P_\kappa \rangle_u \leqslant C\big(\|gu\|_t + \big\|g^{-1} v\big\|_s\big)^2 - (1 - \delta)\langle Q_\kappa^* Q_\kappa \rangle_{gu}, \quad Q_\kappa = \operatorname{Op}^{\mathrm{w}}(q_\kappa). \tag{4.18}$$

Here we use that

$$\operatorname{Op}^{\mathrm{w}}\big(q_\kappa^2 \operatorname{Re}(h_2 - \lambda)\big) = \operatorname{Re}\big((Q_\kappa g)^* Q_\kappa g^{-1}(H - V_3 - \lambda)\big) + R_\kappa,$$
$$R_\kappa \in \Psi\big(\langle \xi/g \rangle_1^2 \hbar^2 \langle x \rangle^{2s'} g^2, g_{\mu,\lambda}\big) \subseteq \Psi\big(\langle \xi/g \rangle_1^2 \langle x \rangle^{2t} g^2, g_{\mu,\lambda}\big),$$

and the fact that R_κ is bounded in $\kappa \in]0, 1]$ in the class $\Psi(\langle \xi/g \rangle_1^2 \langle x \rangle^{2t} g^2, g_{\mu,\lambda})$. Notice that

$$\frac{6}{\epsilon}\big\langle \operatorname{Re}\big((Q_\kappa g)^* Q_\kappa g^{-1}(H - \lambda)\big)\big\rangle_u \leqslant C\|Q_\kappa g u\| \big\|g^{-1} v\big\|_{s'} \leqslant \delta \|Q_\kappa g u\|^2 + C_\delta \big\|g^{-1} v\big\|_s^2,$$

and that the contributions from V_3 and the term R_κ can be treated by (4.12a) and (4.13), respectively.

Now, combining (4.17) and (4.18) we conclude that

$$\|Q_\kappa gu\|^2 \leqslant C\big(\|gu\|_t + \|g^{-1}v\|_s\big)^2$$

uniformly in $\kappa \in]0,1]$. Letting $\kappa \to 0$ completes Step III.

Step IV. Note that (4.11b) is equivalent to the following, seemingly stronger statement:

$$\text{For all } \epsilon > 0, \quad A \in \Psi\big(\langle \xi/g\rangle_1^2, g_{\mu,\lambda}\big) \quad \text{implies} \quad Ag\,\mathrm{Op^w}(F_\epsilon)u \in L^{2,s}. \tag{4.19}$$

We will show (4.19) by induction.

By assumption, $gu \in L^{2,t}$ for a sufficiently small $t \leqslant s$ and consequently, due to Step II, it follows that $Agu \in L^{2,t}$ for all $A \in \Psi(\langle \xi/g\rangle_1^2, g_{\mu,\lambda})$. Consider for all $k \in \mathbb{N}$ the following claim given in terms of $t_k := \min(s, t + (1-\mu/2)(k-1))$:

The bound/localization (4.11b) holds for all $\epsilon > 0$ and all $A \in \Psi(\langle \xi/g\rangle_1^2, g_{\mu,\lambda})$ provided $u \to u_\epsilon := \mathrm{Op^w}(F_{\epsilon/2})u$ and s is replaced by t_k. (Notice that this implies in particular that the state $gu_{2\epsilon} \in L^{2,t_k}$ and, since $\epsilon > 0$ is arbitrary, that $gu_\epsilon \in L^{2,t_k}$.)

We have seen that this claim holds for $k = 1$. So suppose $k > 1$ and that the claim is true for $k \to k-1$. To show the claim for k, we can assume that $t_{k-1} < s$. First, we notice that $v_\epsilon := (H-\lambda)u_\epsilon$ obeys the condition $g^{-1}v_\epsilon \in L^{2,t_k}$ due to the induction hypothesis, (4.13), (4.12a) and (4.12b). Notice at this point that

$$\big[H - V_3 - \lambda, \mathrm{Op^w}(F_{\epsilon/2})\big] \in \Psi\big(g^2\langle \xi/g\rangle_1^2 \hbar, g_{\mu,\lambda}\big),$$

and that in fact (for any $m \in \mathbb{R}$)

$$\begin{gathered}\big[H - V_3 - \lambda, \mathrm{Op^w}(F_{\epsilon/2})\big] = gAg\,\mathrm{Op^w}(F_{\epsilon/4}) + R_m,\\ A \in \Psi\big(\langle \xi/g\rangle_1^2\langle x\rangle^{\mu/2-1}, g_{\mu,\lambda}\big), \qquad R_m \in \Psi\big(\langle \xi/g\rangle_1^2\langle x\rangle^{-m}, g_{\mu,\lambda}\big).\end{gathered}$$

Now, by Step III, (4.11a) applies to $u \to u_\epsilon$, $t \to s_{k-1}$ and with s replaced by $s' = t_k$. Next, by applying Step II to the state $u \to \tilde u_\epsilon := \mathrm{Op^w}(F_\epsilon)u_\epsilon$ (note that as above $g^{-1}(H-\lambda)\tilde u_\epsilon \in L^{2,t_k}$), we conclude that indeed the bound (4.11b) holds with $u \to u_\epsilon$ and s replaced by t_k. The induction is complete.

Finally we obtain, using the above claim, that the bound (4.11b) holds without changing u and with s replaced by t_k. Since clearly $t_k = s$ for k sufficiently large, (4.11b) follows. □

The following corollary follows immediately from Proposition 4.3. At a fixed energy, it strengthens Proposition 4.1(ii).

Corollary 4.4. *Let $\chi \in C_c^\infty(\mathbb{R})$, $\chi = 1$ around 1. Then for any $s > s_0$ we have (with $\lambda \geqslant 0$, and s_0 and s_2 as given in (4.6))*

$$\big\|\langle x\rangle^{s-s_2}\,\mathrm{Op^w}\big((a^2+1)\big(1-\chi(a)\big)\big)R(\lambda \pm \mathrm{i}0)\langle x\rangle^{-s}\big\| \leqslant C. \tag{4.20}$$

The following proposition is similar to Proposition 9.1 stated later, although the flavour is somewhat "global". These results (as well as their proofs) are modifications of [12, Proposition 3.5.1] (and its proof), see also [21] and [11]. The condition (4.21) is similar to (4.11b); it implies that $WF_{\mathrm{sc}}^s(u) \subseteq \{b^2 + \bar c^2 \leqslant 1\}$ and hence that $WF_{\mathrm{sc}}^s(u)$ is compact.

Proposition 4.5. *Let $\lambda \geqslant 0$ and s_0 be defined in* (4.6). *Suppose $u, v \in L^{2,-\infty}$, $(H-\lambda)u = v$, $s \in \mathbb{R}$, $k \in]-1,1[$ and $\{b = k\} \cap WF^s_{\mathrm{sc}}(u) = \emptyset$. Suppose the following condition*:

$$\textit{For all } \delta > 0, \quad \mathrm{Op}^{\mathrm{w}}\big(\langle \xi/g\rangle_1^2 F\big(b^2 + \bar c^2 - 1 > \delta\big)\big)u \in L^{2,s}. \tag{4.21}$$

Define

$$k^+ = \sup\big\{\tilde k \geqslant k \;\big|\; \big\{b \in [k, \tilde k]\big\} \cap WF^s_{\mathrm{sc}}(u) = \emptyset\big\}, \tag{4.22}$$

$$k^- = \inf\big\{\tilde k \leqslant k \;\big|\; \big\{b \in [\tilde k, k]\big\} \cap WF^s_{\mathrm{sc}}(u) = \emptyset\big\}. \tag{4.23}$$

Then

$$k^+ < 1 \quad \Rightarrow \quad \big\{b = k^+\big\} \cap WF^{s+2s_0}_{\mathrm{sc}}(v) \neq \emptyset, \tag{4.24}$$

$$k^- > -1 \quad \Rightarrow \quad \{b = k^-\} \cap WF^{s+2s_0}_{\mathrm{sc}}(v) \neq \emptyset. \tag{4.25}$$

Proof. We shall only deal with the case of superscript "+"; the case of "−" is similar. For convenience we shall assume that $\epsilon_2 \leqslant 2 - \mu$ and divide the proof into two steps.

Step I. We will first show the following weaker statement: Suppose $u \in L^{2,s-\epsilon_2/2}$, $v \in L^{2,s+2s_0}$ and $(H-\lambda)u = v$ (in this case (4.21) follows from Proposition 4.3). Then

$$k^+ \geqslant 1. \tag{4.26}$$

Suppose on the contrary that $k^+ < 1$. By a compactness argument we can then find a point in $WF^s_{\mathrm{sc}}(u)$ of the form $z_1 = (\omega_1, \bar c_1, k^+)$. For $\epsilon > 0$ chosen small enough (less than $(k^+ - k)/2$ suffices here)

$$\big\{b \in \big]k^+ - 2\epsilon, k^+\big[\big\} \cap WF^s_{\mathrm{sc}}(u) = \emptyset. \tag{4.27}$$

We can assume that $J :=]k^+ - 2\epsilon, k^+ + \epsilon[\subseteq]-1,1[$. Pick a non-positive $f \in C_c^\infty(J)$ with $f' \geqslant 0$ on $[k^+ - \epsilon, \infty[$ and $f(k^+) < 0$, and consider for $K > 0$ and $\kappa \in]0,1]$ the symbol

$$b_\kappa = X^{s_0} a_\kappa, \qquad a_\kappa = X^s X_\kappa^{-\epsilon_2/2} F(r > 2)\exp(-Kb) f(b) F\big(b^2 + \bar c^2 < 3\big); \tag{4.28}$$

here X_κ is defined by (4.16).

We compute the Poisson bracket

$$\begin{aligned}\{h_2, b\} &= \frac{g}{r}\bar c^2 + \frac{V_1'(b^2-1)}{g} - \frac{x\cdot\nabla V_2}{g\langle x\rangle} \\ &= \frac{g}{r}\big(\big(1 - rV_1' g^{-2}\big)\bar c^2 + rV_1' g^{-2}\big(b^2 + \bar c^2 - 1\big) + O\big(r^{-\epsilon_2}\big)\big) \qquad (4.29)\\ &= \frac{g}{r}\big(\big(1 - rV_1' g^{-2}\big)\big(1 - b^2\big) + g^{-2}2(h_2 - \lambda) + O\big(r^{-\epsilon_2}\big)\big). \qquad (4.30)\end{aligned}$$

We expand the right-hand side of (4.30) into three terms and notice that due to (2.1) the first term has the following positive lower bound on $\operatorname{supp} b_\kappa$:

$$\cdots \geqslant c\frac{g}{r}; \qquad c = \frac{\tilde{\epsilon}_1}{2}\bigl(1 - \sup\bigl\{t^2 \bigm| t \in \operatorname{supp} f\bigr\}\bigr).$$

First we fix K: A part of the Poisson bracket with b_κ^2 is

$$\bigl\{h_2, X^{2s+2s_0}X_\kappa^{-\epsilon_2}\bigr\} = \frac{g}{r}Y_\kappa b X^{2s+2s_0}X_\kappa^{-\epsilon_2}, \tag{4.31}$$

where $Y_\kappa = Y_\kappa(r)$ is uniformly bounded in κ. We pick $K > 0$ such that for all κ

$$2Kc \geqslant |Y_\kappa| + 2\frac{r}{g}X^{-2s_0} \quad \text{on } \operatorname{supp} b_\kappa.$$

From (4.30), (4.31) and the properties of K and f, we conclude the following bound at $\{f'(b) \geqslant 0\}$:

$$\bigl\{h_2, b_\kappa^2\bigr\} \leqslant -2a_\kappa^2 + g^{-2}(h_2 - \lambda)a_\kappa O\bigl(r^s\bigr) + O\bigl(r^{2s}\bigr)\bigl(F^2\bigr)'\bigl(b^2 + \bar{c}^2 < 3\bigr) + O\bigl(r^{2s-\epsilon_2}\bigr).$$

To use this bound effectively, we introduce a partition of unity: Let $f_1, f_2 \in C_c^\infty(J)$ be chosen such that $\operatorname{supp} f_1 \subseteq]k^+ - 2\epsilon, k^+[$, $\operatorname{supp} f_2 \subseteq]k^+ - \epsilon, k^+ + \epsilon[$ and $f_1^2 + f_2^2 = 1$ on $\operatorname{supp} f$. We multiply both sides by f_2^2 $(= 1 - f_1^2)$ and obtain after a rearrangement

$$\begin{aligned} \bigl\{h_2, b_\kappa^2\bigr\} &\leqslant -2a_\kappa^2 + g^{-2}(h_2 - \lambda)a_\kappa d_\kappa \\ &\quad + K_1 f_1^2 F\bigl(b^2 + \bar{c}^2 < 3\bigr)\langle x\rangle^{2s} - K_2\bigl(F^2\bigr)'\bigl(b^2 + \bar{c}^2 < 3\bigr)\langle x\rangle^{2s} + K_3\langle x\rangle^{2s-\epsilon_2}, \\ d_\kappa &\in S\bigl(\langle x\rangle^s, g_{\mu,\lambda}\bigr); \end{aligned} \tag{4.32}$$

here $K_1, K_2, K_3 > 0$ are independent of κ, and the symbols d_κ are bounded in κ in the indicated class.

We introduce $A_\kappa = \operatorname{Op}^{\mathrm{w}}(a_\kappa)$, $B_\kappa = \operatorname{Op}^{\mathrm{w}}(b_\kappa)$ and the regularization $u_R = F(|x|/R < 1)u$ in terms of a parameter $R > 1$. First we compute

$$\bigl\langle \mathrm{i}\bigl[H, B_\kappa^2\bigr]\bigr\rangle_u = \lim_{R\to\infty}\bigl\langle \mathrm{i}\bigl[H, B_\kappa^2\bigr]\bigr\rangle_{u_R} = -2\operatorname{Im}\bigl\langle v, B_\kappa^2 u\bigr\rangle. \tag{4.33}$$

Using (4.33) and the calculus, cf. [14, Theorems 18.5.4, 18.6.3, 18.6.8], we estimate

$$\bigl|\bigl\langle \mathrm{i}\bigl[H, B_\kappa^2\bigr]\bigr\rangle_u\bigr| \leqslant C_1\|v\|_{s+2s_0}\bigl(\|A_\kappa u\| + \|u\|_{s-\epsilon_2/2}\bigr) \leqslant \frac{1}{2}\|A_\kappa u\|^2 + C_2. \tag{4.34}$$

On the other hand, using (4.21), (4.27) and (4.32), we infer that

$$\begin{aligned} \bigl\langle \mathrm{i}\bigl[H - V_3, B_\kappa^2\bigr]\bigr\rangle_u &= \lim_{R\to\infty}\bigl\langle \mathrm{i}\bigl[H - V_3, B_\kappa^2\bigr]\bigr\rangle_{u_R} \\ &\leqslant -2\|A_\kappa u\|^2 + C_3\bigl\|(H - V_3 - \lambda)u\bigr\|_{s+\mu}\|A_\kappa u\| + C_4, \end{aligned}$$

and whence, using (4.12a) to bound $\|(H - V_3 - \lambda)u\|_{s+\mu} \leqslant C(\|v\|_{s+\mu} + \|u\|_{s-\epsilon_2/2})$, that

$$\langle \mathrm{i}[H - V_3, B_\kappa^2]\rangle_u \leqslant -\frac{3}{2}\|A_\kappa u\|^2 + C_5. \tag{4.35}$$

Clearly another application of (4.12a) yields

$$\langle \mathrm{i}[V_3, B_\kappa^2]\rangle_u \leqslant C_6. \tag{4.36}$$

Combining (4.34)–(4.36) yields

$$\|A_\kappa u\|^2 \leqslant C_7 = C_2 + C_5 + C_6,$$

which in combination with the property that $f(k^+) < 0$ in turn gives a uniform bound

$$\left\| X_\kappa^{-\epsilon_2/2} \operatorname{Op}^{\mathrm{w}}\big(\chi_{z_1} F(r > 2)\big) u\right\|_s^2 \leqslant C_8; \tag{4.37}$$

here χ_{z_1} signifies any phase-space localization factor of the form entering in (4.8) supported in a sufficiently small neighbourhood of the point $z_1 = (\omega_1, \bar{c}_1, k^+)$.

We let $\kappa \to 0$ in (4.37) and infer that $z_1 \notin WF_{\mathrm{sc}}(u)$, which is a contradiction; whence (4.26) is proven.

Step II. We need to remove the conditions of Step I, $u \in L^{2,s-\epsilon_2/2}$ and $v \in L^{2,s+2s_0}$. This will be accomplished by an iteration and modification of the procedure of Step I.

Pick $t_1 \in \mathbb{R}$ such that $v \in L^{2,t_1}$. Pick $t < s$ such that $u \in L^{2,t}$ and define $s_m = \min(s, t + m\epsilon_2/2)$ for $m \in \mathbb{N}$. Let correspondingly k_m^+ be given by (4.22) with $s \to s_m$. Clearly

$$k_m^+ \leqslant k_{m-1}^+; \quad m = 2, 3, \ldots \tag{4.38}$$

If $u \in L^{2,s_m-\epsilon_2/2}$ and $v \in L^{2,s_m+2s_0}$ then (4.24) with $k^+ \to k_m^+$ and $s \to s_m$ follows from Step I. Although we shall not verify these conditions we remark that a suitable micro-local modification will come into play in an inductive procedure, see (4.41) and (4.43) below. We shall indeed (inductively) show (4.24) with $k^+ \to k_m^+$ and $s \to s_m$, i.e. that

$$k_m^+ < 1 \quad \Rightarrow \quad \{b = k_m^+\} \cap WF_{\mathrm{sc}}^{s_m+2s_0}(v) \neq \emptyset. \tag{4.39}$$

Notice that (4.24) follows by using (4.39) for an m taken so large that $s_m = s$.

Let us consider the start of induction given by $m = 1$. In this case obviously $u \in L^{2,s_m-\epsilon_2/2}$. Suppose on the contrary that (4.39) is false. Then we consider the following case:

$$k_m^+ < 1 \quad \text{and} \quad \{b = k_m^+, b^2 + \bar{c}^2 \leqslant 6\} \cap WF_{\mathrm{sc}}^{s_m+2s_0}(v) = \emptyset. \tag{4.40}$$

We let $\epsilon > 0$, J and f be chosen as in Step I with $k^+ \to k_m^+$. Let $\tilde{f} \in C_c^\infty(]k^+ - 3\epsilon, k^+ + 2\epsilon[)$ with $\tilde{f} = 1$ on J. It follows from (4.40), possibly by taking $\epsilon > 0$ smaller than needed in Step I, that

$$I_\epsilon v \in L^{2,s_m+2s_0}; \qquad I_\epsilon = \operatorname{Op}^{\mathrm{w}}\big(\tilde{f}(b) F\big(b^2 + \bar{c}^2 < 6\big)\big). \tag{4.41}$$

Next, we introduce the symbol b_κ by (4.28) (with $s \to s_m$) and proceed as in Step I. As for the bounds (4.34), we can replace v by $I_\epsilon v$ up to addition of a term of the form $C(\|v\|_{t_1}^2 + \|u\|_{s_m-\epsilon_2/2}^2)$. Similarly we can verify (4.35) and (4.36) (using conveniently (4.12b)). So again we obtain (4.37) (with $s \to s_m$), and therefore a contradiction as in Step I. We have shown (4.39) for $m = 1$.

Now suppose $m \geqslant 2$ and that (4.39) is verified for $m - 1$. We need to show the statement for the given m. Due to (4.38) and the induction hypothesis, we can assume that

$$k_m^+ < k_{m-1}^+. \tag{4.42}$$

Again we argue by contradiction assuming (4.40). We proceed as above noticing that it follows from (4.42) that in addition to (4.41) we have

$$I_\epsilon u \in L^{2,s_{m-1}}; \tag{4.43}$$

at this point we possibly need choosing $\epsilon > 0$ even smaller (viz. $\epsilon < (k_{m-1}^+ - k_m^+)/2$). By replacing v by $I_\epsilon v$ and u by $I_\epsilon u$ at various points in the procedure of Step I (using (4.41) and (4.43), respectively) we obtain again a contradiction. Whence (4.39) follows. □

Corollary 4.6. *Let $s \in \mathbb{R}$, $u \in L^{2,-\infty}$, $v \in L^{2,s+2s_0}$, $(H-\lambda)u = v$, $k \in \,]-1,1[$ and $\{b = k\} \cap WF_{\mathrm{sc}}^s(u) = \emptyset$. Then*

$$WF_{\mathrm{sc}}^s(u) \subseteq \{b = 1\} \cup \{b = -1\}. \tag{4.44}$$

Proof. The condition (4.21) is guaranteed by Proposition 4.3. Then we apply Proposition 4.5. □

4.3. Wave front set bounds of the boundary value of the resolvent

Proposition 4.1 implies that the symbol $R(\lambda \pm \mathrm{i}0)$ in many cases can be treated as an operator, although initially it is defined in terms of a quadratic form. Notice that Remark 4.2(2) in one situation gives a slightly different and direct interpretation of $R(\lambda \pm \mathrm{i}0)$ (as a limit of operators and hence avoiding quadratic forms). It will however be convenient to investigate possible other interpretations of states $R(\lambda \pm \mathrm{i}0)v$ (for which in particular Remark 4.2(2) does not apply) and study associated wave front set bounds. The case of $R(\lambda - \mathrm{i}0)$ is similar to that of $R(\lambda + \mathrm{i}0)$ and will not be elaborated regarding proofs.

For sufficiently decaying states v we have (using in (ii) the slightly abused notation $a := b^2 + \bar{c}^2$ for generic points $z = (\omega, \bar{c}, b) = (\omega, b\omega + \bar{c}) \in \mathbb{T}^*$):

Proposition 4.7. *Let $s > s_0$ and $v \in L^{2,s}$. Then the following is true*:

(i) *For any $t > s_0$,*

$$R(\lambda \pm \mathrm{i}0)v = \lim_{\epsilon \searrow 0} R(\lambda \pm \mathrm{i}\epsilon)v \quad \text{exists in } L^{2,-t}.$$

(ii) $WF_{\mathrm{sc}}^{s-s_2}\big(R(\lambda \pm \mathrm{i}0)v\big) \subseteq \{a = 1\}$.

(iii) *For any $\epsilon > 0$,*

$$WF_{\mathrm{sc}}^{s-2s_0-\epsilon}\big(R(\lambda \pm \mathrm{i}0)v\big) \subseteq \{b = \pm 1\}. \tag{4.45}$$

Proof. **Re (i).** This statement follows from Remark 4.2(2); notice that the notation for the limit conforms with Proposition 4.1(i).

Re (ii). We have $(H-\lambda)u = v$. Therefore (ii) follows from Proposition 4.3 (alternatively by using Corollary 4.4).

Re (iii). Let $\chi_- \in C_c^\infty(\mathbb{R})$ such that χ_- is zero around 1. Let $\chi \in C_c^\infty(\mathbb{R})$. Then by Proposition 4.1(iii), for any $\epsilon > 0$

$$\mathrm{Op}^{\mathrm{w}}\big(\chi(a)\chi_-(b)\big)R(\lambda + \mathrm{i}0)v \in L^{2,s-2s_0-\epsilon}. \qquad \square$$

Based completely on Proposition 4.1 one can give a meaning to $R(\lambda \pm \mathrm{i}0)v$ also for some states v with a slower decay provided they have an appropriate phase space localization. (In the statement below $C_0 \geqslant 1$ is given in agreement with Proposition 4.1(ii).)

Proposition 4.8. *Let $s \leqslant s_0$ and $v \in L^{2,s}$. Suppose that for some $t > s_0$ and $k \in]-1,1]$ (or $k \in [-1,1[$)*

$$WF_{\mathrm{sc}}^t(v) \cap \{b < k,\ a < 2C_0\} = \emptyset \quad \big(\text{or } WF_{\mathrm{sc}}^t(v) \cap \{b > k,\ a < 2C_0\} = \emptyset\big). \tag{4.46}$$

(i) *For any $\epsilon > 0$ there exists*

$$R(\lambda + \mathrm{i}0)v = \lim_{\kappa \searrow 0} R(\lambda + \mathrm{i}0)v_\kappa \quad \Big(R(\lambda - \mathrm{i}0)v := \lim_{\kappa \searrow 0} R(\lambda - \mathrm{i}0)v_\kappa\Big) \quad \text{in } L^{2,s-2s_0-\epsilon},$$

where $v_\kappa(x) := F(\kappa|x| < 1)v(x)$.

(ii) $WF_{\mathrm{sc}}^{s-s_2}\big(R(\lambda + \mathrm{i}0)v\big) \subseteq \{a = 1\} \quad \big(WF_{\mathrm{sc}}^{s-s_2}\big(R(\lambda - \mathrm{i}0)v\big) \subseteq \{a = 1\}\big)$.

(iii) *For any $\epsilon > 0$,*

$$WF_{\mathrm{sc}}^{t-2s_0-\epsilon}\big(R(\lambda + \mathrm{i}0)v\big) \cap \{b < k,\ a \leqslant C_0\} = \emptyset$$
$$\Big(WF_{\mathrm{sc}}^{t-2s_0-\epsilon}\big(R(\lambda - \mathrm{i}0)v\big) \cap \{b > k,\ a \leqslant C_0\} = \emptyset\Big). \tag{4.47}$$

Proof. **Re (i).** Let $\chi \in C_c^\infty(]-\infty, 2C_0[)$, $\chi = 1$ around $[0, C_0]$. Let $\chi_- \in C^\infty(\mathbb{R})$ be chosen such that $\chi_- = 1$ around $]-\infty, -1]$ and $\chi_- = 0$ in $[(k-1)/2, \infty[$. Then by the condition (4.46) and the calculus of pseudodifferential operators

$$\mathrm{Op}^{\mathrm{w}}\big(\chi(a)\chi_-(b)\big)v_\kappa \longrightarrow \mathrm{Op}^{\mathrm{w}}\big(\chi(a)\chi_-(b)\big)v \quad \text{in } L^{2,t} \text{ as } \kappa \searrow 0.$$

Whence by Proposition 4.1(i), for any $\epsilon > 0$,

$$u_1 := \lim_{\kappa \searrow 0} R(\lambda + \mathrm{i}0)\,\mathrm{Op}^{\mathrm{w}}\big(\chi(a)\chi_-(b)\big)v_\kappa \quad \text{exists in } L^{2,-s_0-\epsilon}.$$

By Proposition 4.1(ii) we have

$$u_2 := \lim_{\kappa \searrow 0} R(\lambda + \mathrm{i}0)\,\mathrm{Op}^{\mathrm{w}}\big(1 - \chi(a)\big)v_\kappa \quad \text{exists in } L^{2,s-2s_0-\epsilon}.$$

By Proposition 4.1(iii) we have

$$u_3 := \lim_{\kappa\searrow 0} R(\lambda+\mathrm{i}0)\,\mathrm{Op}^{\mathrm{w}}\big(\chi(a)\big(1-\chi_-(b)\big)\big)v_\kappa \quad \text{exists in } L^{2,s-2s_0-\epsilon}.$$

But $s-2s_0\leqslant -s_0$. Hence

$$R(\lambda+\mathrm{i}0)v := \lim_{\kappa\searrow 0} R(\lambda+\mathrm{i}0)v_\kappa = u_1+u_2+u_3 \in L^{2,s-2s_0-\epsilon}.$$

Re (ii). This statement is proven as (ii) of the previous proposition.

Re (iii). Let $\chi^1, \chi^2 \in C_c^\infty(]-\infty, 2C_0[)$, $\chi^2=1$ around $[0, \max(\sup\operatorname{supp}\chi^1, C_0)]$. Let $\chi_-^1 \in C_c^\infty(]-\infty, k[)$ and $\chi_-^2\in C^\infty(\mathbb{R})$ such that $\chi_-^2=1$ around $]-\infty, \sup\operatorname{supp}\chi_-^1]$ and $\operatorname{supp}\chi_-^2\subseteq\,]-\infty,k[$. Then by the condition (4.46)

$$\mathrm{Op}^{\mathrm{w}}\big(\chi^2(a)\chi_-^2(b)\big)v\in L^{2,t}.$$

Whence, by Proposition 4.1(i), noting that $t>s_0$, we obtain

$$R(\lambda+\mathrm{i}0)\,\mathrm{Op}^{\mathrm{w}}\big(\chi^2(a)\chi_-^2(b)\big)v\in L^{2,-s_0-\epsilon}$$

and

$$WF_{\mathrm{sc}}^{t-2s_0-\epsilon}\big(R(\lambda+\mathrm{i}0)\,\mathrm{Op}^{\mathrm{w}}\big(\chi^2(a)\chi_-^2(b)\big)v\big)\subseteq\{b=1\}. \tag{4.48}$$

By Proposition 4.1(iv),

$$\mathrm{Op}^{\mathrm{w}}\big(\chi^1(a)\chi_-^1(b)\big)R(\lambda+\mathrm{i}0)\,\mathrm{Op}^{\mathrm{w}}\big(\chi^2(a)\big(1-\chi_-^2(b)\big)\big)v\in L^{2,\infty}, \tag{4.49}$$

and by Proposition 4.1(v),

$$\mathrm{Op}^{\mathrm{w}}\big(\chi^1(a)\chi_-^1(b)\big)R(\lambda+\mathrm{i}0)\,\mathrm{Op}^{\mathrm{w}}\big(1-\chi^2(a)\big)v\in L^{2,\infty}. \tag{4.50}$$

Now (4.48)–(4.50) yields

$$\mathrm{Op}^{\mathrm{w}}\big(\chi^1(a)\chi_-^1(b)\big)R(\lambda+\mathrm{i}0)v\in L^{2,t-2s_0-\epsilon},$$

which implies (4.47). □

We have yet another interpretation very similar to Proposition 4.7(i):

Proposition 4.9. *Fix real-valued* $\chi\in C_c^\infty(\mathbb{R})$ *and* $\tilde\chi\in C^\infty(\mathbb{R})$ *such that* $\inf\operatorname{supp}\tilde\chi>-1$ (*or* $\sup\operatorname{supp}\tilde\chi<1$). *Let* $A:=\mathrm{Op}^{\mathrm{w}}(\chi(a)\tilde\chi(b))$. *Suppose* $v\in L^{2,s}$ *for some* $s\leqslant s_0$.

For any $\epsilon>0$ *there exists*

$$R(\lambda+\mathrm{i}0)Av=\lim_{\kappa\searrow 0}R(\lambda+\imath\kappa)Av \quad \text{in } L^{2,s-2s_0-\epsilon}$$

$$\big(\text{or } R(\lambda-\mathrm{i}0)Av=\lim_{\kappa\searrow 0}R(\lambda-\imath\kappa)Av \text{ in } L^{2,s-2s_0-\epsilon}\big).$$

Moreover this limit agrees with the interpretation of Proposition 4.8(i).

Proof. We need to invoke an extended version of the bound (4.3e), see [8, Lemma 4.10]. First notice that the symbols g, and hence also a and b, obviously depend on λ. Let $\zeta = \lambda + \imath\kappa$ and define g_ζ, a_ζ and b_ζ by replacing λ by $|\zeta|$ in the definition of g in Section 2.1 and of a and b in (4.1), respectively. Now we have the following extension of the bound (4.3e):

For all $\delta > \frac{1}{2}$ and all $s, t \geqslant 0$, there exists $C > 0$ such that for all $\kappa \in]0, 1]$

$$\big\| \big(\langle x\rangle g_\zeta\big)^{-s} \langle x\rangle^{-t-\delta} g_\zeta^{\frac{1}{2}} R(\zeta) \operatorname{Op}^{\mathrm{w}}\big(\chi_-(a_\zeta)\tilde{\chi}_+(b_\zeta)\big) g_\zeta^{\frac{1}{2}} \langle x\rangle^{t-\delta} \big(\langle x\rangle g_\zeta\big)^{s} \big\| \leqslant C. \tag{4.51}$$

Although this will not be needed, the bound (4.51) is in fact locally uniform in $\lambda \geqslant 0$.

We pick in (4.51) the functions χ_- and $\tilde{\chi}_+$ in agreement with Proposition 4.1(iii) such that in addition $\chi_- = 1$ around $[0, \sup \operatorname{supp} \chi]$ and $\tilde{\chi}_+ = 1$ around $[\min(0, \inf \operatorname{supp} \tilde{\chi}), \infty[$. Using the bounds $g \leqslant g_\zeta$, $a_\zeta \leqslant a$ and $|b_\zeta| \leqslant |b|$ we then obtain that for any $m \in \mathbb{R}$

$$\big(\operatorname{Op}^{\mathrm{w}}\big(\chi_-(a_\zeta)\tilde{\chi}_+(b_\zeta)\big) - 1\big)A \in \Psi\big(\langle x\rangle^m, g_{\mu,\lambda}\big). \tag{4.52}$$

By combining Remark 4.2(2), (4.51) (with $s = 0$, $t = s_0 - s + \frac{\epsilon}{2}$ and $\delta = \frac{1}{2} + \frac{\epsilon}{2}$) and (4.52) we obtain the uniform bound: For all $\kappa \in]0, 1]$

$$\big\| \langle x\rangle^{-t-\delta} g^{\frac{1}{2}} R(\zeta) A g^{\frac{1}{2}} \langle x\rangle^{t-\delta} \big\| \leqslant C. \tag{4.53}$$

Obviously we obtain from (4.53) and a density argument that indeed there exists the limit

$$u := \lim_{\kappa \searrow 0} R(\lambda + \imath\kappa) A v \quad \text{in } L^{2, s-2s_0-\epsilon}.$$

Since $u = R(\lambda + \mathrm{i}0)Av$ for $v \in L^{2,\infty}$ we are done (by using density and interchanging limits). $\square$

4.4. *Sommerfeld radiation condition*

In this subsection we describe a version of the Sommerfeld radiation condition close in spirit to [13, Theorem 30.2.7], [17] and [21].

We introduce for $s > 0$ Besov spaces B_s and corresponding duals B_s^* as in [1] (see [13, Section 14.1] for details about these spaces). They consist of local L^2 functions with a certain (norm) expression being finite.

Throughout this subsection we shall actually only use the duals B_s^*, for which we can take the norm squared to be

$$\|u\|_{B_s^*}^2 := \sup_{R>1} R^{-2s} \int_{|x|<R} |u|^2 \, \mathrm{d}x.$$

An equivalent norm is given by the square root of the expression

$$\int_{|x|<1} |u|^2 \, \mathrm{d}x + \sup_{R>1} R^{-2s} \int_{R/2<|x|<R} |u|^2 \, \mathrm{d}x.$$

In particular we see that for all $s, s' > 0$ the map $X^{s'-s} : B_s^* \to B_{s'}^*$ is bicontinuous.

The subspace $B^*_{s,0} \subseteq B^*_s$ is specified by the additional condition

$$\lim_{R\to\infty} R^{-2s} \int_{|x|<R} |u|^2 \, \mathrm{d}x = 0,$$

or equivalently,

$$\lim_{R\to\infty} R^{-2s} \int_{R/2<|x|<R} |u|^2 \, \mathrm{d}x = 0.$$

There are inclusions

$$L^{2,-s} \subseteq B^*_{s,0} \subseteq B^*_s \subseteq \bigcap_{s'>s} L^{2,-s'}. \tag{4.54}$$

We introduce a notion of scattering wave front set of a distribution $u \in L^{2,-\infty}$ relative to the Besov space $B^*_{s,0}$, $s > 0$, say, denoted by $WF(B^*_{s,0}, u)$. It is the complement within $\mathbb{T}^*$ given by replacing $WF^{-s}_{\mathrm{sc}}(u) \to WF(B^*_{s,0}, u)$ and $L^{2,-s} \to B^*_{s,0}$ in (4.8) (here (4.8) is considered with $s \to -s$). Obviously (4.54) implies the inclusions

$$WF^{-s}_{\mathrm{sc}}(u) \supseteq WF\big(B^*_{s,0}, u\big) \supseteq WF^{-s'}_{\mathrm{sc}}(u); \quad s' > s. \tag{4.55}$$

Proposition 4.10. *Suppose $v \in L^{2,s'_0}$ for some $s'_0 > s_0$ (here s_0 is given in* (4.6)*). Then the equation $(H-\lambda)u = v$ has a unique solution $u \in L^{2,-\infty}$ obeying one of the following conditions*:

(i) $WF^{-s_0}_{\mathrm{sc}}(u) \subseteq \{b > -1\}$,
(ii) $WF(B^*_{s_0,0}, u) \subseteq \{b > 0\}$.

This solution is given by $u = R(\lambda + \mathrm{i}0)v \in L^{2,-s}$ for all $s > s_0$ and $WF^{-s_0}_{\mathrm{sc}}(u) \subseteq \{b = 1\}$.

Similarly, under the same condition on v, the equation $(H-\lambda)u = v$ has a unique solution $u \in L^{2,-\infty}$ obeying one of the following conditions:

(i)′ $WF^{-s_0}_{\mathrm{sc}}(u) \subseteq \{b < 1\}$,
(ii)′ $WF(B^*_{s_0,0}, u) \subseteq \{b < 0\}$;

and this solution is given by $u = R(\lambda - \mathrm{i}0)v \in L^{2,-s}$ for all $s > s_0$ and $WF^{-s_0}_{\mathrm{sc}}(u) \subseteq \{b = -1\}$.

Proof. We shall only consider the first mentioned cases (i) or (ii) (they will be treated in parallel); the other cases can be treated similarly. By Proposition 4.7, the function $u = \tilde{u} := R(\lambda + \mathrm{i}0)v$ is a solution to $(H-\lambda)u = v$ enjoying the stated properties (including (i) and (ii)). Suppose in the sequel that $u \in L^{2,-t}$ for some $t > s_0$, $(H-\lambda)u = v$ and $WF^{-s_0}_{\mathrm{sc}}(u) \subseteq \{b > -1\}$ or $WF(B^*_{s_0,0}, u) \subseteq \{b > 0\}$. It remains to be shown that $u = \tilde{u}$.

Step I. We shall show that $u \in L^{2,-s}$ for all $s > s_0$. By Proposition 4.3,

$$WF_{\mathrm{sc}}^{-s_0}(u) \subseteq \{b^2 + \bar{c}^2 = 1\}, \tag{4.56}$$

$$A\,\mathrm{Op}^{\mathrm{w}}\big(F\big(b^2 + \bar{c}^2 > 3\big)\big)u \in L^{2,-s_0} \quad \text{for all } A \in \Psi\big(\langle \xi/g\rangle_1^2, g_{\mu,\lambda}\big). \tag{4.57}$$

It follows from (4.55), Propositions 4.3 and 4.5 and a compactness argument that

$$WF_{\mathrm{sc}}^{-s}(u) \subseteq \{b = 1\} \quad \text{for all } s > s_0. \tag{4.58}$$

Pick a real-valued decreasing $\psi \in C_c^\infty([0,\infty))$ such that $\psi(r) = 1$ in a small neighbourhood of 0 and $\psi'(r) = -1$ if $1/2 \leqslant r \leqslant 1$. Let $\psi_R(x) = \psi(|x|/R)$; $R > 1$. We also introduce

$$\delta = \max(t - s_0, 2t - 2s_0 + \mu - 2),$$

and check that

$$\delta + s_0' \geqslant t, \quad s_0 + \delta/2 + 1 - \mu/2 \geqslant t \quad \text{and} \quad s_0 + \delta/2 < t.$$

By undoing the commutator we have on one hand that

$$\big\langle \mathrm{i}\big[H, X^{-\delta}\psi_R\big]\big\rangle_u = -2\,\mathrm{Im}\big\langle v, X^{-\delta}\psi_R u\big\rangle, \tag{4.59}$$

yielding the estimate

$$\big|\big\langle \mathrm{i}\big[H, X^{-\delta}\psi_R\big]\big\rangle_u\big| \leqslant C_1\|v\|_{s_0'}\|\|u\|_{-\delta-s_0'} \leqslant C_2\|v\|_{s_0'}\|\|u\|_{-t} = O\big(R^0\big). \tag{4.60}$$

On the other hand

$$\mathrm{i}\big[H, X^{-\delta}\psi_R\big] = \mathrm{Re}\big(g\langle x\rangle h_{\delta,R}\,\mathrm{Op}^{\mathrm{w}}(b)\big);$$
$$h_{\delta,R}(x) = -\delta X^{-2-\delta}\psi_R(x) + X^{-\delta}\big(|x|R\big)^{-1}\psi'\big(|x|/R\big),$$

yielding by using (4.57), (4.58) and the calculus (cf. [14, Theorems 18.5.4, 18.6.3, 18.6.8])

$$\big\langle \mathrm{i}\big[H, X^{-\delta}\psi_R\big]\big\rangle_u = \mathrm{Re}\big\langle g\langle x\rangle h_{\delta,R}\,\mathrm{Op}^{\mathrm{w}}\big(bF(b > 1/2)F\big(b^2 + \bar{c}^2 < 6\big)\big)\big\rangle_u + O\big(R^0\big),$$

which in turn (by the same arguments) implies that

$$\big\langle \mathrm{i}\big[H, X^{-\delta}\psi_R\big]\big\rangle_u \leqslant -\delta 4^{-1}\big\langle g\langle x\rangle X^{-2-\delta}\psi_R\big\rangle_u + O\big(R^0\big). \tag{4.61}$$

By combining (4.60) and (4.61) we obtain

$$\big\langle g\langle x\rangle X^{-2-\delta}\psi_R\big\rangle_u \leqslant C, \tag{4.62}$$

for some constant C which is independent of $R > 1$. Whence, letting $R \to \infty$ we see that $u \in L^{2,-t_1}$; $t_1 := s_0 + \delta/2$.

More generally, we define for $k \in \mathbb{N}$

$$t_k = s_0 + 2^{-1} \max(t_{k-1} - s_0, 2t_{k-1} - 2s_0 + \mu - 2), \quad t_0 := t,$$

and iterate the above procedure. We conclude that $u \in L^{2,-t_k}$, and hence that indeed $u \in L^{2,-s}$ for all $s > s_0$.

Step II. Due to Step I, it suffices to show that $u = 0$ is the only solution to the equation $(H - \lambda)u = 0$ subject to the conditions $u \in L^{2,-s}$ for all $s > s_0$ and either $WF_{\mathrm{sc}}^{-s_0}(u) \subseteq \{b > -1\}$ or $WF(B^*_{s_0,0}, u) \subseteq \{b > 0\}$. In the following Steps III and IV we consider this problem.

Step III. We shall show that $u \in B^*_{s_0,0}$. Under condition (i) the bound (4.58) holds for $s = s_0$ (by Proposition 4.5) which implies that

$$\text{There exists } \epsilon > 0 \quad \text{such that } WF(B^*_{s_0,0}, u) \subseteq \{b > \epsilon\}.$$

Under condition (ii), we have the same conclusion due to (4.56) and a compactness argument. Next, we apply the same scheme as in Step I, now with $\delta = 0$ and using a factor of $F(b > \epsilon)$ instead of a factor of $F(b > 1/2)$. This leads to

$$R^{-1}\big\langle g\langle x\rangle |x|^{-1}\psi'\big(|\cdot|/R\big)\big\rangle_u = o\big(R^0\big),$$

and hence $u \in B^*_{s_0,0}$.

Step IV. We shall show that $u = 0$. For convenience we assume that $\epsilon_2 \leqslant 2 - \mu$. First, letting $s \in]s_0 - \epsilon_2/2, s_0[$ be given arbitrarily, our goal is to show that $u \in L^{2,-s}$. For that consider for $\kappa \in]0, 1/2]$

$$b_\kappa = X^{s_0} a_\kappa; \qquad a_\kappa = \left(\frac{X}{X_\kappa}\right)^{-s} X_\kappa^{-s_0} F(-b > 1/2) F\big(b^2 + \bar{c}^2 < 3\big). \tag{4.63}$$

Here we use the regularization factor of (4.16). We calculate the Poisson bracket

$$\left\{h_2, \left(\frac{X}{X_\kappa}\right)^{2s_0-2s}\right\} = (1-\kappa)(2s_0 - 2s)\langle x\rangle X^{-1} X_\kappa^{-3}\left(\frac{X}{X_\kappa}\right)^{2s_0-2s-1} gb.$$

Obviously this is negative on the support of b_κ, with the (uniform) upper bounds

$$\begin{aligned}\cdots &\leqslant -8^{-1}(2s_0 - 2s)\big(\langle x\rangle X^{2s_0-2} g\big) X_\kappa^{-2}\left(\left(\frac{X}{X_\kappa}\right)^{-s} X_\kappa^{-s_0}\right)^2 \\ &\leqslant -c X_\kappa^{-2}\left(\left(\frac{X}{X_\kappa}\right)^{-s} X_\kappa^{-s_0}\right)^2, \quad c > 0.\end{aligned}$$

Similarly, by (4.29),

$$\begin{aligned}&\big\{h_2, F^2(-b > 1/2)\big\} \\ &\quad = -\frac{g}{r}\big(F^2\big)'(-b > 1/2)\big(\big(1 - rV_1' g^{-2}\big)\bar{c}^2 + \big(rV_1' g^{-2}\big) g^{-2} 2(h_2 - \lambda) + O\big(r^{-\epsilon_2}\big)\big),\end{aligned}$$

where we expand the right-hand side into a sum of three terms and note that the first term is non-positive.

We introduce the quantizations $A_\kappa = \mathrm{Op}^{\mathrm{w}}(a_\kappa)$ and $B_\kappa = \mathrm{Op}^{\mathrm{w}}(b_\kappa)$, and the states $u_R(x) = \psi_R(x)u(x)$, $R > 1$. By Step III,

$$\lim_{R\to\infty} \langle \mathrm{i}[H, B_\kappa^2]\rangle_{u_R} = 0. \tag{4.64}$$

On the other hand, due to the above considerations the expectation of $\mathrm{i}[H, B_\kappa^2]$ in u_R tends to be negative. Keeping the precise upper bounds in mind, we can let $R \to \infty$ (using the calculus, (4.12a), to deal with a contribution from V_3 and (4.64)) obtaining

$$c\|X_\kappa^{-1}A_\kappa u\|^2 \left(= \lim_{R\to\infty} c\|X_\kappa^{-1}A_\kappa u_R\|^2\right) \leqslant C,$$

where the constants c (the one given above) and C are positive and independent of κ. Whence, letting $\kappa \to 0$, we conclude that

$$\mathrm{Op}^{\mathrm{w}}\big(F(-b > 1/2)F\big(b^2 + \bar{c}^2 < 3\big)\big)u \in L^{2,-s}. \tag{4.65}$$

Upon replacing the factor $F(-b > 1/2)$ in (4.63) by $F(b > 1/2)$, we can argue similarly and obtain

$$\mathrm{Op}^{\mathrm{w}}\big(F(b > 1/2)F\big(b^2 + \bar{c}^2 < 3\big)\big)u \in L^{2,-s}. \tag{4.66}$$

In combination with Proposition 4.5, the bounds (4.65) and (4.66) and the fact that (4.56) holds with s_0 replaced by s (note this is trivial since, by assumption, now $v = 0$) yield that $u \in L^{2,-s}$.

Next, the above procedure can be iterated: Assuming that $u \in L^{2,-s}$ for all $s > t_k := s_0 - k\epsilon_2/2$ (for some $k \in \mathbb{N}$), the procedure leads to $u \in L^{2,-s}$ for all $s > t_{k+1}$. Consequently, $u \in L^{2,s}$ for all $s \in \mathbb{R}$. In particular $u \in L^2$, and therefore $u = 0$. □

5. Fourier integral operators

In this section we construct and study certain modifiers in the form of Fourier integral operators; they will enter in the construction of wave operators in Section 6.

5.1. The WKB-ansatz

Assume first that Condition 1.1 holds. Fix $\sigma_0 \in]0, 2[$. Recall from Lemma 3.1 that there exists a decreasing function $]0, \infty[\ni \lambda \mapsto R_0(\lambda)$ such that on the set

$$\big\{(x,\xi) \in \mathbb{R}^d \times \big(\mathbb{R}^d \setminus \{0\}\big) \;\big|\; x \in \Gamma^+_{R_0(|\xi|^2/2),\sigma_0}(\hat{\xi})\big\}$$

we can construct a solution ϕ^+ of the eikonal equation satisfying the (non-uniform in energy) bounds (3.3).

We fix $0 < \sigma < \sigma' < \sigma_0$. Next we introduce smoothed out characteristic functions

$$\chi_1(r) = \begin{cases} 1, & \text{for } r \geqslant 2, \\ 0, & \text{for } r \leqslant 1, \end{cases} \tag{5.1}$$

and

$$\chi_2(l) = \begin{cases} 1, & \text{for } l \geqslant 1-\sigma, \\ 0, & \text{for } l \leqslant 1-\sigma'. \end{cases} \tag{5.2}$$

Define

$$a_0^+(x,\xi) := \chi_2(\hat{x}\cdot\hat{\xi})\chi_1\big(|x|/R_0\big(|\xi|^2/2\big)\big).$$

The basic idea of Isozaki–Kitada is to use the modifier given by a Fourier integral operator J_0^+ on $L^2(\mathbb{R}^d)$ of the form

$$\big(J_0^+ f\big)(x) = (2\pi)^{-d/2}\int \mathrm{e}^{\mathrm{i}\phi^+(x,\xi)} a_0^+(x,\xi)\hat{f}(\xi)\,\mathrm{d}\xi, \tag{5.3}$$

where

$$\hat{f}(\xi) := (2\pi)^{-d/2}\int \mathrm{e}^{-\mathrm{i}x\cdot\xi} f(x)\,\mathrm{d}x$$

denotes the (unitary) Fourier transform of f.

If we assume that the potentials satisfy Conditions 2.1 and 2.2, then we can assume that the function $R_0(\lambda)$ is the constant R_0 given by Lemma 3.2. Thus in this case the solution $\phi^+(x,\omega,\lambda)$ of the eikonal equation is defined in $\Gamma^+_{R_0,\sigma_0}\times[0,\infty[$ (here σ_0 is also given by Lemma 3.2; possibly it is much smaller than 2), and the amplitude a_0 is simply given by

$$a_0^+(x,\xi) := \chi_2(\hat{x}\cdot\hat{\xi})\chi_1\big(|x|/R_0\big).$$

5.2. *The improved WKB-ansatz*

The modifier J_0^+ (and its incoming counterpart, say J_0^-) is sufficient only for the most basic purposes, such as the existence of the outgoing (incoming) wave operator. To study finer properties of wave operators it is useful to use a more refined construction suggested by the WKB method.

This more refined construction is possible and useful already under Condition 1.1. However, for simplicity of presentation, in the remaining part of the section we will assume that the potentials satisfy the more restrictive Conditions 2.1 and 2.2. These conditions allow us to extend this and related constructions (see Section 5.5) down to (and including) $\lambda = 0$. Therefore, it will be convenient to switch between the two notations $\phi^+(x,\xi)$ and $\phi^+(x,\omega,\lambda)$. This will be done tacitly in the following, and in fact, we shall often slightly abuse notation by writing $(x,\xi)\in\Gamma^+_{R_0,\sigma_0}$ instead of $(x,\omega,\lambda)\in\Gamma^+_{R_0,\sigma_0}\times[0,\infty[$.

The WKB method suggests to approximate the wave operator by a Fourier integral operator J^+ on $L^2(\mathbb{R}^d)$ of the form

$$\big(J^+ f\big)(x) = (2\pi)^{-d/2} \int \mathrm{e}^{\mathrm{i}\phi^+(x,\xi)} a^+(x,\xi) \hat{f}(\xi)\,\mathrm{d}\xi, \tag{5.4}$$

where the symbol $a^+(x,\xi)$ is supported in $\Gamma^+_{R_0,\sigma_0}$ and constructed by an iterative procedure to make the difference $T^+ := \mathrm{i}(HJ^+ - J^+H_0)$ small in an outgoing region $\Gamma^+_{R,\sigma}$ for some $R > R_0$, $\sigma < \sigma_0$. We have

$$\big(T^+ f\big)(x) = (2\pi)^{-d/2} \int \mathrm{e}^{\mathrm{i}\phi^+(x,\xi)} t^+(x,\xi) \hat{f}(\xi)\,\mathrm{d}\xi, \tag{5.5}$$

where

$$t^+(x,\xi) = \bigg(\big(\nabla_x \phi^+(x,\xi)\big)\cdot\nabla_x + \frac{1}{2}\big(\triangle_x \phi^+(x,\xi)\big)\bigg) a^+(x,\xi) - \frac{\mathrm{i}}{2}\triangle_x a^+(x,\xi). \tag{5.6}$$

As it is well known from the WKB method, it is possible to improve on the ansatz by putting (here we need $\xi \neq 0$)

$$a^+(x,\xi) := \big(\det \nabla_\xi \nabla_x \phi^+(x,\xi)\big)^{1/2} b^+(x,\xi), \tag{5.7}$$

$$t^+(x,\xi) := \big(\det \nabla_\xi \nabla_x \phi^+(x,\xi)\big)^{1/2} r^+(x,\xi). \tag{5.8}$$

We have

$$\bigg(\big(\nabla_x \phi^+(x,\xi)\big)\cdot\nabla_x + \frac{1}{2}\big(\triangle_x \phi^+(x,\xi)\big)\bigg)\big(\det \nabla_\xi \nabla_x \phi^+(x,\xi)\big)^{1/2} = 0,$$

and therefore

$$\begin{aligned} r^+(x,\xi) &= \big(\nabla_x \phi^+(x,\xi)\big)\cdot\nabla_x b^+(x,\xi) \\ &\quad - \big(\det \nabla_\xi \nabla_x \phi^+(x,\xi)\big)^{-1/2} \frac{\mathrm{i}}{2} \triangle_x \big(\det \nabla_\xi \nabla_x \phi^+(x,\xi)\big)^{1/2} b^+(x,\xi). \end{aligned}$$

It is useful to introduce

$$\zeta^+(x,\xi) = \ln\big(\det \nabla_\xi \nabla_x \phi(x,\xi)\big)^{1/2}; \quad \xi \neq 0. \tag{5.9}$$

Note that it satisfies the equation

$$\big(\nabla_x \phi(x,\xi)\big)\cdot\nabla_x \zeta^+(z,\xi) + \frac{1}{2}\triangle_x \phi(x,\xi) = 0. \tag{5.10}$$

Proposition 5.1. *For* $(x,\xi)\in\Gamma^+_{R,\sigma}$, $\xi\neq 0$,

$$\zeta^+(x,\xi)=\frac{1}{2}\int_1^\infty \triangle_y\phi^+\big(y^+(t;x,\xi),\xi\big)\,\mathrm{d}t. \tag{5.11}$$

Proof. Both $\zeta^+(x,\xi)$ and the right-hand side of (5.11) satisfy the first order Eq. (5.10). Both go to zero as $|x|\to\infty$. In particular, they go to zero along the characteristics $t\to y^+(t,x,\xi)$. Therefore, they coincide. □

Lemma 5.2. *There exist the uniform limits*

$$\lim_{\lambda\searrow 0}\partial_\omega^\delta\partial_x^\gamma\big(\zeta^+(x,\xi)-\zeta^+_{\mathrm{sph}}(x,\xi)\big).$$

Besides, we have uniform estimates with $\breve\epsilon$ *given as in Proposition* 3.3

$$\partial_\omega^\delta\partial_x^\gamma\big(\zeta^+(x,\xi)-\zeta^+_{\mathrm{sph}}(x,\xi)\big)=O\big(|x|^{-|\gamma|-\breve\epsilon}\big),\quad |\delta|+|\gamma|\geqslant 0.$$

Proof. Below div and ∇ will always involve the derivatives with respect to the first argument. We compute:

$$\begin{aligned}\zeta^+(x,\xi)-\zeta^+_{\mathrm{sph}}(x,\xi)&=\int_1^\infty\frac{1}{2}\big(\operatorname{div}F^+\big(y^+(t),\xi\big)-\operatorname{div}F^+_{\mathrm{sph}}\big(y^+_{\mathrm{sph}}(t),\xi\big)\big)\,\mathrm{d}t\\&=\int_1^\infty\mathrm{d}t\,\frac{1}{2}\int_0^1\nabla\operatorname{div}F^+\big(y^+_l(t),\xi\big)\cdot\big(y^+(t)-y^+_{\mathrm{sph}}(t)\big)\,\mathrm{d}l\\&\quad+\int_1^\infty\frac{1}{2}\big(\operatorname{div}F^+\big(y^+_{\mathrm{sph}}(t),\xi\big)-\operatorname{div}F^+_{\mathrm{sph}}\big(y^+_{\mathrm{sph}}(t),\xi\big)\big)\,\mathrm{d}t\\&=I+II,\end{aligned}$$

where $y^+_l(t)=ly^+(t)+(1-l)y^+_{\mathrm{sph}}(t)$.

Now I can be estimated (cf. (3.5f) and [6, (6.43)]) by

$$\begin{aligned}C_1\int_1^\infty\big|y^+\big|^{-2}g\big(\big|y^+\big|\big)t^{\alpha-\epsilon}\,\mathrm{d}t&\leqslant C_2\int_{|x|}^\infty\big|y^+\big|^{-2}\big|y^+\big|^{(\alpha-\epsilon)/\alpha}\,\mathrm{d}\big|y^+\big|\\&=O\big(|x|^{-\epsilon/\alpha}\big)=O\big(|x|^{-\breve\epsilon}\big).\end{aligned}\tag{5.12}$$

Here $\alpha=2/(2+\mu)$ and $\epsilon>0$ is specified in [6, Subsection 6.1]. We used that

$$\frac{\mathrm{d}|y^+|}{\mathrm{d}t}\geqslant cg\big(\big|y^+\big|\big),\quad \big|y^+\big|\geqslant ct^\alpha,\ c>0.$$

Splitting the time-integral as $\int_1^{T_0} \mathrm{d}t + \int_{T_0}^{\infty} \mathrm{d}t$, the argument above yields (uniform) smallness of the second term (provided T_0 is chosen big). As for the contribution from the first term, we can apply the dominated convergence theorem; whence we obtain the existence of $\lim_{\lambda\searrow 0} I$.

Next $\partial_\omega^\delta \partial_x^\gamma I$ is a sum integrals of terms of the following form:

$$\partial_\omega^{\delta_1}\partial_x^{\gamma_1} y_l^+ \cdots \partial_\omega^{\delta_n}\partial_x^{\gamma_n} y_l^+ \partial_{y_l^+}^n \partial_\omega^\nu \nabla \operatorname{div} F\big(y_l^+, \xi\big) \cdot \partial_\omega^\alpha \partial_x^\beta \big(y^+(t) - y_{\mathrm{sph}}^+(t)\big),$$

where $\delta_1 + \cdots + \delta_n + \nu + \alpha = \delta$ and $\gamma_1 + \cdots + \gamma_n + \beta = \gamma$. This can be estimated (cf. (3.5f) and [6, (4.41) and (6.43)]) by

$$C|x|^{-|\gamma|}\big|y^+\big|^{-2} g\big(\big|y^+\big|\big) t^{\alpha-\epsilon}.$$

We argue as above to obtain uniform bounds on $\partial_\omega^\delta \partial_x^\gamma I$, as well as the existence of $\lim_{\lambda\searrow 0} \partial_\omega^\delta \partial_x^\gamma I$.

Now II is bounded (cf. (3.5g)) by

$$C_1 \int_1^\infty \big|y^+\big|^{-1-\breve{\epsilon}} g\big(\big|y^+\big|\big)\,\mathrm{d}t \leqslant C_2 \int_{|x|}^\infty \big|y^+\big|^{-1-\breve{\epsilon}}\,\mathrm{d}\big|y^+\big| = O\big(|x|^{-\breve{\epsilon}}\big). \tag{5.13}$$

Then we apply the dominated convergence theorem as above, and we obtain the existence of $\lim_{\lambda\searrow 0} II$.

$\partial_\omega^\delta \partial_x^\gamma II$ is a sum of integrals of terms of the form

$$\partial_\omega^{\delta_1}\partial_x^{\gamma_1} y^+ \cdots \partial_\omega^{\delta_n}\partial_x^{\gamma_n} y^+ \partial_{y^+}^n \partial_\omega^\nu \big(\operatorname{div} F^+\big(y^+, \xi\big) - \operatorname{div} F_{\mathrm{sph}}^+\big(y^+, \xi\big)\big),$$

where $\delta_1 + \cdots + \delta_n + \nu = \delta$ and $\gamma_1 + \cdots + \gamma_n = \gamma$. This can be estimated (cf. (3.5g) and [6, (4.41) and (6.43)]) by

$$C|x|^{-|\gamma|}\big|y^+\big|^{-1-\breve{\epsilon}} g\big(\big|y^+\big|\big).$$

Then we can argue as above. □

Define

$$\tilde{\zeta}^+(x,\omega,\lambda) := \zeta^+\big(x, \sqrt{2\lambda}\omega\big) - \ln(2\lambda)^{(2-d)/4}.$$

Proposition 5.3.

(i) *There exist* (*uniform*) *estimates*

$$\big|\tilde{\zeta}^+(x,\omega,\lambda) - \ln g\big(|x|\big)^{(d-2)/2}\big| \leqslant C, \tag{5.14a}$$

$$\partial_\omega^\delta \partial_x^\gamma \tilde{\zeta}^+(x,\omega,\lambda) = O\big(|x|^{-|\gamma|}\big), \quad \textit{for } |\delta| + |\gamma| \geqslant 1. \tag{5.14b}$$

(ii) *There exist (uniform) estimates*

$$(2\lambda)^{(d-2)/4}\partial_\omega^\delta\partial_x^\gamma\big(\det\nabla_\xi\nabla_x\phi^+(x,\xi)\big)^{1/2}=g\big(|x|\big)^{(d-2)/2}O\big(|x|^{-|\gamma|}\big),$$
$$\textit{for } |\delta|+|\gamma|\geqslant 0. \tag{5.14c}$$

(iii) *There exist the locally uniform limits*

$$\partial_\omega^\delta\partial_x^\gamma\tilde\zeta^+(x,\omega,0):=\lim_{\lambda\searrow 0}\partial_\omega^\delta\partial_x^\gamma\tilde\zeta^+(x,\omega,\lambda).$$

Proof. Let us first prove the estimates (5.14b) for $|\delta|=0$, $|\gamma|\geqslant 1$ in the spherically symmetric case. $\partial_x^\gamma\zeta_{\mathrm{sph}}^+(x,\xi)$ is an integral of terms of the form

$$\partial_x^{\gamma_1}y\cdots\partial_x^{\gamma_n}y\,\partial_y^n\operatorname{div}F_{\mathrm{sph}}^+\big(y^+(t),\xi\big),$$

where $\gamma_1+\cdots+\gamma_n=\gamma$. Using $\partial_x^\gamma y^+=O(|x|^{1-|\gamma|}g(|x|)g(|y^+|)^{-1})$, cf. [6, Proposition 4.9], these integrals are bounded by

$$C_1\int_1^\infty |x|^{-|\gamma|+n}g\big(|x|\big)^n g\big(\big|y^+\big|\big)^{-n+1}\big|y^+\big|^{-n-1}\,\mathrm{d}t$$
$$\leqslant C_2\int_{|x|}^\infty |x|^{-|\gamma|+n}g\big(|x|\big)^n g\big(\big|y^+\big|\big)^{-n}\big|y^+\big|^{-n-1}\,\mathrm{d}\big|y^+\big|=O\big(|x|^{-|\gamma|}\big).$$

Thus

$$\partial_x^\gamma\zeta_{\mathrm{sph}}^+(x,\xi)=O\big(|x|^{-|\gamma|}\big),\quad \text{for } |\gamma|\geqslant 1.$$

Clearly we can argue as above for $|\delta|>0$ as well. If $|\gamma|=0$, we can use the formula (valid due to spherical symmetry)

$$\zeta_{\mathrm{sph}}^+(x,R_\eta\xi)=\zeta_{\mathrm{sph}}^+\big(R_\eta^{-1}x,\xi\big),$$

for any d-dimensional rotation R_η. Clearly this converts ω-derivatives to x-derivatives, and consequently we have shown (5.14b) in the general case.

Taking into account Lemma 5.2 we obtain the estimates (5.14b) in the general case (when V is not necessarily radial).

We have

$$\tilde\zeta_{\mathrm{sph}}^+(x,\xi)=\tilde\zeta_{\mathrm{sph}}^+\big(x,\sqrt{2\lambda}\hat x\big)+\int_0^\theta\nabla_\omega\tilde\zeta_{\mathrm{sph}}^+\big(x,\sqrt{2\lambda}\omega(l)\big)\cdot\omega^\perp(l)\,\mathrm{d}l,$$

where $[0,\theta]\ni l\mapsto\omega(l)$ is the arc joining $\hat x$ and ω and $\omega^\perp(l)$ is the tangent vector. Using (3.16) and (5.14b) with $|\delta|=1$, $|\gamma|=0$ and Lemma 5.2 we obtain (5.14a).

The above arguments in conjunction with the proof of Lemma 5.2 can be used to prove that there exist the limits

$$\lim_{\lambda \searrow 0} \partial_\omega^\delta \partial_x^\gamma \tilde{\zeta}^+(x, \omega, \lambda), \quad |\delta| + |\gamma| \geqslant 1.$$

We know from the explicit formula (3.13) that $\lim_{\lambda \searrow 0} \tilde{\zeta}^+_{\mathrm{sph}}(x, \hat{x}, \lambda)$ exists locally uniformly in x. Hence so does $\lim_{\lambda \searrow 0} \tilde{\zeta}^+(x, \omega, \lambda)$ locally uniformly in $(x, \omega) \in \Gamma^+$.

As for the bounds (5.14c), we use (5.14a) and (5.14b). □

5.3. Solving transport equations

Introduce the operator

$$\begin{aligned} M &= \left(\det \nabla_\xi \nabla_x \phi^+(x, \xi)\right)^{-1/2} \frac{\mathrm{i}}{2} \triangle_x \left(\det \nabla_\xi \nabla_x \phi^+(x, \xi)\right)^{1/2} \\ &= \mathrm{e}^{-\tilde{\zeta}^+(x,\xi)} \frac{\mathrm{i}}{2} \triangle_x \mathrm{e}^{\tilde{\zeta}^+(x,\xi)} \\ &= \frac{\mathrm{i}}{2}\left(\triangle_x + 2\nabla_x \zeta^+(x, \xi) \cdot \nabla_x + \triangle_x \zeta^+(x, \xi) + \nabla_x \zeta^+(x, \xi)^2\right). \end{aligned}$$

Notice that due to Proposition 5.3 this operator is well defined at $\lambda = 0$ (more precisely, for $(x, \omega, \lambda) \in \Gamma^+_{R_0,\sigma_0} \times \{0\}$).

We define inductively for $(x, \xi) \in \Gamma^+_{R,\sigma_0}$:

$$b_0^+(x, \xi) := 1;$$

$$b_{m+1}^+(x, \xi) := \int_1^\infty M b_m^+\left(y(t, x, \xi, t), \xi\right) \mathrm{d}t.$$

Proposition 5.4. *There exist the following (uniform) estimates*:

$$\partial_\omega^\delta \partial_x^\gamma b_m^+(x, \xi) = O\left(|x|^{-m(1-\mu/2)-|\gamma|}\right), \tag{5.15a}$$

$$\partial_\omega^\delta \partial_x^\gamma M b_m^+(x, \xi) = O\left(|x|^{-2-m(1-\mu/2)-|\gamma|}\right). \tag{5.15b}$$

Proof. For a given m, (5.15a) easily implies (5.15b).

Integrating $\partial_\omega^\delta \partial_x^\gamma M b_m(x, \xi)$ we can bound $\partial_\omega^\delta \partial_x^\gamma b_{m+1}(x, \xi)$ by

$$\begin{aligned} \int_1^\infty \left|y^+\right|^{-2-m(1-\mu/2)-|\gamma|} \mathrm{d}t &\leqslant C_1 \int_{|x|}^\infty \left|y^+\right|^{-2-m(1-\mu/2)-|\gamma|} g\left(\left|y^+\right|\right)^{-1} \mathrm{d}\left|y^+\right| \\ &\leqslant C_2 \int_{|x|}^\infty \left|y^+\right|^{-2-m(1-\mu/2)-|\gamma|+\mu/2} \mathrm{d}\left|y^+\right| = O\left(|x|^{-(m+1)(1-\mu/2)-|\gamma|}\right). \end{aligned}$$

This shows the induction step. □

We set

$$b^+(x,\xi) := \chi_2(\hat{x}\cdot\omega)\breve{b}^+(x,\xi), \qquad \breve{b}^+(x,\xi) = \sum_{m=0}^{\infty} b_m^+(x,\xi)\chi_1\big(|x|/R_m\big)$$

for an appropriately chosen sequence $R_m \to \infty$ (this is an example of the so-called Borel construction, cf. [13, Proposition 18.1.3]). There are (uniform) bounds

$$\partial_\omega^\delta \partial_x^\gamma b^+(x,\xi) = O\big(|x|^{-|\gamma|}\big).$$

We introduce

$$\begin{aligned} r^+(x,\xi) &= \big(\nabla_x\phi^+(x,\xi)\cdot\nabla_x + M\big)b^+(x,\xi),\\ r_{\rm pr}^+(x,\xi) &= \chi_2(\hat{x}\cdot\omega)\big(\nabla_x\phi^+(x,\xi)\cdot\nabla_x + M\big)\breve{b}^+(x,\xi),\\ r_{\rm bd}^+(x,\xi) &= r^+(x,\xi) - r_{\rm pr}^+(x,\xi). \end{aligned} \tag{5.16}$$

(The subscript pr stands for the *propagation* and bd stands for the *boundary*.)

Proposition 5.5. *There exist* (*uniform*) *bounds*

$$\partial_\omega^\delta \partial_x^\gamma r_{\rm pr}^+(x,\xi) = O\big(|x|^{-\infty}\big),$$

and $r_{\rm bd}^+(x,\xi)$ *is supported away from* $\Gamma_{R_0,\sigma}^+$ *and*

$$\partial_\omega^\delta \partial_x^\gamma r_{\rm bd}^+(x,\xi) = O\big(g\big(|x|\big)|x|^{-1-|\gamma|}\big).$$

5.4. Constructions in incoming region

Using the phase function $\phi^- = \phi^-(x,\omega,\lambda)$ given in (3.6) we can construct a symbol $a^- = \mathrm{e}^{\zeta^-}b^-$ with $t^- = \mathrm{e}^{\zeta^-}(r_{\rm pr}^- + r_{\rm bd}^-)$, $r_{\rm pr}^- = O(|x|^{-\infty})$ and the symbol $r_{\rm bd}^- = O(g(|x|)|x|^{-1})$ vanishing on a given $\Gamma_{R,\sigma}^- \subseteq \Gamma_{R_0,\sigma_0}^-$ and obeying appropriate analogues of the conditions of the previous subsection.

Similar to (5.4) we consider the Fourier integral operator J^- on $L^2(\mathbb{R}^d)$ given by

$$(J^- f)(x) = (2\pi)^{-d/2}\int \mathrm{e}^{\mathrm{i}\phi^-(x,\xi)}a^-(x,\xi)\hat{f}(\xi)\,\mathrm{d}\xi. \tag{5.17}$$

5.5. Fourier integral operators at fixed energies

For all $\tau \in L^2(S^{d-1})$ we introduce

$$\big(J^\pm(\lambda)\tau\big)(x) := (2\pi)^{-d/2}\int \mathrm{e}^{\mathrm{i}\phi^\pm(x,\omega,\lambda)}\tilde{a}^\pm(x,\omega,\lambda)\tau(\omega)\,\mathrm{d}\omega, \tag{5.18}$$

$$\big(T^\pm(\lambda)\tau\big)(x) := (2\pi)^{-d/2}\int \mathrm{e}^{\mathrm{i}\phi^\pm(x,\omega,\lambda)}\tilde{t}^\pm(x,\omega,\lambda)\tau(\omega)\,\mathrm{d}\omega, \tag{5.19}$$

where

$$\tilde{a}^{\pm}(x,\omega,\lambda) := (2\lambda)^{(d-2)/4} a^{\pm}\big(x, \sqrt{2\lambda}\omega\big),$$
$$\tilde{t}^{\pm}(x,\omega,\lambda) := (2\lambda)^{(d-2)/4} t^{\pm}\big(x, \sqrt{2\lambda}\omega\big).$$

The functions $\tilde{a}^{\pm}$ and $\tilde{t}^{\pm}$ are continuous in $(x,\omega,\lambda) \in \mathbb{R}^d \times S^{d-1} \times [0,\infty)$. This fact will be very important in the forthcoming sections. Due to these properties we can *define* $J^{\pm}(\lambda)$ and $T^{\pm}(\lambda)$ at $\lambda = 0$ by the expressions (5.18) and (5.19), respectively. We can split $T^{\pm}(\lambda) = T^{\pm}_{\mathrm{bd}}(\lambda) + T^{\pm}_{\mathrm{pr}}(\lambda)$ in agreement with the decomposition (5.16) (cf. (5.8)).

Throughout this subsection $\breve{\epsilon}$ signifies the $\breve{\epsilon} > 0$ appearing in Proposition 3.3 (it is tacitly assumed that $\breve{\epsilon} < 1 - \mu/2$)). For the problems at hand we can use coordinates for $\omega \in S^{d-1}$ sufficiently close to the dth standard vector $e_d \in \mathbb{R}^d$ specified as follows (using a partition of unity in the $\hat{x}$-variable and a rotation of coordinates this is without loss of generality):

$$\omega = \omega_\perp + \omega_d e_d; \qquad \omega_d = \sqrt{1-\omega_\perp^2}, \quad \omega_\perp \in \mathbb{R}^{d-1},\ |\omega_\perp| \text{ is small}. \tag{5.20}$$

Proposition 5.6. *There exist a (large) $R \geqslant R_0$ and a (small) $\tilde{\sigma} \in \,]0,\sigma_0]$ such that for all $|x| \geqslant R$ there exists a unique $\omega \in S^{d-1}$ satisfying $\omega \cdot \hat{x} \geqslant 1 - \tilde{\sigma}$ (alternatively: $x \in \Gamma^+_{R,\tilde{\sigma}}(\omega)$) and $\partial_\omega \phi^+(x,\omega,\lambda) = 0$. We introduce the notation $\omega^+_{\mathrm{crt}} = \omega^+_{\mathrm{crt}}(x,\lambda)$ for this vector. It is smooth in x and we have*

$$\partial_x^\gamma\big(\omega^+_{\mathrm{crt}} - \hat{x}\big) = O\big(|x|^{-\breve{\epsilon}-|\gamma|}\big).$$

Let

$$\phi(x,\lambda) = \phi^+\big(x, \omega^+_{\mathrm{crt}}(x,\lambda), \lambda\big). \tag{5.21}$$

This function solves the eikonal equation

$$\big(\partial_x \phi(x,\lambda)\big)^2/2 + V(x) = \lambda.$$

In the spherically symmetric case we have $\omega^+_{\mathrm{crt}} = \hat{x}$ and

$$\phi_{\mathrm{sph}}(x,\lambda) = \sqrt{2\lambda} R_0 + \int_{R_0}^{|x|} \sqrt{2\lambda - 2V(r)}\,\mathrm{d}r. \tag{5.22}$$

The proposition is obvious in the case $V_2 = 0$, cf. (3.9). The general case follows by an application of the fixed point theorem, cf. the proof of the similar statement [15, Lemma 4.1]. At this point one needs some control of the Hessian; we refer the reader to the proof of Theorem 5.7.

Of course, there is an analogue of Proposition 5.6 in the $-$ case; we then need to replace ϕ^+ with ϕ^-, and $\hat{x}$ with $-\hat{x}$. We obtain $\omega^-_{\mathrm{crt}}(x,\lambda) = -\omega^+_{\mathrm{crt}}(x,\lambda)$. Note the identity

$$\phi(x,\lambda) = -\phi^-\big(x, \omega^-_{\mathrm{crt}}(x,\lambda), \lambda\big).$$

Theorem 5.7. *Let* $\tau \in C^\infty(S^{d-1})$*. Then*

$$\big(J^\pm(\lambda)\tau\big)(x) = (2\pi)^{-\frac{1}{2}} \mathrm{e}^{\mp \mathrm{i}\pi\frac{d-1}{4}} g^{-\frac{1}{2}}(r,\lambda) r^{-\frac{d-1}{2}} \big(\mathrm{e}^{\pm \mathrm{i}\phi(x,\lambda)}\tau(\pm\hat{x}) + O\big(r^{-\breve{\epsilon}}\big)\big). \tag{5.23}$$

Moreover (5.23) *is uniform in* $(\hat{x},\lambda) \in S^{d-1} \times [0,\infty[$*. The same asymptotics holds for*

$$\pm g^{-1}\hat{x} \cdot pJ^\pm(\lambda)\tau(x).$$

Proof. We invoke the method of stationary phase (with a parameter given by the expression $h = h(r)$ of (3.14)), cf. [14, Theorem 7.7.6] or [15, Theorem 4.3]. For simplicity we consider only the $+$ case and we abbreviate $\omega_{\mathrm{crt}} = \omega^+_{\mathrm{crt}}$. This method yields (up to a minor point that is resolved below) that

$$\begin{aligned}\big(J^+(\lambda)\tau\big)(x) = (2\pi)^{-\frac{d}{2}} \mathrm{e}^{-\mathrm{i}\pi\frac{d-1}{4}} \big|\det\big(\partial^2_\omega \phi^+(x,\omega_{\mathrm{crt}},\lambda)/2\pi\big)\big|^{-\frac{1}{2}} \\ \times \mathrm{e}^{\mathrm{i}\phi^+(x,\omega_{\mathrm{crt}},\lambda)}\big(\tilde{a}^+(x,\omega_{\mathrm{crt}},\lambda)\tau(\omega_{\mathrm{crt}}) + g^{\frac{d-2}{2}} O\big(r^{-\breve{\epsilon}}\big)\big).\end{aligned} \tag{5.24}$$

Let us consider the Hessian. We first compute it in the case $V_2 = 0$ choosing coordinates such that $\hat{x} = e_d$ and using (5.20):

$$\partial^2_{\omega_\perp}\phi^+_{\mathrm{sph}}(\omega = \hat{x}) = -\partial_{\omega_\perp}\partial_{\hat{x}}\phi^+_{\mathrm{sph}}(\omega = \hat{x}),$$

and using the fact that

$$\partial_{\omega_\perp}\partial_{\hat{x}}\phi^+_{\mathrm{sph}}(\omega = \hat{x}) = hI, \tag{5.25}$$

cf. the computation (3.12) (here I refers to the form on $TS^{d-1}_{\hat{x}=\omega} \times TS^{d-1}_\omega$ given by the Euclidean metric), we obtain that

$$\partial^2_{\omega_\perp}\phi^+_{\mathrm{sph}}(\omega = \hat{x}) = -hI. \tag{5.26}$$

In particular the critical point is non-degenerate in this case.

Since ω_{crt} is a critical point, the second derivative has an invariant geometric meaning. Therefore, we can drop the reference to the special coordinates $\omega_\perp$ and we can write simply ∂^2_ω for $\partial^2_{\omega_\perp}$ in the left-hand side of (5.26). The formula (5.26) is then valid for all $\hat{x} \in S^{d-1}$.

The general case is similar. In particular, after applying Proposition 3.3 and (5.26), we obtain

$$\big|\det\big(\partial^2_\omega\phi^+(x,\omega_{\mathrm{crt}},\lambda)\big)\big| = h^{d-1}\big(1 + O\big(r^{-\breve{\epsilon}}\big)\big). \tag{5.27}$$

We conclude by combining (3.13), Lemma 5.2, Proposition 5.3, (5.27) and the construction of the symbol $\tilde{a}^+$ that (5.24) and indeed also (5.23) hold.

The second part of the theorem follows similarly. □

6. Wave matrices

In this section we study (modified) wave matrices. We prove that they have a limit at zero energy, in the sense of maps into an appropriate weighted space. This implies asymptotic oscillatory formulas for the standard short-range and Dollard scattering matrices.

6.1. Wave operators

The following theorem is essentially well known (follows from (3.3)). It describes a construction of modified wave operators similar to that of Isozaki–Kitada [18,19]. Notice, however, that the original construction involved energies strictly bounded away from zero. Notice also that the construction of $J^{\pm}$ in Section 5, although given under Conditions 2.1 and 2.2, in fact can be done under Condition 1.1 as well.

Theorem 6.1. *Suppose that V satisfies Condition* 1.1. *Then*

$$W^{\pm} f = \lim_{t\to\pm\infty} \mathrm{e}^{\mathrm{i}tH} J_0^{\pm} \mathrm{e}^{-\mathrm{i}tH_0} f = \lim_{t\to\pm\infty} \mathrm{e}^{\mathrm{i}tH} J^{\pm} \mathrm{e}^{-\mathrm{i}tH_0} f; \quad \hat{f} \in C_c\big(\mathbb{R}^d \setminus \{0\}\big). \tag{6.1}$$

The "wave operator" $W^{\pm}$ extends to an isometric operator on $L^2(\mathbb{R}^d)$ satisfying $HW^{\pm} = W^{\pm} H_0$, and its range is the absolutely continuous spectral subspaces of H. Moreover,

$$0 = \lim_{t\to\mp\infty} \mathrm{e}^{\mathrm{i}tH} J_0^{\pm} \mathrm{e}^{-\mathrm{i}tH_0} f = \lim_{t\to\mp\infty} \mathrm{e}^{\mathrm{i}tH} J^{\pm} \mathrm{e}^{-\mathrm{i}tH_0} f; \quad \hat{f} \in C_c\big(\mathbb{R}^d \setminus \{0\}\big). \tag{6.2}$$

Remarks. We know that $J_0^{\pm} 1_{]\epsilon,\infty[}(H_0)$ and $J^{\pm} 1_{]\epsilon,\infty[}(H_0)$ are bounded for any $\epsilon > 0$, but we *do not* know if $J_0^{\pm}$ and $J^{\pm}$ are bounded (not even under Conditions 2.1 and 2.2). This is the reason for restricting the choice of vectors in (6.1) and (6.2). An alternative, and equivalent, definition of $W^{\pm}$ as a bounded operator on $L^2(\mathbb{R}^d)$ is the following:

$$W^{\pm} = \text{s-}\lim_{\epsilon\searrow 0} \text{s-}\lim_{t\to\pm\infty} \mathrm{e}^{\mathrm{i}tH} J^{\pm} 1_{]\epsilon,\infty[}(H_0) \mathrm{e}^{-\mathrm{i}tH_0}.$$

The following general fact serves as the basic formula in stationary scattering theory, see Appendix A for a derivation.

Lemma 6.2. *Suppose there are densely defined operators $\breve{J}^{\pm}$ and $\breve{T}^{\pm}$ on $L^2(\mathbb{R}^d)$ such that $\breve{J}^{\pm} 1_{]\epsilon,\infty[}(H_0)$ and $\breve{T}^{\pm} 1_{]\epsilon,\infty[}(H_0)$ are bounded for any $\epsilon > 0$ and that $\breve{T}^{\pm} f = i(H\breve{J}^{\pm} - \breve{J}^{\pm} H_0) f$ for any $f \in L^2(\mathbb{R}^d)$ with $\hat{f} \in C_c(\mathbb{R}^d \setminus \{0\})$. Suppose there exists*

$$\breve{W}^{\pm} f := \lim_{t\to\pm\infty} \mathrm{e}^{\mathrm{i}tH} \breve{J}^{\pm} \mathrm{e}^{-\mathrm{i}tH_0} f, \quad \hat{f} \in C_c\big(\mathbb{R}^d \setminus \{0\}\big).$$

Then we have the following formula

$$\breve{W}^{\pm} f = \lim_{\epsilon\searrow 0} \int \big(\breve{J}^{\pm} + \mathrm{i}\, R(\lambda \mp \mathrm{i}\epsilon) \breve{T}^{\pm}\big) \delta_\epsilon(\lambda) f \, \mathrm{d}\lambda, \tag{6.3}$$

where $\delta_\epsilon(\lambda) = \frac{R_0(\lambda+\mathrm{i}\epsilon) - R_0(\lambda-\mathrm{i}\epsilon)}{2\pi\imath} = \frac{\epsilon}{\pi}((H_0 - \lambda)^2 + \epsilon^2)^{-1}$.

6.2. Wave matrices at positive energies

For any $s \in \mathbb{R}$ we recall the definition of weighted spaces $L^{2,s}(\mathbb{R}^d) := (1 + x^2)^{-s/2} L^2(\mathbb{R}^d)$.

Let Δ_ω denote the Laplace–Beltrami operator on the sphere S^{d-1}. For $n \in \mathbb{R}$ we define the Sobolev spaces on the sphere $L^{2,n}(S^{d-1}) := (1 - \Delta_\omega)^{-n/2} L^2(S^{d-1})$.

For $\lambda > 0$ we introduce $\mathcal{F}_0(\lambda)$ by

$$\mathcal{F}_0(\lambda) f(\omega) = (2\lambda)^{(d-2)/4} \hat{f}\big(\sqrt{2\lambda}\omega\big).$$

Let $s > \frac{1}{2}$ and $n \geqslant 0$. Note that $\mathcal{F}_0(\lambda)$ is a bounded operator in the space $\mathcal{B}(L^{2,s+n}(\mathbb{R}^d), L^{2,n}(S^{d-1}))$ and depends continuously on $\lambda > 0$. Likewise, $\mathcal{F}_0(\lambda)^* \in \mathcal{B}(L^{2,-n}(S^{d-1}), L^{2,-s-n}(\mathbb{R}^d))$ and it also depends continuously on $\lambda > 0$. Note also that the operator

$$\int \oplus \mathcal{F}_0(\lambda)\, \mathrm{d}\lambda : L^2\big(\mathbb{R}^d\big) \to \int_0^\infty \oplus L^2\big(S^{d-1}\big)\, \mathrm{d}\lambda \tag{6.4}$$

is unitary; consequently the operators $\mathcal{F}_0(\lambda)$ diagonalize the operator H_0. Finally,

$$\operatorname*{s-lim}_{\epsilon \searrow 0} \delta_\epsilon(\lambda) = \mathcal{F}_0(\lambda)^* \mathcal{F}_0(\lambda) \quad \text{in } \mathcal{B}\big(L^{2,s}\big(\mathbb{R}^d\big), L^{2,-s}\big(\mathbb{R}^d\big)\big). \tag{6.5}$$

Due to the limiting absorption principle we have the following partial analogue of (6.5) for the full Hamiltonian, defined under Condition 1.1: Let $s > \frac{1}{2}$ and

$$\delta_\epsilon^V(\lambda) := \frac{R(\lambda + \mathrm{i}\epsilon) - R(\lambda - \mathrm{i}\epsilon)}{2\pi \imath}. \tag{6.6}$$

Then there exists

$$\delta^V(\lambda) := \operatorname*{s-lim}_{\epsilon \searrow 0} \delta_\epsilon^V(\lambda) \quad \text{in } \mathcal{B}\big(L^{2,s}\big(\mathbb{R}^d\big), L^{2,-s}\big(\mathbb{R}^d\big)\big). \tag{6.7}$$

The operator-valued function $\delta^V(\cdot)$ is a strongly continuous function of $\lambda > 0$.

If Conditions 2.1–2.3 are true then we can extend the definition of $\delta^V(\lambda)$ to include $\lambda = 0$ if we demand that $s > \frac{1}{2} + \frac{\mu}{4}$, and the corresponding operator-valued function will be a strongly continuous (in fact, norm continuous) function of $\lambda \geqslant 0$, cf. Remark 4.2(2).

In the remaining part of this section we shall assume that the positive parameter σ' in (5.2) is sufficiently small (this requirement can be fulfilled uniformly in $\lambda \geqslant 0$). Notice that the condition conforms well with Lemma 3.2; we need it at various points, see for example the proof of Lemma 6.9.

Formally, we have $J^\pm(\lambda) = J^\pm \mathcal{F}_0(\lambda)^*$ and $T^\pm(\lambda) = T^\pm \mathcal{F}_0(\lambda)^*$. This suggests that (6.3) can be used to define wave operators at a fixed energy. This idea is used in the following theorem (which is essentially well known).

Theorem 6.3. *Suppose that the potential satisfies Condition* 1.1. *Let* $\epsilon > 0$, $n \geqslant 0$ *and* $\lambda > 0$. *Then*

$$W^\pm(\lambda) := J^\pm(\lambda) + \mathrm{i}\, R(\lambda \mp \mathrm{i}\, 0) T^\pm(\lambda) \tag{6.8}$$

defines a bounded operator in $\mathcal{B}(L^{2,-n}(S^{d-1}), L^{2,-\frac{1}{2}-\epsilon-n}(\mathbb{R}^d))$*, which depends continuously on* $\lambda > 0$*. It depends only on the splitting of the potential* V *into* V_1 *and* V_3 (*but does not depend on the details of the construction of* $J^\pm$). *For all* $f \in L^{2,\frac{1}{2}+\epsilon}(\mathbb{R}^d)$ *and* $g \in C_c(]0,\infty[)$*, we have*

$$W^\pm g(H_0) f = \int_0^\infty g(\lambda) W^\pm(\lambda) \mathcal{F}_0(\lambda) f \, \mathrm{d}\lambda. \tag{6.9}$$

Moreover,

$$W^\pm(\lambda) W^\pm(\lambda)^* = \delta^V(\lambda). \tag{6.10}$$

We set

$$w^\pm(\omega, \lambda) = W^\pm(\lambda)\delta_\omega,$$

where δ_ω *denotes the delta-function at* $\omega \in S^{d-1}$*. Then for all multiindices* δ *the function*

$$S^{d-1} \times]0,\infty[\ni (\omega, \lambda) \mapsto \partial_\omega^\delta w^\pm(\omega, \lambda) \in L^{2,-p}\big(\mathbb{R}^d\big); \quad p > |\delta| + d/2,$$

is continuous.

Remark. The operator $W^\pm(\lambda) : \mathcal{D}'(S^{d-1}) \to L^{2,-\infty}$ is called the *wave matrix at the energy* λ. Its range consists of generalized eigenfunction at the energy λ. The function $w^\pm(\omega,\lambda)$ (which belongs to $W^\pm(\lambda) L^{2,\frac{1}{2}-p}(S^{d-1})$ for $p > \frac{d}{2}$) is called the *generalized eigenfunction at the energy* λ *and outgoing* (*or incoming*) *asymptotic normalized velocity* ω.

Let us explain the steps of a proof of Theorem 6.3 (in the case of "+"-superscript only); our (main) results contained in Theorems 6.5 and 6.6 will be proved by a parallel procedure.

First one introduces a partition of unity of the form

$$\begin{aligned} I &= \mathrm{Op}^{\mathrm{r}}\big(\chi_+(a)\big) + \mathrm{Op}^{\mathrm{r}}\big(\chi_-(a)\tilde{\chi}_-(b)\big) + \mathrm{Op}^{\mathrm{r}}\big(\chi_-(a)\tilde{\chi}_+(b)\big) \\ &=: \mathrm{Op}^{\mathrm{r}}(\chi_1) + \mathrm{Op}^{\mathrm{r}}(\chi_2) + \mathrm{Op}^{\mathrm{r}}(\chi_3). \end{aligned} \tag{6.11}$$

Here a and b are the symbols introduced in (4.4) (rather than in (4.1) since we do not here impose Conditions 2.1–2.3) and χ_+ is a real-valued function as in Proposition 4.1(ii) such that $\chi_+(t) = 1$ for $t \geqslant 2C_0$, and $\chi_- = 1 - \chi_+$. Moreover, $\tilde{\chi}_-, \tilde{\chi}_+ \in C^\infty(\mathbb{R})$ are real-valued functions obeying $\tilde{\chi}_- + \tilde{\chi}_+ = 1$ and

$$\operatorname{supp} \tilde{\chi}_- \subseteq (-\infty, 1 - \bar{\sigma}], \tag{6.12}$$

$$\operatorname{supp} \tilde{\chi}_+ \subseteq [1 - 2\bar{\sigma}, \infty[. \tag{6.13}$$

The number $\bar{\sigma}$ needs to be taken (small) positive depending on the parameter σ of Section 5.1. (For the proof of Theorems 6.5 and 6.6 to be elaborated on later we refer at this point to (6.38) for the precise requirement.)

The proof of Theorem 6.3 is based on the following lemma:

Lemma 6.4. *Suppose that the potential satisfies Condition* 1.1.

(i) *For all* $n \geqslant 0$ *and* $\epsilon > 0$, $J^+(\lambda)$ *is a continuous function in* $\lambda > 0$ *with values in* $\mathcal{B}(L^{2,-n}(S^{d-1}), L^{2,-\frac{1}{2}-\epsilon-n}(\mathbb{R}^d))$.
(ii) *For all* $n \in \mathbb{R}$ *and* $\epsilon > 0$, $T^+_{\mathrm{bd}}(\lambda)$ *is a continuous function in* $\lambda > 0$ *with values in* $\mathcal{B}(L^{2,-n}(S^{d-1}), L^{2,\frac{1}{2}-\epsilon-n}(\mathbb{R}^d))$.
(iii) *For all* $m, n \in \mathbb{R}$, $\mathrm{Op}^{\mathrm{r}}(\chi_3)T^+_{\mathrm{bd}}(\lambda)$ *is a continuous function in* $\lambda > 0$ *with values in* $\mathcal{B}(L^{2,-n}(S^{d-1}), L^{2,m}(\mathbb{R}^d))$.
(iv) *For all* $m, n \in \mathbb{R}$, $T^+_{\mathrm{pr}}(\lambda)$ *is a continuous function in* $\lambda > 0$ *with values in* $\mathcal{B}(L^{2,-n}(S^{d-1}), L^{2,m}(\mathbb{R}^d))$.

More general statements than Lemma 6.4 (i)–(iv) will be given and proven in the context of treating small energies (see Lemma 6.8); these statements are under Conditions 2.1 and 2.2. Let us here use (i)–(iv) in an

Outline of the proof of Theorem 6.3. The expression (6.8) is a well-defined element of $\mathcal{B}(L^{2,-n}(S^{d-1}), L^{2,-\frac{1}{2}-\epsilon-n}(\mathbb{R}^d))$ due to the positive energy version of Proposition 4.8 and Lemma 6.4; this is for any $\epsilon > 0$ and $n \geqslant 0$. (Notice that (4.46) holds for any $t \in \mathbb{R}$ by Lemma 6.4.) Effectively, this argument is based on the following scheme (to be used below): We insert the right-hand side of (6.11) to the right of the resolvent in (6.8) and expand into three terms. Whence, by using Remark 4.2(4) and Lemma 6.4, we see that $W^+(\lambda)$ is a sum of four well-defined operators in $\mathcal{B}(L^{2,-n}(S^{d-1}), L^{2,-\frac{1}{2}-\epsilon-n}(\mathbb{R}^d))$, hence well-defined.

Next note that $\lambda \mapsto W^+(\lambda)$ is norm continuous, due to the norm continuity of each of the above mentioned four operators, which in turn may be seen by combining the continuity statements of Remark 4.2(4) and Lemma 6.4.

The statement on the independence of details of construction of $J^\pm$ is based on the positive energy version of Proposition 4.10; the interested reader will realize this by using arguments from the proof of Lemma 6.10 stated later.

The formula (6.9) can be verified by combining (6.3) with arguments used above, see Appendix A for an abstract approach. The identity (6.10) is a consequence of (6.9).

Finally, due to the fact that $\partial^\delta_\omega \delta_\omega \in L^{2,\frac{1}{2}-p}(S^{d-1})$ for $p > |\delta| + \frac{d}{2}$ (with continuous dependence of $\omega \in S^{d-1}$), we conclude that indeed $\partial^\delta_\omega w^+(\omega, \lambda) \in L^{2,-p}(\mathbb{R}^d)$ with a continuous dependence of ω and λ.

6.3. Wave matrices at low energies

Until the end of this section we assume that Conditions 2.1–2.3 are true. The main new result of this section is expressed in the following two theorems which concern the low-energy behaviour of the wave matrices of Theorem 6.3:

Theorem 6.5. *For* $s > \frac{1}{2} + \frac{\mu}{4}$ *and* $n \geqslant 0$,

$$W^\pm(0) := J^\pm(0) + \mathrm{i}\, R(\mp \mathrm{i}0) T^\pm(0) \tag{6.14}$$

defines a bounded operator in $\mathcal{B}(L^{2,-n}(S^{d-1}), L^{2,-s-n(1-\mu/2)}(\mathbb{R}^d))$. It depends only on the splitting of the potential V into V_1+V_2 and V_3 (but does not depend on the details of the construction of $J^\pm$). We have

$$W^\pm(0)W^\pm(0)^* = \delta^V(0). \tag{6.15}$$

If we set

$$w^\pm(\omega,0) = W^\pm(0)\delta_\omega,$$

then we obtain an element of $L^{2,-p}(\mathbb{R}^d)$ with $p > \frac{d}{2}+\frac{\mu}{2}-\frac{d\mu}{4}$ depending continuously on ω. In fact, more generally, $\partial_\omega^\delta w^\pm(\omega,0) \in L^{2,-p}(\mathbb{R}^d)$ with $p > (|\delta|+\frac{d}{2})(1-\frac{\mu}{2})+\frac{\mu}{2}$ with continuous dependence on ω.

Theorem 6.6. *For all $\epsilon>0$ and $n \geqslant 0$,*

$$\big(\langle x\rangle g\big)^{-n}\langle x\rangle^{-\frac12-\epsilon} g^{\frac12} W^\pm(\lambda) \tag{6.16}$$

is a continuous $\mathcal{B}(L^{2,-n}(S^{d-1}), L^2(\mathbb{R}^d))$-valued function in $\lambda \in [0,\infty[$.

For all $\epsilon>0$ and all multiindices δ, the function

$$S^{d-1}\times[0,\infty[\ \ni(\omega,\lambda)\mapsto \big(\langle x\rangle g\big)^{-|\delta|+\frac12-\frac{d}{2}}\langle x\rangle^{-\frac12-\epsilon} g^{\frac12}\partial_\omega^\delta w^\pm(\omega,\lambda)\in L^2\big(\mathbb{R}^d\big)$$

is continuous.

The following corollary interprets Theorem 6.6 in terms of the usual weighted spaces:

Corollary 6.7. *Let $n \geqslant 0$. We have*

$$W^\pm(0) = \lim_{\lambda\searrow 0} W^\pm(\lambda)$$

in the sense of operators in $\mathcal{B}(L^{2,-n}(S^{d-1}), L^{2,-\tilde s_n}(\mathbb{R}^d))$, where $\tilde s_n > \frac12 + n + \max(0, \frac{\mu}{4} - n\frac{\mu}{2})$. For all multiindices δ, the function

$$S^{d-1}\times[0,\infty[\ \ni(\omega,\lambda)\mapsto \partial_\omega^\delta w^\pm(\omega,\lambda)\in L^{2,-\tilde p}\big(\mathbb{R}^d\big)$$

is continuous, with $\tilde p > \frac{d}{2}+|\delta|$ for $d \geqslant 2$ and $\tilde p > \frac12 + |\delta| + \max(0, (1-2|\delta|)\frac{\mu}{4})$ for $d=1$.

The proof of Theorems 6.5 and 6.6 is based on the following analogue of Lemma 6.4 (for convenience we focus as before on the case of "+"-superscript only). The symbol χ_3 appearing in the statement (iii) below is specified as before, i.e. by (6.11) and the subsequent discussion.

Lemma 6.8.

(i) *For all $n \geqslant 0$ and $\epsilon > 0$,*

$$\big(\langle x\rangle g\big)^{-n}\langle x\rangle^{-\frac{1}{2}-\epsilon} g^{\frac{1}{2}} J^{+}(\lambda) \tag{6.17a}$$

is a continuous $\mathcal{B}(L^{2,-n}(S^{d-1}), L^2(\mathbb{R}^d))$-valued function in $\lambda \in [0,\infty[$.

(ii) *For all $n \in \mathbb{R}$ and $\epsilon > 0$,*

$$\big(\langle x\rangle g\big)^{-n}\langle x\rangle^{\frac{1}{2}-\epsilon} g^{-\frac{1}{2}} T^{+}_{\mathrm{bd}}(\lambda) \tag{6.17b}$$

is a continuous $\mathcal{B}(L^{2,-n}(S^{d-1}), L^2(\mathbb{R}^d))$-valued function in $\lambda \in [0,\infty[$.

(iii) *For all $m, n \in \mathbb{R}$,*

$$\langle x\rangle^{m}\,\mathrm{Op}^{\mathrm{r}}(\chi_3) T^{+}_{\mathrm{bd}}(\lambda) \tag{6.17c}$$

is a continuous $\mathcal{B}(L^{2,-n}(S^{d-1}), L^2(\mathbb{R}^d))$-valued function in $\lambda \in [0,\infty[$.

(iv) *For all $m, n \in \mathbb{R}$,*

$$\langle x\rangle^{m} T^{+}_{\mathrm{pr}}(\lambda) \tag{6.17d}$$

is a continuous $\mathcal{B}(L^{2,-n}(S^{d-1}), L^2(\mathbb{R}^d))$-valued function in $\lambda \in [0,\infty[$.

Later on we will actually need a slightly stronger bound than the one of Lemma 6.8(i) with $n = 0$, which we state below (referring to notation of (4.6) and (4.54)):

Lemma 6.9. *For all $\tau \in L^2(S^{d-1})$, $J^{+}(\lambda)\tau \in B^{*}_{s_0}$. In fact, with a bounding constant independent of $\lambda \geqslant 0$,*

$$g^{\frac{1}{2}} J^{+}(\lambda) \in \mathcal{B}\big(L^2\big(S^{d-1}\big), B^{*}_{\frac{1}{2}}\big).$$

Proof. We need to bound the operator $P_R := R^{-1} J^{+}(\lambda)^{*} g 1_{\{|x|<R\}} J^{+}(\lambda)$ independently of $R > 1$ and $\lambda \geqslant 0$. Writing $P_R = R^{-1}\int_0^R \mathrm{d}r \int_{S_r} Q_r\,\mathrm{d}x$ with $S_r = \{|x| = r\}$, it thus suffices to bound the operator $\int_{S_r} Q_r\,\mathrm{d}x$ independently of $r > 0$ and $\lambda \geqslant 0$.

Step I. Analysis of $\int_{S_r} Q_r\,\mathrm{d}x$. The kernel of Q_r is given by

$$Q_r(\omega,\omega') = \mathrm{e}^{\mathrm{i}(\phi^{+}(x,\omega',\lambda)-\phi^{+}(x,\omega,\lambda))} a(x,\omega,\omega',\lambda),$$

where

$$a(x,\omega,\omega',\lambda) = (2\pi)^{-d} g\big(|x|,\lambda\big)\overline{\tilde{a}^{+}(x,\omega,\lambda)}\tilde{a}^{+}(x,\omega',\lambda).$$

For simplicity, we shall henceforth omit the superscript $+$, $r > 0$ and $\lambda \geqslant 0$ in the notation.

Our goal is to show that $\int_{S_r} Q_r \,\mathrm{d}x$ is a PsDO on $L^2(S^{d-1})$ with symbol $b(\omega,\omega',z)$ obeying uniform bounds (uniform in $r>0$ and $\lambda \geqslant 0$)

$$\left|\partial_\omega^{\beta_1}\partial_{\omega'}^{\beta_2}\partial_z^{\alpha} b\right| \leqslant C_{\beta_1,\beta_2,\alpha}\langle z\rangle^{-|\alpha|}. \tag{6.18}$$

Clearly this would prove the lemma.

We can use a partition of unity on S^{d-1}, and therefore we can assume that the vectors ω,ω' and $\hat{x}$ are close to the dth standard vector $e_d \in \mathbb{R}^d$. Consequently, we can use coordinates

$$\omega = \omega_\perp + \omega_d e_d, \qquad \omega_d = \sqrt{1-\omega_\perp^2}, \tag{6.19}$$

$$x = x_\perp + x_d e_d, \qquad x_d = \sqrt{r^2 - x_\perp^2}. \tag{6.20}$$

Next we write

$$\phi(x,\omega') - \phi(x,\omega) = (\omega_\perp - \omega'_\perp)\cdot z, \qquad z = -\int_0^1 \partial_{\omega_\perp}\phi\big(x, s(\omega'-\omega)+\omega\big)\,\mathrm{d}s.$$

Step II. We shall show that the map

$$S_r \supset \mathcal{U} \ni x \to Tx = z \in \mathbb{R}^{d-1} \text{ is a diffeomorphism onto its range.} \tag{6.21}$$

Here $\mathcal{U}$ is an open neighbourhood of e_d containing the supports of $a(\cdot,\omega,\omega')$.

To this end we investigate the bilinear form $\partial_x\partial_\omega\phi(x,\omega)$ on $TS_x^{d-1}\times TS_\omega^{d-1}$. Note that

$$\partial_x\partial_\omega\phi^+_{\mathrm{sph}}(\hat{x}=\omega) = r^{-1}hI, \tag{6.22}$$

cf. (5.25).

In the coordinates (6.19) and (6.20), the identity (6.22) reads for $z_{\mathrm{sph}} = (Tx)_{\mathrm{sph}}$ (here we consider the case where $V_2 = 0$)

$$\partial_{x_j} z_{\mathrm{sph},\,i}(\omega=\omega'=\hat{x}) = -r^{-1}h\big(\delta_{ij} + \omega_d^{-2}\omega_i\omega_j\big), \quad i,j \leqslant d-1. \tag{6.23}$$

Due to (3.15), Proposition 3.3 and (6.23) we obtain the more general result

$$\partial_{x_j} z_i = -r^{-1}h\big(\delta_{ij} + \omega_d^{-2}\omega_i\omega_j + O(\sigma') + O\big(r^{-\check{\epsilon}}\big)\big), \quad i,j \leqslant d-1. \tag{6.24}$$

Here $O(\sigma')$ refers to a term obeying $|O(\sigma')| \leqslant C\sigma'$, where $\sigma' > 0$ is given in (5.2) (assumed to be small).

In particular, T is a local diffeomorphism with inverse determinant

$$|\partial_{x_j} z_i|^{-1} = \big(-r^{-1}h\big)^{1-d}\big(\omega'_d\big)^2\big(1 + O(\sigma') + O\big(r^{-\check{\epsilon}}\big)\big). \tag{6.25}$$

For a later application we note the uniform bounds

$$\partial_\omega^{\beta_1}\partial_{\omega'}^{\beta_2}\partial_x^{\alpha}|\partial_{x_j} z_i|^{-1} = g^{1-d}r^{-|\alpha|}O\big(r^0\big). \tag{6.26}$$

Also, T is injective: Suppose $Tx^1 = Tx^2$, then

$$0 = \int_0^1 \partial_{x_j} z_i\big(s\big(x^1 - x^2\big) + x^2\big)\big(x_j^1 - x_j^2\big)\,\mathrm{d}s$$
$$= -r^{-1}h\big(\big(\delta_{ij} + \omega_d^{-2}\omega_i\omega_j\big) + O(\sigma') + O\big(r^{-\check{\epsilon}}\big)\big)\big(x_j^1 - x_j^2\big).$$

Using the invertibility of the matrix $\delta_{ij} + \omega_d^{-2}\omega_i\omega_j$, it follows that $x^1 = x^2$.

Step III. Analysis of symbol b. Due to Step II, we can change coordinates and obtain that $\int_{S_r} Q_r\,\mathrm{d}x$ is a PsDO with a symbol $b = |\partial_{x_j} z_i|^{-1}a$. It remains to show (6.18). For zero indices $\beta_1 = \beta_2 = \alpha = 0$, we obtain the bound by combining Proposition 5.3 and (6.25). For derivatives, we note the bounds

$$\big|\partial_\omega^{\beta_1}\partial_{\omega'}^{\beta_2}\partial_x^\alpha z\big| \leqslant C_{\beta_1,\beta_2,\alpha} g r^{1-|\alpha|}, \tag{6.27}$$

which by a little bookkeeping yields

$$\big|\partial_\omega^{\beta_1}\partial_{\omega'}^{\beta_2}\partial_z^\gamma x\big| \leqslant C_{\beta_1,\beta_2,\gamma} r\langle z\rangle^{-|\gamma|}. \tag{6.28}$$

Another bookkeeping using Proposition 5.3, (6.25) and (6.28) yields (6.18). □

Proof of Lemma 6.8. We drop the superscript "+" and the parameter λ in the notation. We first prove uniform boundedness on any compact interval $[0, \lambda_1]$.

Re (i). We replace $J = J(\cdot)$ by $J\chi(\omega)$, where $\chi \in C^\infty(S^{d-1})$ with a sufficiently small support. We can assume that n is a non-negative integer. Instead of studying $J(1 - \Delta_\omega)^{n/2}$, it then suffices to study $J\partial_\omega^\nu$ for $|\nu| \leqslant n$.

Integrating by parts, we observe that the corresponding integral kernel equals

$$C\partial_\omega^\nu\big(\mathrm{e}^{\mathrm{i}\phi(x,\omega)}\tilde{a}(x,\omega)\big) = \mathrm{e}^{\mathrm{i}\phi(x,\omega)}\tilde{a}_\nu(x,\omega),$$

where $\tilde{a}_\nu$ is a linear combinations of terms of the form

$$\partial_\omega^{\nu_1}\phi(x,\omega)\cdots\partial_\omega^{\nu_k}\phi(x,\omega)\partial_\omega^{\nu_0}\tilde{a}(x,\omega),$$

with $\nu_0 + \nu_1 + \cdots + \nu_k = \nu$. Thus, using that $|\partial_\omega^\delta\phi| \leqslant C\langle x\rangle g$ (cf. (3.11d)) and Proposition 5.3, we obtain

$$\partial_\omega^\delta\partial_x^\gamma\tilde{a}_\nu(x,\omega) = O\big(\langle x\rangle^{n-|\gamma|}g^{n+\frac{d-2}{2}}\big). \tag{6.29}$$

Then we follow the proof of Lemma 6.9.

Re (ii). Assume first that $n \geqslant 0$. Then we follow the same scheme as above. The bound on the relevant kernel needs to be replaced by

$$\partial_\omega^\delta\partial_x^\gamma\tilde{t}_\nu(x,\omega) = O\big(\langle x\rangle^{n-1-|\gamma|}g^{n+\frac{d}{2}}\big), \tag{6.30}$$

cf. Proposition 5.5. Using (6.30) we can proceed as before.

Assume next that $n < 0$. We can assume that n is a negative integer. For fixed x, we decompose $\omega = \omega_\perp + \sqrt{1-\omega_\perp^2}\,\hat{x}$, where $\omega_\perp \cdot x = 0$. By (3.11c), we have the uniform lower bound

$$\left|\nabla_{\omega_\perp}\phi(x,\omega)\right| \geqslant c|x|g \quad \text{for } \hat{x}\cdot\omega \leqslant 1-\sigma, \tag{6.31}$$

and by (3.11d) the uniform upper bounds

$$\left|\partial_{\omega_\perp}^{\delta}\phi(x,\omega)\right| \leqslant C|x|g. \tag{6.32}$$

We apply the non-stationary method based on the identity

$$\left(\mathrm{i}\frac{\nabla_{\omega_\perp}\phi}{|\nabla_{\omega_\perp}\phi|^2}\cdot\nabla_{\omega_\perp}\right)^{-n}\mathrm{e}^{\mathrm{i}\phi^+(x,\omega)} = \mathrm{e}^{\mathrm{i}\phi(x,\omega)}.$$

After performing $-n$ integrations by parts, the bounds (6.31) and (6.32) yield

$$T\chi\tau = \sum_{|\nu|\leqslant -n}\int \tilde{t}_\nu(x,\omega)\partial_{\omega_\perp}^{\nu}\tau(\omega)\,\mathrm{d}\omega,$$

where the functions $\tilde{t}_\nu$ also satisfy the bounds (6.30). Then we proceed as before.

Re (iii). The kernel of $\mathrm{Op}^{\mathrm{r}}(\chi_3)T_{\mathrm{bd}}(\cdot)$ is given by the integral

$$\int \mathrm{d}\xi\,\mathrm{e}^{\mathrm{i}x\cdot\xi}\int \mathrm{e}^{\mathrm{i}(\phi(y,\omega)-y\cdot\xi)}k(\omega,y,\xi)\,\mathrm{d}y, \qquad k(\omega,y,\xi) = (2\pi)^{-3d/2}\chi_3(y,\xi)\tilde{t}_{\mathrm{bd}}(y,\omega).$$

It suffices to show that

$$\left|\partial_\xi^\beta\partial_\omega^\delta\int \mathrm{e}^{\mathrm{i}(\phi(y,\omega)-y\cdot\xi)}k(\omega,y,\xi)\,\mathrm{d}y\right| \leqslant C_{\beta,\delta} \quad \text{uniformly in } \xi, \omega \text{ and } \lambda. \tag{6.33}$$

Notice that the symbol k is compactly supported in ξ. First we observe that (using notation of Section 4.1)

$$k = k_{\omega,\lambda} \in S_{\mathrm{unif}}\big(g^{\frac{d}{2}}\langle x\rangle^{-1}, g_{\mu,\lambda}\big).$$

We can substitute $k \to k = F(|y| > 2\bar{R})k(\omega,y,\xi)$.

Next we integrate by parts, writing first

$$\left(\mathrm{i}\frac{\xi-\nabla_y\phi}{|\xi-\nabla_y\phi|^2}\cdot\nabla_y\right)^{\ell}\mathrm{e}^{\mathrm{i}(\phi(y,\omega)-y\cdot\xi)} = \mathrm{e}^{\mathrm{i}(\phi(y,\omega)-y\cdot\xi)}.$$

We need to argue that $\xi - \partial_y\phi \neq 0$ on the support of the involved symbol. For that we recall the following elementary inequality valid for all $z_1, z_2 \in \mathbb{R}^d$ and $\kappa_1, \kappa_2 > 0$:

$$|z_1 - z_2|^2 \geqslant \min\big(\kappa_1^2/2, \kappa_2 - \kappa_2^2/2\big)\big(|z_1|^2 + |z_2|^2\big), \tag{6.34}$$

provided one of the following three conditions holds:

$$|z_2| \leqslant (1-\kappa_1)|z_1|, \qquad |z_1| \leqslant (1-\kappa_1)|z_2| \quad \text{or} \quad z_1 \cdot z_2 \leqslant (1-\kappa_2)|z_1||z_2|.$$

Now, on the support of the symbol k we have $(1-\sigma')|y| \leqslant y \cdot \omega \leqslant (1-\sigma)|y|$, cf. (5.2). We use these inequalities in (3.5c) and (3.5d), yielding

$$1 - C\sigma' - C|y|^{-\breve{\epsilon}} \leqslant \frac{\nabla_y \phi(y,\omega)}{|\nabla_y \phi(y,\omega)|} \cdot \hat{y} \leqslant 1 - c\sigma + C|y|^{-\breve{\epsilon}},$$

which in turn (if $\bar{R}$ is taken large enough) implies that

$$1 - 2C\sigma' \leqslant \frac{\nabla_y \phi(y,\omega)}{g(|y|)} \cdot \frac{y}{\langle y \rangle} \leqslant 1 - \frac{c}{2}\sigma. \tag{6.35}$$

We claim that there exists a small $c' = c'(\sigma,\sigma') > 0$ such that

$$\left|\xi - \nabla_y \phi(y,\omega)\right| \geqslant c'\left(|\xi| + \left|\nabla_y \phi(y,\omega)\right|\right) \tag{6.36}$$

on the support of k (showing in particular that $\xi - \partial_y \phi \neq 0$).

Obviously, (6.36) follows from (6.34) with

$$z_1 = \frac{\xi}{g(|y|)} \quad \text{and} \quad z_2 = \frac{\nabla_y \phi(y,\omega)}{g(|y|)},$$

provided one of the above three conditions hold. If all of those conditions fail, so that intuitively $z_1 \approx z_2$, we can replace z_2 in (6.35) by z_1 yielding

$$1 - 3C\sigma' \leqslant b(x,\xi) \leqslant 1 - \frac{c}{3}\sigma. \tag{6.37}$$

Here we applied (6.34) for some κ_1 and κ_2, depending on σ and σ'. Now, the second inequality of (6.37) is violated on the support of $\tilde{\chi}_+(b(y,\xi))$, provided that $\bar{\sigma} > 0$ of (6.13) is chosen such that

$$2\bar{\sigma} < \frac{c}{3}\sigma. \tag{6.38}$$

We have shown the bound (6.36) on the support of the symbol k, and therefore in particular on the support of the relevant symbol, after performing the y-integrations by parts. The estimate (6.33) follows.

Re (iv). First we assume that $n \geqslant 0$. Integrating by parts in ω, as in the proof of (i), and using Proposition 5.5, which says that t_{pr} with all its derivatives is $O(\langle x \rangle^{-\infty})$, we obtain that $\langle x \rangle^m T_{\mathrm{pr}}(\lambda)$ is in $\mathcal{B}(L^{2,-n}(S^{d-1}), L^2(\mathbb{R}^d))$ for any m. The case $n < 0$ then follows trivially.

Let us now prove the continuity. Consider for instance (i). Let $\tau \in C^\infty(S^{d-1})$ and set

$$J_{n,\epsilon}(\lambda) := \left(\langle x \rangle g\right)^{-n} \langle x \rangle^{-\frac{1}{2}-\epsilon} g^{\frac{1}{2}} J(\lambda).$$

Clearly, for (small) $\kappa > 0$,

$$J_{n,\epsilon}(\lambda)\tau = F\bigl(\kappa|x| < 1\bigr) J_{n,\epsilon}(\lambda)\tau + F\bigl(\kappa|x| > 1\bigr)\langle x\rangle^{-\epsilon/2} J_{n,\epsilon/2}(\lambda)\tau. \tag{6.39}$$

We know that $J_{n,\epsilon/2}(\lambda)$ is bounded uniformly in λ. Hence the second term on the right of (6.39) is $O(\kappa^{\epsilon/2})$.

We know that $a(x,\omega,\lambda)$, $\phi(x,\omega,\lambda)$ and $g(x,\lambda)^{\pm 1}$ are continuous down to $\lambda = 0$. The first term on the right of (6.39) involves only variables in a compact set. Therefore it is continuous in λ. Hence $J_{n,\epsilon}(\lambda)\tau$ is continuous as the uniform limit of continuous functions.

By the uniform bound, which we proved before, we conclude that $J_{n,\epsilon}(\lambda)$ is strongly continuous in $\mathcal{B}(L^{2,-n}(S^{d-1}), L^2(\mathbb{R}^d))$.

Now

$$J_{n,\epsilon}(\lambda) = g^{\epsilon/2} J_{n+\epsilon/2,\epsilon/2}(\lambda)(1-\Delta_\omega)^{-\epsilon/4}(1-\Delta_\omega)^{\epsilon/4},$$

where $g^{\epsilon/2}$ is strongly continuous, $J_{n+\epsilon/2,\epsilon/2}(\lambda)$ is strongly continuous in $\mathcal{B}(L^{2,-n-\epsilon/2}(S^{d-1}), L^2(\mathbb{R}^d))$, $(1-\Delta_\omega)^{-\epsilon/4}$ is a compact operator on $L^{2,-n-\epsilon/2}(S^{d-1})$ and $(1-\Delta_\omega)^{\epsilon/4}$ is a unitary element of $\mathcal{B}(L^{2,-n}(S^{d-1}), L^{2,-n-\epsilon/2}(S^{d-1}))$. We invoke the general fact that the product of a strongly continuous operator-valued function and a compact operator is norm continuous. Whence we obtain the norm continuity of $J_{n,\epsilon}(\lambda)$ in $\mathcal{B}(L^{2,-n}(S^{d-1}), L^2(\mathbb{R}^d))$.

The proof of the norm continuity of the operators in the remaining parts of the lemma is similar. □

Outline of the proof of Theorems 6.5 and 6.6. The proof goes along the lines of the proof of Theorem 6.3. In particular this amounts to inserting the right-hand side of (6.11) to the right of the resolvent in (6.8) and expanding into three terms. Next, using Proposition 4.1 and Lemma 6.8, we conclude that $W^+(\lambda)$ is well defined as a sum of four operators, say $T_j(\lambda)$. In fact, all of the four maps

$$[0,\infty[\ \ni \lambda \to \bigl(\langle x\rangle g\bigr)^{-n}\langle x\rangle^{-\frac12-\epsilon} g^{\frac12} T_j(\lambda) \in \mathcal{B}\bigl(L^{2,-n}\bigl(S^{d-1}\bigr), L^2\bigl(\mathbb{R}^d\bigr)\bigr)$$

are continuous.

For the independence of $W^+(\lambda)$ of cutoffs, we use Propositions 4.8 and 4.10 in the same way as in the arguments for deducing (6.40) stated below.

The formula (6.15) follows by combining (6.10), Remark 4.2(2) and the shown continuity properties of $W^+(\lambda)$ and $W^+(\lambda)^*$. □

Lemma 6.10. *For any $\lambda \geqslant 0$, $R(\lambda \pm \mathrm{i}0)T^{\pm}(\lambda)$ is well defined as a map from $\mathcal{D}'(S^{d-1})$ to $L^{2,-\infty}$ and*

$$0 = J^{\pm}(\lambda) + \mathrm{i}\, R(\lambda \pm \mathrm{i}0) T^{\pm}(\lambda). \tag{6.40}$$

Proof. Note that we can extend Lemma 6.8 as follows: Let $\chi_- \in C_c^\infty(\mathbb{R})$ and $\tilde\chi_- \in C_c^\infty(\mathbb{R})$ with $\operatorname{supp}\tilde\chi_- \subseteq\ ]-\infty, 2\bar\sigma - 1[$ for some small $\bar\sigma > 0$. Then, for all $m, n \in \mathbb{R}$,

$$\mathrm{Op}^{\mathrm{r}}\bigl(\chi_-(a)\tilde\chi_-(b)\bigr)T^+_{\mathrm{bd}}(\lambda),\ \mathrm{Op}^{\mathrm{r}}\bigl(\chi_-(a)\tilde\chi_-(b)\bigr)J^+(\lambda) \in \mathcal{B}\bigl(L^{2,-n}\bigl(S^{d-1}\bigr), L^{2,m}\bigl(\mathbb{R}^d\bigr)\bigr),$$

cf. (6.37) (recall the standing hypothesis of this subsection that the positive parameter σ' in (5.2) is sufficiently small).

Therefore, for all $\tau \in \mathcal{D}'(S^{d-1})$ and $s \in \mathbb{R}$,

$$\big(WF^s_{\mathrm{sc}}\big(T^+(\lambda)\tau\big) \cup WF^s_{\mathrm{sc}}\big(J^+(\lambda)\tau\big)\big) \cap \{b < \bar{\sigma} - 1\} = \emptyset. \tag{6.41}$$

By the definition of $T^+(\lambda)$,

$$(H-\lambda)J^+(\lambda)\tau = -\mathrm{i}\,T^+(\lambda)\tau = -\mathrm{i}(H-\lambda)R(\lambda+\mathrm{i}0)T^+(\lambda)\tau. \tag{6.42}$$

Notice that due to (6.41) and Proposition 4.8(iii), the vector $u = R(\lambda+\mathrm{i}0)T^+(\lambda)\tau$ is in fact well-defined and

$$WF^s_{\mathrm{sc}}(u) \cap \{b < \bar{\sigma} - 1\} = \emptyset. \tag{6.43}$$

Using (6.41)–(6.43) and Proposition 4.10, we conclude that the generalized eigenfunction satisfies

$$J^+(\lambda)\tau + \mathrm{i}\,R(\lambda+\mathrm{i}0)T^+(\lambda)\tau = 0. \qquad \square \tag{6.44}$$

Remark. There exists an alternative time-dependent proof of Lemma 6.10 that avoids the use of Proposition 4.10: Due to (6.2)

$$0 = \lim_{\epsilon \searrow 0} \int \big(J^\pm + \mathrm{i}\,R(\lambda \pm \mathrm{i}\epsilon)T^\pm\big)\delta_\epsilon(\lambda) f \,\mathrm{d}\lambda, \quad \hat{f} \in C_c\big(\mathbb{R}^d \setminus \{0\}\big),$$

cf. Lemma 6.2 or Appendix A. The right-hand is given by

$$\int \big(J^\pm + \mathrm{i}\,R(\lambda \pm \mathrm{i}0)T^\pm\big)\delta_0(\lambda) f \,\mathrm{d}\lambda,$$

cf. Appendix A. Whence, by a density argument, (6.40) follows.

We complete this subsection by discussing a certain refined mapping property of $W^\pm(\lambda)$. Besides its own interest its application (see Corollary 6.12 stated below) will be needed in Section 8. The result is related to the fact that the continuity in λ of the operators in (6.16) and (6.17a) is proven only for $n \geqslant 0$ while the continuity in λ of the operator in (6.17b) is valid for all $n \in \mathbb{R}$.

Theorem 6.11. *Fix real-valued* $\chi, \tilde{\chi}_- \in C_c^\infty(\mathbb{R})$ *and* $\chi_+ \in C^\infty(\mathbb{R})$ *such that* $\operatorname{supp}\tilde{\chi}_- \subset]-1,1[$, $\chi_+' \in C_c^\infty(\mathbb{R})$ *and* $\operatorname{supp}\chi_+ \subset]C_0,\infty[$. *Let* $\tilde{A} := \mathrm{Op}^{\mathrm{w}}(\chi(a)\tilde{\chi}_-(b))$ *and* $A_+ := \mathrm{Op}^{\mathrm{w}}(\chi_+(a))$ *for* $\lambda \geqslant 0$. *For all* $n \in \mathbb{R}$, $\epsilon > 0$ *and with* $A = \tilde{A}$ *or* $A = A_+$,

$$W^\pm_{n,\epsilon}(\lambda) := \big(\langle x\rangle g\big)^{-n} \langle x\rangle^{-\frac{1}{2}-\epsilon} g^{\frac{1}{2}} A W^\pm(\lambda) \tag{6.45}$$

is a continuous $\mathcal{B}(L^{2,-n}(S^{d-1}), L^2(\mathbb{R}^d))$*-valued function in* $\lambda \in [0,\infty[$.

Proof. With reference (4.2) (this class of symbols is used extensively in [8])

$$B(\lambda) := \big(\langle x\rangle g\big)^{-n}\langle x\rangle^{-\frac{1}{2}-\epsilon} g^{\frac{1}{2}} A g^{-\frac{1}{2}}\langle x\rangle^{\frac{1}{2}+\frac{\epsilon}{2}}\big(\langle x\rangle g\big)^{n} \in \Psi_{\mathrm{unif}}\big(\langle x\rangle^{-\frac{\epsilon}{2}}, g_{\mu,\lambda}\big).$$

Whence, by the calculus, $B(\lambda) \in \mathcal{B}(L^2(\mathbb{R}^d))$ with a bound locally independent of $\lambda \geqslant 0$, and in fact $B(\cdot)$ is norm continuous. By using this continuity and Theorem 6.6, we conclude that it suffices to consider the case $n < 0$.

Re $A = \tilde{A}$. Since the construction of $W^+(\lambda)$ is independent of the (small) parameters σ and σ' in (5.2), we can take them smaller (if needed) to assure that

$$\sup \operatorname{supp} \chi_- < 1 - 3C\sigma'. \tag{6.46}$$

Here we refer to the left-hand side of (6.37).

Now, to show that $W^+_{n,\epsilon}(\lambda)$ is an element of $\mathcal{B}(L^{2,-n}(S^{d-1}), L^2(\mathbb{R}^d))$, we consider for $\lambda > 0$ the two terms of (6.8) separately (if $\lambda = 0$ we use instead (6.14)): The contribution from the first term (i.e. from $J^+(\lambda)$) has better mapping properties than specified, cf. Lemma 6.8(iii). In fact, using (6.46) we can mimic the proof of Lemma 6.8(iii) to handle this contribution. As for the contribution from the second term (i.e. from $\mathrm{i}\, R(\lambda - \mathrm{i}0)T^+(\lambda)$), we combine Lemma 6.8 (ii) and (iv) and Proposition 4.1(iii).

By the same arguments, continuity in $\lambda \geqslant 0$ is valid for the contribution from each of the mentioned two terms, hence for $W^+_{n,\epsilon}(\lambda)$.

Re $A = A_+$. Again we consider for $\lambda > 0$ the two terms of (6.8) separately (if $\lambda = 0$ we use instead (6.14)). The contribution from the first term $J^+(\lambda)$ has again better mapping properties than needed. More precisely, we have the following analogue of Lemma 6.8(iii):

For all $m \in \mathbb{R}$ the family of operators $\langle x\rangle^m A_+ J^+(\lambda)$ constitutes a continuous $\mathcal{B}(L^{2,-n}(S^{d-1}), L^2(\mathbb{R}^d))$-valued function of $\lambda \in [0, \infty[$.

To show this, we can again follow the proof of Lemma 6.8(iii). It suffices to show locally uniform boundedness in the indicated topology and we may replace $A_+ \to \mathrm{Op}^{\mathrm{r}}(\chi_+(a))$. The kernel of $\mathrm{Op}^{\mathrm{r}}(\chi_+(a))J^+(\lambda)$ is given by the integral

$$\int \mathrm{d}\xi\, \mathrm{e}^{\mathrm{i}x\cdot\xi} \int \mathrm{e}^{\mathrm{i}(\phi(y,\omega)-y\cdot\xi)} k_{\omega,\lambda}(y,\xi)\,\mathrm{d}y,$$

$$k_{\omega,\lambda}(y,\xi) = (2\pi)^{-3d/2}\chi_+\big(\xi^2/g\big(|y|,\lambda\big)^2\big)\tilde{a}^+(y,\omega,\lambda).$$

It suffices to show that

$$\langle\xi\rangle^{d+1}\left|\partial_\xi^\beta \partial_\omega^\delta \int \mathrm{e}^{\mathrm{i}(\phi(y,\omega)-y\cdot\xi)} k_{\omega,\lambda}(y,\xi)\,\mathrm{d}y\right| \leqslant C_{\beta,\delta} \quad \text{uniformly in } \xi, \omega \text{ and } \lambda. \tag{6.47}$$

For that we notice that

$$k = k_{\omega,\lambda} \in S_{\mathrm{unif}}\big(g^{\frac{d}{2}-1}, g_{\mu,\lambda}\big).$$

It suffices to show (6.47) with $k \to k = F(|y| > 2\bar{R})k_{\omega,\lambda}(y,\xi)$.

Next we integrate by parts, writing first

$$\left(\mathrm{i}\frac{\xi - \nabla_y\phi}{|\xi - \nabla_y\phi|^2}\cdot\nabla_y\right)^{\ell} \mathrm{e}^{\mathrm{i}(\phi(y,\omega)-y\cdot\xi)} = \mathrm{e}^{\mathrm{i}(\phi(y,\omega)-y\cdot\xi)},$$

and then we invoking the uniform bounds

$$C|\xi| \geqslant \left|\xi - \nabla_y \phi(y,\omega)\right| \geqslant c\left(|\xi| + \left|\nabla_y \phi(y,\omega)\right|\right), \tag{6.48}$$

which are valid on the support of k (provided $\bar{R}$ is chosen sufficiently large). Clearly, we obtain (6.47) by this procedure if ℓ (i.e. the number of integrations by parts) is chosen sufficiently large.

As for the contribution from the second term $\mathrm{i}\,R(\lambda - \mathrm{i}\,0)T^+(\lambda)$, we combine Lemma 6.8 (ii) and (iv) and Proposition 4.1(ii). □

We can extend the identities (6.10) and (6.15) (which below corresponds to $s = 0$) as follows:

Corollary 6.12. *Let $\chi, \tilde{\chi}_- \in C_c^\infty(\mathbb{R})$ be given as in Theorem 6.11. Fix $\lambda \geqslant 0$. Let again $\tilde{A} := \mathrm{Op}^{\mathrm{w}}(\chi(a)\tilde{\chi}_-(b))$. For all $\delta > \frac{1}{2}$ and $s \leqslant 0$, there exists the strong limit*

$$\operatorname*{s-lim}_{\epsilon \searrow 0} g^{\frac{1}{2}} \delta_\epsilon^V(\lambda)\tilde{A} g^{\frac{1}{2}} = g^{\frac{1}{2}} \delta^V(\lambda)\tilde{A} g^{\frac{1}{2}} = g^{\frac{1}{2}} W^\pm(\lambda) W^\pm(\lambda)^* \tilde{A} g^{\frac{1}{2}} \tag{6.49}$$

in $\mathcal{B}(L^{2,s+\delta}(\mathbb{R}^d), L^{2,s-\delta}(\mathbb{R}^d))$.

Proof. It follows from Proposition 4.9 that indeed there exists the limit

$$B := \operatorname*{s-lim}_{\epsilon \searrow 0} g^{\frac{1}{2}} \delta_\epsilon^V(\lambda)\tilde{A} g^{\frac{1}{2}} \quad \text{in } \mathcal{B}\left(L^{2,s+\delta}\left(\mathbb{R}^d\right), L^{2,s-\delta}\left(\mathbb{R}^d\right)\right).$$

Let $n = s/s_1$, where s_1 is given as in (4.6). Due to Theorem 6.11

$$W^\pm(\lambda)^* \tilde{A} g^{\frac{1}{2}} = \left(g^{\frac{1}{2}} \tilde{A} W^\pm(\lambda)\right)^* \in \mathcal{B}\left(L^{2,s+\delta}\left(\mathbb{R}^d\right), L^{2,n}\left(S^{d-1}\right)\right),$$

and due to Theorem 6.6

$$g^{\frac{1}{2}} W^\pm(\lambda) \in \mathcal{B}\left(L^{2,n}\left(S^{d-1}\right), L^{2,s-\delta}\left(\mathbb{R}^d\right)\right).$$

We have shown that

$$g^{\frac{1}{2}} W^\pm(\lambda) W^\pm(\lambda)^* \tilde{A} g^{\frac{1}{2}} \in \mathcal{B}\left(L^{2,s+\delta}\left(\mathbb{R}^d\right), L^{2,s-\delta}\left(\mathbb{R}^d\right)\right).$$

Since

$$Bv = g^{\frac{1}{2}} W^\pm(\lambda) W^\pm(\lambda)^* \tilde{A} g^{\frac{1}{2}} v \quad \text{for } v \in L^{2,\infty},$$

cf. (6.10) and (6.15), we are done by a density argument. □

6.4. Asymptotics of short-range wave matrices

Clearly, if $\mu > 1$, there exists

$$W_{\mathrm{sr}}^{\pm} f = \lim_{t\to\pm\infty} \mathrm{e}^{\mathrm{i}tH}\mathrm{e}^{-\mathrm{i}tH_0} f, \tag{6.50}$$

which is the usual definition of wave operators in the short-range case. In the case $\mu \in]1,2[$, we can compare our wave matrices with the wave matrices defined by (6.50).

Recall $\hat{p} := p/|p|$.

Theorem 6.13. *For $\mu \in]1,2[$, the operators*

$$\psi_{\mathrm{sr}}^{+}(p) := \mathrm{i}\int_{R_0}^{\infty} \big(|p| - F^{+}\big(l\hat{p}, \hat{p}, p^2/2\big)\cdot \hat{p}\big)\,\mathrm{d}l,$$

$$\psi_{\mathrm{sr}}^{-}(p) := -\mathrm{i}\int_{R_0}^{\infty} \big(|p| + F^{+}\big(-l\hat{p}, -\hat{p}, p^2/2\big)\cdot \hat{p}\big)\,\mathrm{d}l$$

are well-defined. If $V_2 = 0$, then $\psi_{\mathrm{sr}}^{\pm}(p) = \psi_{\mathrm{sr}}^{\pm}(|p|)$ with

$$\psi_{\mathrm{sr}}^{\pm}\big(|p|\big) = \pm\mathrm{i}\int_{R_0}^{\infty} \Big(|p| - \sqrt{p^2 - 2V_1(r)}\Big)\,\mathrm{d}r.$$

We have

$$W_{\mathrm{sr}}^{+} = W^{+}\mathrm{e}^{\mathrm{i}\psi_{\mathrm{sr}}^{+}(p)}, \tag{6.51a}$$

$$W_{\mathrm{sr}}^{-} = W^{-}\mathrm{e}^{\mathrm{i}\psi_{\mathrm{sr}}^{-}(p)}. \tag{6.51b}$$

Whence in particular, for all $\lambda > 0$,

$$W_{\mathrm{sr}}^{+}(\lambda) = W^{+}(\lambda)\mathrm{e}^{\mathrm{i}\psi_{\mathrm{sr}}^{+}(\sqrt{2\lambda}\cdot)}, \tag{6.52a}$$

$$W_{\mathrm{sr}}^{-}(\lambda) = W^{-}(\lambda)\mathrm{e}^{\mathrm{i}\psi_{\mathrm{sr}}^{-}(\sqrt{2\lambda}\cdot)}. \tag{6.52b}$$

Proof. One can readily show the theorem from well-known properties of the free evolution and the fact that

$$\phi^{+}(x,\omega,\lambda) + \int_{R_0}^{\infty} \big(\sqrt{2\lambda} - F^{+}(l\omega,\omega,\lambda)\cdot\omega\big)\,\mathrm{d}l = \sqrt{2\lambda}\omega\cdot x + o\big(|x|^0\big), \tag{6.53}$$

which in turn follows from [6, (4.50)] and a change a contour of integration. The asymptotics is locally uniform in $(\omega,\lambda) \in S^{d-1} \times]0,\infty[$. $\square$

Remark 6.14. $\psi_{\mathrm{sr}}^{\pm}$ is indeed oscillatory. Notice that for $V_1(r) = -\gamma r^{-\mu}$, as $\lambda \to 0^+$, we have

$$\psi_{\mathrm{sr}}^{+}(\sqrt{2\lambda}) = \int_{R_0}^{\infty} \left(\sqrt{2\lambda} - \sqrt{2\left(\lambda + \gamma r^{-\mu}\right)}\right) \mathrm{d}r$$

$$= (2\lambda)^{\frac{1}{2}-\frac{1}{\mu}} \int_{R_0(2\lambda)^{\frac{1}{\mu}}}^{\infty} \left(1 - \sqrt{1 + 2\gamma s^{-\mu}}\right) \mathrm{d}s$$

$$= (2\lambda)^{\frac{1}{2}-\frac{1}{\mu}} \int_{0}^{\infty} \left(1 - \sqrt{1 + 2\gamma s^{-\mu}}\right) \mathrm{d}s + O\left(\lambda^0\right),$$

cf. [28, (7.11)]. See Remark 6.16 for a similar result.

6.5. *Asymptotics of Dollard-type wave matrices*

For $\mu > \frac{1}{2}$ and $\mu + \epsilon_2 > 1$, the Dollard-type wave operators are given by

$$W_{\mathrm{dol}}^{\pm} f = \lim_{t \to \pm\infty} \mathrm{e}^{\mathrm{i}tH} U_{\mathrm{dol}}(t) f,$$

where

$$U_{\mathrm{dol}}(t) = \mathrm{e}^{-\mathrm{i}\int_0^t (p^2/2 + V_1(sp)1_{\{|sp| \geqslant R_0\}})\,\mathrm{d}s}.$$

We have the following analogue of Theorem 6.13.

Theorem 6.15. *For $\frac{1}{2} < \mu < 2$, $\epsilon_2 < 1$ and $\mu + \epsilon_2 > 1$, the operators*

$$\psi_{\mathrm{dol}}^{+}(p) = \mathrm{i} \int_{R_0}^{\infty} \left(|p| - F^+\left(l\hat{p}, \hat{p}, p^2/2\right) \cdot \hat{p} - |p|^{-1} V_1(l)\right) \mathrm{d}l,$$

$$\psi_{\mathrm{dol}}^{-}(p) = -\mathrm{i} \int_{R_0}^{\infty} \left(|p| + F^+\left(-l\hat{p}, -\hat{p}, p^2/2\right) \cdot \hat{p} - |p|^{-1} V_1(l)\right) \mathrm{d}l$$

are well-defined. If $V_2 = 0$, then $\psi_{\mathrm{dol}}^{\pm}(p) = \psi_{\mathrm{dol}}^{\pm}(|p|)$ and

$$\psi_{\mathrm{dol}}^{\pm}\left(|p|\right) = \pm\mathrm{i} \int_{R_0}^{\infty} \left(|p| - \sqrt{p^2 - 2V_1(r)} - |p|^{-1} V_1(r)\right) \mathrm{d}r.$$

We have

$$W^+_{\mathrm{dol}} = W^+ \mathrm{e}^{\mathrm{i}\,\psi^+_{\mathrm{dol}}(p)}, \tag{6.54a}$$

$$W^-_{\mathrm{dol}} = W^- \mathrm{e}^{\mathrm{i}\,\psi^-_{\mathrm{dol}}(p)}. \tag{6.54b}$$

Whence in particular, for all $\lambda > 0$

$$W^+_{\mathrm{dol}}(\lambda) = W^+(\lambda)\mathrm{e}^{\mathrm{i}\,\psi^+_{\mathrm{dol}}(\sqrt{2\lambda}\cdot)}, \tag{6.55a}$$

$$W^-_{\mathrm{dol}}(\lambda) = W^-(\lambda)\mathrm{e}^{\mathrm{i}\,\psi^-_{\mathrm{dol}}(\sqrt{2\lambda}\cdot)}. \tag{6.55b}$$

Proof. First we notice that $\psi^\pm_{\mathrm{dol}}$ are well-defined due to the fact that

$$\big(F^+ - F^+_{\mathrm{sph}}\big)(l\omega, \omega, \lambda) = O\big(l^{-\delta}\big)$$

for any $\delta < \min(\mu + \epsilon_2, 2\mu)$, and hence integrable. Here F^+_{sph} refers to the F^+ for the case $V_2 = 0$, whence $F^+_{\mathrm{sph}}(l\omega, \omega, \lambda) = g(l, \lambda)\omega$. For this estimate, we refer to [6, Remarks 6.2 2)] and the proof of [6, Lemma 6.4]. It appears stronger at the price of not being uniform in (small) λ. There is an extension of this estimate that allows us to integrate along the line segment joining x and $R\omega$ and taking the limit:

$$\begin{aligned}\int_x^{\infty\omega} \big(F^+ - F^+_{\mathrm{sph}}\big)(\bar{x}, \omega, \lambda)\cdot d\bar{x} &= \lim_{R\to\infty} \int_x^{R\omega} \big(F^+ - F^+_{\mathrm{sph}}\big)(\bar{x}, \omega, \lambda)\cdot \mathrm{d}\bar{x} \\ &= o\big(|x|^0\big).\end{aligned} \tag{6.56}$$

Introduce the auxillary phases

$$\phi^\pm_{\mathrm{dol}}(x, \omega, \lambda) = \sqrt{2\lambda}x\cdot\omega \mp (2\lambda)^{-\frac{1}{2}} \int_{R_0}^{\pm x\cdot\omega} V_1(l)\,\mathrm{d}l,$$

$$\phi^\pm_{\mathrm{aux}}(x, \omega, \lambda) = \phi^\pm_{\mathrm{aux}} = \phi^\pm_{\mathrm{dol}} - \int_x^{\pm\infty\omega} \big(F^+_{\mathrm{sph}} - \nabla_x\phi^\pm_{\mathrm{dol}}\big)\cdot \mathrm{d}\bar{x},$$

and corresponding modifiers

$$\big(J^\pm_\sharp f\big)(x) = (2\pi)^{-d/2} \int \mathrm{e}^{\mathrm{i}\,\phi^\pm_\sharp(x,\xi)} \chi(x, \pm\hat{\xi}) \hat{f}(\xi)\,\mathrm{d}\xi; \quad \xi = \sqrt{2\lambda}\omega.$$

Here we can take the function χ of the form $\chi(x, \omega) = \chi_1(|x|/R)\chi_2(\hat{x}\cdot\omega)$ with χ_1 and χ_2 given as in (5.1) and (5.2), respectively.

By the stationary phase method, [14, Theorem 7.7.6], one derives the following asymptotics in $L^2(\mathbb{R}^d)$ for any state f with $\hat{f} \in C_c^\infty(\mathbb{R}^d \setminus \{0\})$:

$$U_{\mathrm{dol}}(t) f \asymp J^\pm_{\mathrm{dol}} \mathrm{e}^{\mathrm{i}tH_0} f \asymp J^\pm_{\mathrm{aux}} \mathrm{e}^{\mathrm{i}tH_0} f \quad \text{as } t \to \pm\infty.$$

Next we notice the following analogue of (6.53), cf. (6.56):

$$\phi^{\pm}(x,\omega,\lambda)+\int_{R_0}^{\infty}\big(\nabla\phi^{+}_{\mathrm{dol}}-F^{+}\big)(\pm l\omega,\pm\omega,\lambda)\cdot\omega\,\mathrm{d}l$$
$$=\phi^{\pm}_{\mathrm{aux}}(x,\omega,\lambda)+o\big(|x|^0\big).$$

Again this asymptotics is locally uniform in $(\omega,\lambda)\in S^{d-1}\times\,]0,\infty[$. □

Remark 6.16. The first factor on the right-hand side of (7.11) is oscillatory. Let us state the following asymptotics for the special case where $V_1(r)=-\gamma r^{-\mu}$ for $r\geqslant R_0$:

$$\psi^{+}_{\mathrm{dol}}\big(\sqrt{2\lambda}\big)=\int_{R_0}^{\infty}\Big(\sqrt{2\lambda}-\sqrt{2\big(\lambda+\gamma r^{-\mu}\big)}+(2\lambda)^{-\frac12}\gamma r^{-\mu}\Big)\,\mathrm{d}r$$
$$=(2\lambda)^{\frac12-\frac1\mu}\int_{R_0(2\lambda)^{\frac1\mu}}^{\infty}\Big(1-\sqrt{1+2\gamma s^{-\mu}}+\gamma s^{-\mu}\Big)\,\mathrm{d}s.$$

For $\lambda\searrow 0$, this behaves as

$$\begin{aligned}
&(2\lambda)^{\frac12-\frac1\mu}C_\mu+O\big(\lambda^{-\frac12}\big), && \tfrac12<\mu<1;\\
&-\gamma(2\lambda)^{-\frac12}\ln 2\lambda+(2\lambda)^{-\frac12}C_1+O(1), && \mu=1;\\
&(2\lambda)^{-\frac12}\frac{R_0^{1-\mu}\gamma}{\mu-1}+O\big(\lambda^{\frac12-\frac1\mu}\big), && 1<\mu<2.
\end{aligned}$$

Here

$$C_\mu:=\int_0^{\infty}\Big(1-\sqrt{1+2\gamma s^{-\mu}}+\gamma s^{-\mu}\Big)\,\mathrm{d}s,$$

$$C_1:=\int_1^{\infty}\Big(1-\sqrt{1+2\gamma s^{-1}}+\gamma s^{-1}\Big)\,\mathrm{d}s+\int_0^{1}\Big(1-\sqrt{1+2\gamma s^{-1}}\Big)\,\mathrm{d}s-\gamma\ln R_0.$$

7. Scattering matrices

In this section we study (modified) scattering matrices. We prove that they have a limit at zero energy. This implies low energy oscillatory asymptotics for the standard short-range and Dollard scattering matrices.

7.1. Scattering matrices at positive energies

The scattering operator commutes with H_0, which is diagonalized by the direct integral decomposition (6.4). Because of that, the general theory of decomposable operators says that there exists a measurable family $]0,\infty[\ \ni \lambda \mapsto S(\lambda)$, with $S(\lambda)$ unitary operators on $L^2(S^{d-1})$ defined for almost all λ, such that

$$S \simeq \int_0^\infty \oplus S(\lambda)\,\mathrm{d}\lambda, \tag{7.1}$$

using the decomposition (6.4).

The following theorem is (essentially) well known:

Theorem 7.1. *Assume Condition* 1.1. *Then*

$$S(\lambda) = -2\pi J^+(\lambda)^* T^-(\lambda) + 2\pi \mathrm{i}\, T^+(\lambda)^* R(\lambda + \mathrm{i}0) T^-(\lambda) \tag{7.2a}$$

$$= -2\pi W^+(\lambda)^* T^-(\lambda) \tag{7.2b}$$

defines a unitary operator on $L^2(S^{d-1})$ depending strongly continuously on $\lambda > 0$. Moreover, (7.1) *is true. Furthermore, for all $n \in \mathbb{R}$ and $\epsilon > 0$,*

$$S(\lambda) \in \mathcal{B}\big(L^{2,n}\big(S^{d-1}\big), L^{2,n-\epsilon}\big(S^{d-1}\big)\big),$$

depending norm continuously on $\lambda > 0$. (Hence in particular $S(\lambda)$ maps $C^\infty(S^{d-1})$ into itself.)

For a derivation of the formula (7.2a) we refer the reader to Appendix A. For the remaining part of the theorem we refer the reader to the proof of Theorem 7.2 stated below (one can use Theorem 6.3 and Lemma 6.4 as substitutes for Theorem 6.6 and Lemma 6.8, respectively).

7.2. Scattering matrices at low energies

Until the end of this section we assume that Conditions 2.1–2.3 are true. The main new result of this section is the following theorem:

Theorem 7.2. *The result of Theorem* 7.1 *is true for all $\lambda \in [0,\infty[$. Specifically, if we define*

$$S(0) = -2\pi J^+(0)^* T^-(0) + 2\pi \mathrm{i}\, T^+(0)^* R(+\mathrm{i}0) T^-(0) \tag{7.3a}$$

$$= -2\pi W^+(0)^* T^-(0), \tag{7.3b}$$

then $S(0)$ is unitary, $\text{s-lim}_{\lambda\searrow 0} S(\lambda) = S(0)$ *in the sense of $\mathcal{B}(L^2(S^{d-1}))$ and* $\lim_{\lambda\searrow 0} S(\lambda) = S(0)$ *in the sense of $\mathcal{B}(L^{2,n}(S^{d-1}), L^{2,n-\epsilon}(S^{d-1}))$ for any $n \in \mathbb{R}$ and $\epsilon > 0$.*

Proof. First we notice that the expression

$$S(\lambda) = -2\pi W^+(\lambda)^* T^-(\lambda) \in \mathcal{B}\big(L^{2,n}\big(S^{d-1}\big), L^{2,n-\epsilon}\big(S^{d-1}\big)\big) \quad \text{for } n > 0,$$

has a norm continuous dependence of $\lambda \geqslant 0$. Indeed, fix $n > 0$ and $\epsilon \in]0, n]$, and pick $\epsilon_1, \epsilon_2 \in \mathbb{R}$ such that $\epsilon\frac{\mu}{2} < \epsilon_1 < \epsilon$ and $\epsilon_2 = \frac{1}{2}(\epsilon - \epsilon_1)$. We write

$$\begin{aligned} &W^+(\lambda)^* T^-(\lambda) \\ &\quad = \left(W^+(\lambda)^* g^{\frac{1}{2}} \langle x\rangle^{-\frac{1}{2}-\epsilon_2} \left(\langle x\rangle g\right)^{-n+\epsilon}\right)\left(g^{-\epsilon}\langle x\rangle^{-\epsilon_1}\right)\left(\left(\langle x\rangle g\right)^n \langle x\rangle^{\frac{1}{2}-\epsilon_2} g^{-\frac{1}{2}} T^-(\lambda)\right). \end{aligned} \tag{7.4}$$

We shall use the analogues of Lemma 6.8 (ii) and (iv) with $T^+(\lambda)$ replaced by $T^-(\lambda)$ (proved in the same way). The third factor on the right of (7.4) is continuous in λ with values in $\mathcal{B}(L^{2,n}(S^{d-1}), L^2(\mathbb{R}^d))$. The second factor is continuous in λ as an operator on $L^2(\mathbb{R}^d)$. The first factor is continuous in λ as an operator in $\mathcal{B}(L^2(\mathbb{R}^d), L^{2,n-\epsilon}(S^{d-1}))$ due to Theorem 6.6. This proves the norm continuity of $S(\lambda)$ in $\mathcal{B}(L^{2,n}(S^{d-1}), L^{2,n-\epsilon}(S^{d-1}))$ for $n > 0$.

Let us prove the same property for $n \leqslant 0$ using a slight extension of the above scheme: Notice that the positive sign condition above entered only in the condition $n - \epsilon \geqslant 0$ needed for applying Theorem 6.6. Since $n \leqslant 0$ we have $n - \epsilon < 0$ and therefore we need a substitute for Theorem 6.6. This is provided by Theorem 6.11 and an analogue of Lemma 6.8 for $T^-(\lambda)$. In fact, choose for (small) $\bar\sigma > 0$ real-valued $\tilde\chi_- \in C_c^\infty(\mathbb{R})$ and $\chi_+ \in C^\infty(\mathbb{R})$ such that $\operatorname{supp}\tilde\chi_- \subset]-1, 1[$, $\tilde\chi_- = 1$ in $[\bar\sigma - 1, 1 - \bar\sigma]$, $\operatorname{supp}\chi_+ \subset]C_0, \infty[$ and $\chi_+ = 1$ in $[2C_0, \infty[$. Let $\chi = 1 - \chi_+$, $\tilde A = \mathrm{Op}^{\mathrm{w}}(\chi(a)\tilde\chi_-(b))$, $A_+ = \mathrm{Op}^{\mathrm{w}}(\chi_+(a))$ and $\bar A = \mathrm{Op}^{\mathrm{w}}(\chi(a)(1 - \tilde\chi_-(b)))$. We insert the identity $I = \tilde A + A_+ + \bar A$

$$W^+(\lambda)^* T^-(\lambda) = \left((\tilde A + A_+) W^+(\lambda)\right)^* T^-(\lambda) + W^+(\lambda)^* \left(\bar A T^-(\lambda)\right). \tag{7.5}$$

Due to Theorem 6.11 the above argument can be repeated for the first term on the right-hand side, and if $\bar\sigma > 0$ is chosen sufficiently small we have the following analogue of Lemma 6.8 (iii) and (iv) (here stated in combination): For all $m \in \mathbb{R}$ the family of operators $\langle x\rangle^m \bar A T^-(\lambda)$ constitutes a continuous $\mathcal{B}(L^{2,-n}(S^{d-1}), L^2(\mathbb{R}^d))$-valued function of $\lambda \in [0, \infty[$. By choosing $m > \frac{1}{2} + \frac{\mu}{4}$ and using Theorem 6.6 we conclude norm continuity of the second term of (7.5).

But from the isometricity of S we see that $S(\lambda)$ is isometric for almost all λ as a map on $L^2(S^{d-1})$. Therefore, it is isometric and strongly continuous as a map on $L^2(S^{d-1})$ for all $\lambda \geqslant 0$.

By repeating this argument for S^* (not to be elaborated on) we obtain that $S(\lambda)^*$ is isometric and strongly continuous in $\lambda \geqslant 0$ as a map on $L^2(S^{d-1})$. Whence $S(\lambda)$ is unitary as a map on $L^2(S^{d-1})$. □

Remark. There is an alternative and completely stationary approach to proving the unitarity of the scattering matrices. In fact taking (7.2b) and (7.3b) as definitions the unitarity is a consequence of the formula (8.11), which in turn can be verified directly along the lines of Section 8.

7.3. Asymptotics of short-range scattering matrices

In the case $\mu \in]1, 2[$ we can compare $S(\lambda)$ with the S-matrix $S_{\mathrm{sr}}(\lambda)$ defined similarly

$$S_{\mathrm{sr}} = W_{\mathrm{sr}}^{+\,*} W_{\mathrm{sr}}^- \simeq \int_0^\infty \oplus S_{\mathrm{sr}}(\lambda)\,\mathrm{d}\lambda.$$

Under the condition of radial symmetry Yafaev considered in [28] the component of $S_{\mathrm{sr}}(\lambda)$ for each sector of fixed angular momentum. He computed an explicit oscillatory behaviour as $\lambda \to 0$.

The following result is a consequence of Theorem 6.13. In combination with Theorem 7.2, it yields oscillatory behaviour in a more general situation than considered in [28].

Theorem 7.3. *For $\mu \in]1,2[$, the operators S_{sr} and S are related by*

$$S_{\mathrm{sr}} = \mathrm{e}^{-\mathrm{i}\,\psi_{\mathrm{sr}}^{+}(p)} S \mathrm{e}^{\mathrm{i}\,\psi_{\mathrm{sr}}^{-}(p)}. \tag{7.6}$$

In particular, for all $\lambda > 0$,

$$S_{\mathrm{sr}}(\lambda) = \mathrm{e}^{-\mathrm{i}\,\psi_{\mathrm{sr}}^{+}(\sqrt{2\lambda}\cdot)} S(\lambda) \mathrm{e}^{\mathrm{i}\,\psi_{\mathrm{sr}}^{-}(\sqrt{2\lambda}\cdot)}, \tag{7.7}$$

and if $V_2 = 0$ then

$$S_{\mathrm{sr}}(\lambda) = e^{-\mathrm{i}\,2\int_{R_0}^{\infty}(\sqrt{2\lambda}-\sqrt{2(\lambda - V_1(r))})\,\mathrm{d}r} S(\lambda). \tag{7.8}$$

7.4. Asymptotics of Dollard-type scattering matrices

For $\mu > \frac{1}{2}$ and $\mu + \epsilon_2 > 1$, the Dollard-type S-matrix is diagonalized as before:

$$S_{\mathrm{dol}} = W_{\mathrm{dol}}^{+*} W_{\mathrm{dol}}^{-} \simeq \int_0^{\infty} \oplus S_{\mathrm{dol}}(\lambda)\,\mathrm{d}\lambda.$$

We have the following analogue of Theorem 7.3, cf. Theorem 6.15:

Theorem 7.4. *For $\frac{1}{2} < \mu < 2$, $\epsilon_2 < 1$ and $\mu + \epsilon_2 > 1$, the operators S_{dol} and S are related by*

$$S_{\mathrm{dol}} = \mathrm{e}^{-\mathrm{i}\,\psi_{\mathrm{dol}}^{+}(p)} S \mathrm{e}^{\mathrm{i}\,\psi_{\mathrm{dol}}^{-}(p)}. \tag{7.9}$$

In particular, for all $\lambda > 0$,

$$S_{\mathrm{dol}}(\lambda) = \mathrm{e}^{-\mathrm{i}\,\psi_{\mathrm{dol}}^{+}(\sqrt{2\lambda}\cdot)} S(\lambda) \mathrm{e}^{\mathrm{i}\,\psi_{\mathrm{dol}}^{-}(\sqrt{2\lambda}\cdot)}, \tag{7.10}$$

and if $V_2 = 0$ then

$$S_{\mathrm{dol}}(\lambda) = \mathrm{e}^{-\mathrm{i}\,2\int_{R_0}^{\infty}(\sqrt{2\lambda}-\sqrt{2(\lambda - V_1(r)} - (2\lambda)^{-1/2} V_1(r))\,\mathrm{d}r} S(\lambda). \tag{7.11}$$

Example 7.5. For the purely Coulombic case $V = -\gamma r^{-1}$ in dimension $d \geqslant 3$ one can compute

$$S(0) = \mathrm{e}^{\mathrm{i}\,c} P, \quad c \in \mathbb{R}, \tag{7.12}$$

where $(P\tau)(\omega) = \tau(-\omega)$. This formula can be verified using (7.11) and Remark 6.16, the explicit formula [30, (4.3)] for the Coulombic (Dollard) scattering matrix (slightly different from our definition), asymptotics of the Gamma function (see for example the reference [3] of [30]) and, for example, the stationary phase formula [14, Theorem 7.7.6] (alternatively one can use the formula [30, (3.4)]). It also follows (up to a compact term) from [7], where the constant c is computed as $c = 4\sqrt{2\gamma R_0} - \pi\frac{d-2}{2}$.

It follows from (7.12) that the singularities of the kernel $S(0)(\omega, \omega')$ in this particular case are located at $\{(\omega, \omega') \in S^{d-1} \times S^{d-1} \mid \omega = -\omega'\}$. We devote Section 9 to an extension of this result.

We also note that for the purely Coulombic case there is in fact a complete asymptotic expansion $S(\lambda) \asymp \sum_{j=0}^{\infty} S_j \lambda^{j/2}$. Here (of course) S_0 is given by (7.12), and one can readily check that $S_1 \neq 0$. In particular we see that $S(\lambda)$ is not smooth at $\lambda = 0$, cf. Remark 4.2(3). We refer to [2] (and references cited therein) for explicit expansions of the generalized purely Coulombic eigenfunctions at zero energy (for $d = 3$); those are also in $\sqrt{\lambda}$.

8. Generalized eigenfunctions

Throughout this section we impose Conditions 2.1–2.3. For any $\lambda \geqslant 0$, we define

$$\mathcal{V}^{-\infty}(\lambda) = \big\{u \in L^{2,-\infty} \bigm| (H - \lambda)u = 0\big\} \subseteq \mathcal{S}'\big(\mathbb{R}^d\big).$$

Elements of $\mathcal{V}^{-\infty}(\lambda)$ will be called generalized eigenfunctions of H at energy λ. In this section we study all generalized eigenfunctions of H.

Remark. Note that by Proposition 4.3, for any $u \in V^{-\infty}(\lambda)$ and $s \in \mathbb{R}$,

$$WF^s_{\mathrm{sc}}(u) \subseteq \big\{b^2 + \bar{c}^2 = 1\big\}. \tag{8.1}$$

8.1. Representations of generalized eigenfunctions

In this subsection we show that all generalized eigenfunctions can be represented by their incoming or outgoing data.

Theorem 8.1. *For any $\lambda \geqslant 0$ the map*

$$W^{\pm}(\lambda) : \mathcal{D}'\big(S^{d-1}\big) \to \mathcal{V}^{-\infty}(\lambda)\big(\subseteq L^{2,-\infty}\big)$$

is continuous and bijective.

Proof. *Step I.* Clearly $W^{\pm}(\lambda) : \mathcal{D}'(S^{d-1}) \to \mathcal{V}^{-\infty}(\lambda)$ is well defined and continuous, cf. Theorem 6.6.

Step II. We show that $W^{\pm}(\lambda)$ is onto. Let $u \in \mathcal{V}^{-\infty}(\lambda)$ be given. Let

$$\chi^{\pm} = \chi_-(a)\tilde{\chi}_{\pm}(b) + \frac{1}{2}\chi_+(a), \tag{8.2}$$

where $\chi_+ = 1 - \chi_-$ is a real-valued function as in Proposition 4.1(ii) such that $\chi_+(t) = 1$ for $t \geqslant 2C_0$, and $\tilde{\chi}_-, \tilde{\chi}_+ \in C^\infty(\mathbb{R})$ are real-valued functions obeying $\tilde{\chi}_- + \tilde{\chi}_+ = 1$ and

$$\operatorname{supp} \tilde{\chi}_- \subseteq]-\infty, 1/2[, \tag{8.3}$$

$$\operatorname{supp} \tilde{\chi}_+ \subseteq]-1/2, \infty[. \tag{8.4}$$

Now

$$\lim_{\epsilon\downarrow 0} R(\lambda \pm \mathrm{i}\epsilon)(H-\lambda)\,\mathrm{Op}^{\mathrm{r}}\big(\chi^{\pm}\big)u$$
$$= \mathrm{Op}^{\mathrm{r}}\big(\chi^{\pm}\big)u \pm \lim_{\epsilon\downarrow 0} \mathrm{i}\epsilon R(\lambda \pm \mathrm{i}\epsilon)\,\mathrm{Op}^{\mathrm{r}}\big(\chi^{\pm}\big)u. \tag{8.5}$$

Note that $\lim_{\epsilon\downarrow 0} R(\lambda \pm \mathrm{i}\epsilon)\,\mathrm{Op}^{\mathrm{r}}(\chi^{\pm})u$ exists, due to Propositions 4.3, 4.7, and 4.9. Therefore the second term on the right of (8.5) is zero. Therefore, we have

$$0 = \mathrm{Op}^{\mathrm{r}}\big(\chi^{\pm}\big)u - R(\lambda \pm \mathrm{i}0)(H-\lambda)\,\mathrm{Op}^{\mathrm{r}}\big(\chi^{\pm}\big)u. \tag{8.6}$$

Adding the two equations of (8.6) yields

$$u = 2\pi \imath \delta^{V}(\lambda)(H-\lambda)\,\mathrm{Op}^{\mathrm{r}}\big(\chi^{+}\big)u,$$

which in turn in conjunction with Proposition 4.3, (6.10), (6.15) and Corollary 6.12 yields

$$u = W^{\pm}(\lambda)\tau, \qquad \tau = \pm 2\pi \mathrm{i}\, W^{\pm}(\lambda)^{*}\big[H, \mathrm{Op}^{\mathrm{r}}\big(\chi^{\pm}\big)\big]u \in \mathcal{D}'\big(S^{d-1}\big). \tag{8.7}$$

Step III. We show that $W^{\pm}(\lambda)$ is injective. For convenience we shall only treat the case of superscript $+$. By (8.7) we need to show that for all $\tau \in \mathcal{D}'(S^{d-1})$

$$\tau = 2\pi \mathrm{i}\, W^{+}(\lambda)^{*}(H-\lambda)\,\mathrm{Op}^{\mathrm{r}}\big(\chi^{+}\big)W^{+}(\lambda)\tau. \tag{8.8}$$

By continuity it suffices to verify (8.8) for $\tau \in C^{\infty}(S^{d-1})$. This can be done as follows. Pick non-negative $f \in C_c^{\infty}(\mathbb{R})$ with $\int_0^{\infty} f(s)\,\mathrm{d}s = 1$, and let $F_R(t) = 1 - \int_0^{t/R} f(s)\,\mathrm{d}s$; $R > 1$. We write the right-hand side of (8.8) as

$$\text{w-}\lim_{R\to\infty} 2\pi \mathrm{i}\, W^{+}(\lambda)^{*} F_R\big(\langle x\rangle\big)(H-\lambda)\,\mathrm{Op}^{\mathrm{r}}\big(\chi^{+}\big)W^{+}(\lambda)\tau \tag{8.9}$$

and pull the factor $(H-\lambda)$ to the left. Thus (8.9) equals

$$\text{w-}\lim_{R\to\infty} 2\pi R^{-1} W^{+}(\lambda)^{*} f\big(\langle x\rangle/R\big) g\,\mathrm{Op}^{\mathrm{r}}\big(b\chi^{+}\big)W^{+}(\lambda)\tau.$$

If $\lambda \geqslant 0$, we insert (6.8) for $W^{+}(\lambda)$ (if $\lambda = 0$, we use instead (6.14)). By Proposition 4.1 (ii) and (iii) and Lemma 6.8 (ii) and (iv), we can replace each factor of $W^{+}(\lambda)$ by a factor of $J^{+}(\lambda)$, cf. the proof of Theorem 6.11. Moreover, we can replace the factor $\mathrm{Op}^{\mathrm{r}}(b\chi^{+})$ by the operator $g^{-1}\hat{x}\cdot p$. Therefore, (8.9) becomes

$$\text{w-}\lim_{R\to\infty} 2\pi R^{-1} J^{+}(\lambda)^{*} f\big(\langle x\rangle/R\big)\hat{x}\cdot p J^{+}(\lambda)\tau. \tag{8.10}$$

By Theorem 5.7, (8.10) equals τ. The identity (8.8) follows. □

Remarks.

(1) A somewhat similar representation formula has been derived for representing positive solutions to a PDE, see for example [22]. This involves the so-called Martin boundary. In our case, the notion analogous to the "Martin boundary" would be S^{d-1}.

(2) For $V_3 = 0$, we have

$$\mathcal{V}^{-\infty}(\lambda) = \{u \in \mathcal{S}'(\mathbb{R}^d) \mid (H - \lambda)u = 0\},$$

and hence the set $\mathcal{V}^{-\infty}(\lambda)$ is closed in $\mathcal{S}'(\mathbb{R}^d)$ (with respect to the weak-$*$ topology of $\mathcal{S}'(\mathbb{R}^d)$). Moreover, in this case $W^{\pm}(\lambda)$ maps $\mathcal{D}'(S^{d-1})$ bicontinuously onto $\mathcal{V}^{-\infty}(\lambda)$.
In fact, suppose $u \in \mathcal{S}'(\mathbb{R}^d)$ obeys $(H - \lambda)u = 0$. Then for some $m \in \mathbb{N}$ we have $\langle p\rangle^{-2m} u \in L^{2,-\infty}$. But $(H - \lambda + \mathrm{i})^{-m}\langle p\rangle^{2m}$ is bounded on any $L^{2,s}$. Whence, showing that indeed $u \in \mathcal{V}^{-\infty}(\lambda)$,

$$\mathrm{i}^{-m} u = (H - \lambda + \mathrm{i})^{-m} u = (H - \lambda + \mathrm{i})^{-m}\langle p\rangle^{2m}\big(\langle p\rangle^{-2m} u\big) \in L^{2,-\infty}.$$

8.2. Scattering matrices – an alternative construction

The construction of scattering matrices given in Sections 7.1 and 7.2 involved a detailed knowledge of appropriate operators, see the proof of Theorem 7.2. However, given the theory of wave matrices developed in Section 8.1 and the basic formulas (6.10) and (6.15) for the spectral resolution, we could have constructed the scattering matrix more easily.

Recall from Theorem 8.1 that $W^{\pm}(\lambda) : \mathcal{D}'(S^{d-1}) \to L^{2,-\infty}$ is injective. Hence, $W^{\pm}(\lambda)^*: L^{2,\infty} \to C^{\infty}(S^{d-1})$ has a dense range.

For $\tau \in L^2(S^{d-1})$ of the form $\tau = W^-(\lambda)^* v$ with $v \in L^{2,\infty}$, we define $S(\lambda)\tau := W^+(\lambda)^* v$. By (6.10) and (6.15), we know that

$$\big\|W^+(\lambda)^* v\big\|^2 = \big\|W^-(\lambda)^* v\big\|^2 = \big\langle v, \delta^V(\lambda) v\big\rangle.$$

Hence $S(\lambda)$ is indeed well-defined and isometric. But $W^{\pm}(\lambda)^* L^{2,\infty}$ is dense in $C^{\infty}(S^{d-1})$, and therefore also in $L^2(S^{d-1})$. Whence $S(\lambda)$ extends to an isometric operator on $L^2(S^{d-1})$. Reversing the role of $+$ and $-$, we obtain that $S(\lambda)$ is actually unitary. By construction, it satisfies

$$S(\lambda) W^-(\lambda)^* = W^+(\lambda)^*, \quad \lambda \geqslant 0. \tag{8.11}$$

8.3. Geometric scattering matrices

The following type of result was proved for a class of constant coefficient Hamiltonians (with no potential) in [1], and generalized to Schrödinger operators with long-range potentials (for a class including the one given by Condition 1.1) at positive energies by [9]. It gives a characterization of the space $W^{\pm}(\lambda) L^2(S^{d-1})$, which in turn yields yet another characterization of the scattering matrix $S(\lambda)$.

Let $s_0 = s_0(\lambda)$ be given as in (4.6), and introduce in terms of a dual Besov space

$$\mathcal{V}^{-s_0}(\lambda) := B^*_{s_0} \cap \mathcal{V}^{-\infty}(\lambda)$$

endowed with the topology of $B^*_{s_0}$. The statement (iv) below is given in terms of the phase function $\phi = \phi(x, \lambda)$ of (5.21).

Theorem 8.2.

(i) *For all* $\tau \in L^2(S^{d-1})$,

$$WF_{\mathrm{sc}}^{-s_0}\big(W^{\pm}(\lambda)\tau\big) \subseteq \{b=-1\} \cup \{b=1\}.$$

(ii) *The operator* $W^{\pm}(\lambda)$ *maps* $L^2(S^{d-1})$ *bijectively and bicontinuously onto* $\mathcal{V}^{-s_0}(\lambda)$.
(iii) *The operator* $W^{\pm}(\lambda)^*$ *(defined a priori on* $B_{s_0}^{**} \supseteq B_{s_0}$*) maps* B_{s_0} *onto* $L^2(S^{d-1})$.
(iv) *For all* $\tau \in L^2(S^{d-1})$,

$$W^{-}(\lambda)\tau(x) - \frac{\mathrm{e}^{\mathrm{i}\pi\frac{d-1}{4}}\mathrm{e}^{-\mathrm{i}\phi(x,\lambda)}\tau(-\hat{x}) + \mathrm{e}^{-\mathrm{i}\pi\frac{d-1}{4}}\mathrm{e}^{\mathrm{i}\phi(x,\lambda)}(S(\lambda)\tau)(\hat{x})}{(2\pi)^{\frac{1}{2}}g^{\frac{1}{2}}(r,\lambda)r^{\frac{d-1}{2}}} \in B_{s_0,0}^{*}, \tag{8.12}$$

$$W^{+}(\lambda)\tau(x) - \frac{\mathrm{e}^{-\mathrm{i}\pi\frac{d-1}{4}}\mathrm{e}^{\mathrm{i}\phi(x,\lambda)}\tau(\hat{x}) + \mathrm{e}^{\mathrm{i}\pi\frac{d-1}{4}}\mathrm{e}^{-\mathrm{i}\phi(x,\lambda)}(S(\lambda)^*\tau)(-\hat{x})}{(2\pi)^{\frac{1}{2}}g^{\frac{1}{2}}(r,\lambda)r^{\frac{d-1}{2}}} \in B_{s_0,0}^{*}, \tag{8.13}$$

$$\|\tau\|^2_{L^2(S^{d-1})} = \lim_{R\to\infty} R^{-1} \int\limits_{r<R} \big|\sqrt{\pi}\, g^{\frac{1}{2}}(r,\lambda)W^{\pm}(\lambda)\tau\big|^2\,\mathrm{d}x. \tag{8.14}$$

Proof. Re (i). Again we concentrate on the case of superscript $+$. Let $\tau \in L^2(S^{d-1})$ be given. We shall use the partition (6.11), as in the proof of Theorems 6.5 and 6.6, so let $\bar{\sigma} > 0$ be given as before, cf. (6.12) and (6.13). As for the partition functions (8.2), we modify (8.3) and (8.4) by replacing here $\tilde{\chi}_{\pm} \to \tilde{\chi}_{\pm,\mathrm{righ}}$

$$\operatorname{supp} \tilde{\chi}_{-,\mathrm{righ}} \subseteq \left]-\infty, 1-\bar{\sigma}/4\right[, \tag{8.15}$$

$$\operatorname{supp} \tilde{\chi}_{+,\mathrm{righ}} \subseteq \left]1-\bar{\sigma}/2, \infty\right[. \tag{8.16}$$

Then it follows from Propositions 4.1 and 4.3 and Lemmas 6.8 and 6.9 that

$$\mathrm{Op}^{\mathrm{r}}\big(\chi^{+}_{\mathrm{righ}}\big)W^{+}(\lambda) \in \mathcal{B}\big(L^2\big(S^{d-1}\big), B^{*}_{s_0}\big). \tag{8.17}$$

(The fact that this bound holds for $W^{+}(\lambda) \to J^{+}(\lambda)$ is indeed a consequence of Lemma 6.9 due to interpolation, cf. [13, Theorem 14.1.4], but it can also be proved concretely along the lines of the proofs of Lemma 6.9 and Theorem 6.11.)

Since $\langle W^{+}(\lambda)\tau, \mathrm{i}[H, F_R\,\mathrm{Op}^{\mathrm{r}}(\chi^{+}_{\mathrm{righ}})]W^{+}(\lambda)\tau\rangle = 0$, we conclude from (4.30) and (8.17) that

$$\sup_{R>1} \mathrm{Re}\big\langle W^{+}(\lambda)\tau, \mathrm{Op}^{\mathrm{w}}\big(F_R\chi_{-}(a)\tilde{\chi}'_{\mathrm{righ}}(b)gr^{-1}\big)W^{+}(\lambda)\tau\big\rangle \leqslant C\|\tau\|^2. \tag{8.18}$$

Here we used the calculus of pseudodifferential operators, cf. [14, Theorem 18.6.8].

In combination with Propositions 4.3 and 4.5, we conclude that

$$\{-1<b<1\} \cap WF_{\mathrm{sc}}^{-s_0}\big(W^{+}(\lambda)\tau\big) = \emptyset. \tag{8.19}$$

Re (ii) (Boundedness).

To proceed from here we change (8.15) and (8.16) as follows:

$$\operatorname{supp}\tilde{\chi}_{-,\mathrm{lef}} \subseteq]-\infty, -1+\bar{\sigma}/2[, \tag{8.20}$$

$$\operatorname{supp}\tilde{\chi}_{+,\mathrm{lef}} \subseteq]-1+\bar{\sigma}/4, \infty[. \tag{8.21}$$

With these cutoffs we can show analogously that

$$\mathrm{Op}^{\mathrm{r}}(\chi_{\mathrm{lef}}^{-})W^{-}(\lambda) \in \mathcal{B}\big(L^2\big(S^{d-1}\big), B_{s_0}^{*}\big). \tag{8.22}$$

Using (8.11), this leads to

$$\mathrm{Op}^{\mathrm{r}}(\chi_{\mathrm{lef}}^{-})W^{+}(\lambda) \in \mathcal{B}\big(L^2\big(S^{d-1}\big), B_{s_0}^{*}\big). \tag{8.23}$$

Finally, writing (with $\chi_{\mathrm{middle}} := 1 - \chi_{\mathrm{righ}}^{+} - \chi_{\mathrm{lef}}^{-}$)

$$W^{+}(\lambda) = \mathrm{Op}^{\mathrm{r}}\big(\chi_{\mathrm{righ}}^{+}\big)W^{+}(\lambda) + \mathrm{Op}^{\mathrm{r}}(\chi_{\mathrm{lef}}^{-})W^{+}(\lambda) + \mathrm{Op}^{\mathrm{r}}(\chi_{\mathrm{middle}})W^{+}(\lambda),$$

we conclude from (4.54), (8.17), (8.19) and (8.23) that indeed

$$W^{+}(\lambda) \in \mathcal{B}\big(L^2\big(S^{d-1}\big), B_{s_0}^{*}\big). \tag{8.24}$$

Whence $W^{+}(\lambda)$ maps $L^2(S^{d-1})$ continuously into $\mathcal{V}^{-s_0}(\lambda)$.

Re (ii) (Bijectiveness). We shall show that $W^{+}(\lambda)$ maps $L^2(S^{d-1})$ onto $\mathcal{V}^{-s_0}(\lambda)$. Using the expression (8.7) for the inverse $\tau \in \mathcal{D}'(S^{d-1})$, mimicking the first part of Step III in the proof of Theorem 8.1 and using the Riesz' representation theorem (see for example [33]) in conjunction with (8.24), we obtain that indeed $\tau \in L^2(S^{d-1})$. This argument also shows that

$$W^{+}(\lambda)^{-1} \in \mathcal{B}\big(\mathcal{V}^{-s_0}(\lambda), L^2\big(S^{d-1}\big)\big). \tag{8.25}$$

Re (iii). The result follows from (ii) by the Banach's closed range theorem, see [33].

Re (iv). Let

$$u_{\pm,\tau}(x) = (2\pi)^{-\frac{1}{2}} \mathrm{e}^{\mp\mathrm{i}\pi\frac{d-1}{4}} g^{-\frac{1}{2}}(r,\lambda) r^{-\frac{d-1}{2}} \mathrm{e}^{\pm\mathrm{i}\phi(x,\lambda)} \tau(\pm\hat{x}).$$

Clearly $u_{\pm,\tau} \in B_{s_0}^{*}$ with a continuous dependence on τ. We claim (with reference to (8.2)) that

$$\mathrm{Op}^{\mathrm{r}}\big(\chi^{\pm}\big)W^{\pm}(\lambda)\tau - u_{\pm,\tau} \in B_{s_0,0}^{*}. \tag{8.26}$$

Notice that also the first term is in $B_{s_0}^{*}$ with a continuous dependence on τ, cf. (8.17) and (8.19), hence it suffices to show (8.26) for $\tau \in C^{\infty}(S^{d-1})$, in which case the asymptotics follows from Theorem 5.7, cf. Step III of the proof of Theorem 8.1.

Now, combining (8.26) and the identity (8.11), we obtain

$$\mathrm{Op}^{\mathrm{r}}\big(\chi^{+}\big)W^{-}(\lambda)\tau - u_{+,S(\lambda)\tau}, \qquad \mathrm{Op}^{\mathrm{r}}\big(\chi^{-}\big)W^{+}(\lambda)\tau - u_{-,S(\lambda)^{*}\tau} \in B_{s_0,0}^{*}. \tag{8.27}$$

By (8.26) and (8.27),

$$W^{-}(\lambda)\tau - (u_{-,\tau} + u_{+,S(\lambda)\tau}), \qquad W^{+}(\lambda)\tau - (u_{+,\tau} + u_{-,S(\lambda)^{*}\tau}) \in B_{s_0,0}^{*},$$

showing (8.12) and (8.13).

As for (8.14) we use (8.12) and (8.13); notice that the cross terms do not contribute to the limit which can be seen by an integration by parts with respect to the variable $r = |x|$, invoking Proposition 3.3. □

On the basis of Theorem 8.2, we can characterize the scattering matrix $S(\lambda)$ geometrically as follows:

Corollary 8.3. *For all $\tau^- \in L^2(S^{d-1})$, there exist a uniquely determined $u \in \mathcal{V}^{-s_0}(\lambda)$ and $\tau^+ \in L^2(S^{d-1})$ such that*

$$u - \frac{\mathrm{e}^{\mathrm{i}\pi\frac{d-1}{4}}\mathrm{e}^{-\mathrm{i}\phi(x,\lambda)}\tau^-(-\hat{x}) + \mathrm{e}^{-\mathrm{i}\pi\frac{d-1}{4}}\mathrm{e}^{\mathrm{i}\phi(x,\lambda)}\tau^+(\hat{x})}{(2\pi)^{\frac{1}{2}}g^{\frac{1}{2}}(r,\lambda)r^{\frac{d-1}{2}}} \in B^*_{s_0,0}. \tag{8.28}$$

We have $\tau^+ = S(\lambda)\tau^-$, $u = W^-(\lambda)\tau^- = W^+(\lambda)\tau^+$.

Proof. The existence part (with $\tau^+ = S(\lambda)\tau^-$) follows from (8.12).

To show the uniqueness, suppose that u_i, τ_i^+, $i = 1, 2$, satisfy the requirements of (8.28) with the same τ_-. Then for the difference, $u = u_1 - u_2$, we have $(H - \lambda)u = 0$ and $WF(B^*_{s_0,0}, u) \subseteq \{b = 1\}$. Hence by Proposition 4.10, $u = 0$. □

Corollary 8.4. *Let $d \geqslant 2$ and $\lambda \geqslant 0$. Suppose (in addition to Conditions 2.1 and 2.3) that V_2 and V_3 are spherically symmetric and that $\int_0^\infty r|V_3(r)|\,\mathrm{d}r < \infty$. (Condition 2.2 is not needed since V_2 can be absorbed into V_1). Then there exists a real-valued continuous function $\sigma_l(\cdot)$ such that for all spherical harmonics Y of order l we have $S(\lambda)Y = \mathrm{e}^{\mathrm{i}2\sigma_l(\lambda)}Y$.*

Let $u_l(r)$ denote the regular solution of the reduced Schrödinger equation on the half-line $]0,\infty[$

$$-u'' + V_l u = 0, \quad V_l(r) = 2\big(V(r) - \lambda\big) + \frac{(l + \frac{d}{2} - 1)^2 - 4^{-1}}{r^2}, \quad l \geqslant 0;$$

where "regular" refers to the asymptotics $u(r) \asymp r^{l+\frac{d-1}{2}}$ as $r \to 0$. Then $\sigma_l(\cdot)$ is uniquely determined mod 2π *by the asymptotics*

$$\frac{u_l(r)}{r^{\frac{d-1}{2}}} - C\frac{\sin\big(\int_{R_0}^r \sqrt{2(\lambda - V(r'))}\,\mathrm{d}r' + \sqrt{2\lambda R_0} - \frac{d-3+2l}{4}\pi + \sigma_l(\lambda)\big)}{(\lambda - V(r))^{\frac{1}{4}}r^{\frac{d-1}{2}}} \in B^*_{s_0,0}, \tag{8.29}$$

where $C = C(l,\lambda)$ is a (uniquely determined) positive constant.

Proof. Let Y be a spherical harmonic of order l. Note that its parity is $(-1)^l$, i.e. $Y(-\omega) = (-1)^l Y(\omega)$. Besides, $u := r^{-\frac{d-1}{2}}u_l(r)Y(\hat{x})$ solves $(H - \lambda)u = 0$. We apply Corollary 8.3 with this u and with $\tau^- = Y$, so that $\tau^+ = \mathrm{e}^{\mathrm{i}2\sigma_l(\lambda)}Y$. Then

$$\begin{aligned}
&\mathrm{e}^{\mathrm{i}\pi\frac{d-1}{4}}\mathrm{e}^{-\mathrm{i}\phi(x,\lambda)}\tau^-(-\hat{x}) + \mathrm{e}^{-\mathrm{i}\pi\frac{d-1}{4}}\mathrm{e}^{\mathrm{i}\phi(x,\lambda)}\tau^+(\hat{x}) \\
&\quad = \big(\mathrm{e}^{\mathrm{i}\pi\frac{d-1}{4} - \mathrm{i}\phi(x,\lambda) + \mathrm{i}\pi l} + \mathrm{e}^{-\mathrm{i}\pi\frac{d-1}{4} + \mathrm{i}\phi(x,\lambda) + \mathrm{i}2\sigma_l(\lambda)}\big)Y(\hat{x}) \\
&\quad = 2\mathrm{e}^{\mathrm{i}\pi\frac{l}{2} + \mathrm{i}\sigma_l(\lambda)}\sin\bigg(\phi(x,\lambda) - \frac{d-3+2l}{4}\pi + \sigma_l(\lambda)\bigg)Y(\hat{x}).
\end{aligned}$$

We finish the proof using (5.22). □

Let us remark that, because of the spherical symmetry of the potential, the asymptotics (8.29) can be improved:

$$\big(\lambda - V(r)\big)^{\frac{1}{4}} u_l(r) - C \sin\left(\int_{R_0}^{r} \sqrt{2\big(\lambda - V(r')\big)}\, \mathrm{d}r' + \sqrt{2\lambda R_0} - \frac{d-3+2l}{4}\pi + \sigma_l(\lambda)\right)$$
$$\to 0 \quad \text{for } r \to \infty. \tag{8.30}$$

The equivalence of (8.29) and (8.30) follows from the 1-dimensional WKB-method described for instance in [24] (see also [7]).

9. Homogeneous potentials – location of singularities of $S(0)$

In this section we impose Conditions 2.1–2.3 with $d \geqslant 2$ and the condition $V_1(r) = -\gamma r^{-\mu}$ for $r \geqslant 1$ and hence $V(r) = -\gamma r^{-\mu} + O(r^{-\mu-\epsilon_2})$, cf. (1.23). Throughout the section $g = g(\lambda = 0) = \sqrt{-2V_1}$.

Our goal is to prove a statement about the localization of the singularities of the (Schwartz) kernel $S(0)(\omega, \omega')$. The purely Coulombic case for which $\mu = 1$ and $d \geqslant 3$ was treated explicitly in Example 7.5. Under an additional condition we can write down a fairly explicit integral that carries the singularities.

This section is also closely related to our recent paper [7], which is, however, restricted to radial potentials.

9.1. Reduced classical equations

Consider the classical system given by the Hamiltonian $h_1(x, \xi) = \frac{1}{2}\xi^2 - \gamma |x|^{-\mu}$ for $x \neq 0$. The equations of motion for $h_1(x, \xi)$ are invariant with respect to the transformation

$$(x, \xi) \mapsto \big(\lambda x, \lambda^{-\mu/2}\xi\big), \quad \lambda \in \mathbb{R}_+, \tag{9.1}$$

upon rescaling of time $t \mapsto t\lambda^{1+\mu/2}$.

Let

$$\mathbb{T}^* := \big(\mathbb{R}^d \setminus \{0\}\big) \times \mathbb{R}^d / \sim,$$

where $(x_1, \xi_1) \sim (x_2, \xi_2)$ iff there exists $\lambda > 0$ such that $(x_1, \xi_1) = (\lambda x_2, \lambda^{-\mu/2}\xi_2)$. Note that $\mathbb{T}^*$ can be conveniently identified with $T^*(S^{d-1}) \times \mathbb{R}$. We shall introduce coordinates of $\mathbb{T}^*$ by setting $b = \hat{x} \cdot \frac{\xi}{g} \in \mathbb{R}$ and $\bar{c} = (I - |\hat{x}\rangle\langle\hat{x}|)\frac{\xi}{g} \in T^*_{\hat{x}}(S^{d-1})$ with $\hat{x} \in S^{d-1}$. (At this point we are slightly abusing the notation of Section 4.2, however as noticed there the b and $\bar{c}$ given by (4.7) agree with the above definition for $r \geqslant 1$.) The equations of motion for the Hamiltonian h_1 can be reduced to $\mathbb{T}^*$. Introducing the "new time" τ by $\frac{\mathrm{d}\tau}{\mathrm{d}t} = g/r$ we have the following system of reduced equations of motion:

$$\begin{cases} \frac{\mathrm{d}}{\mathrm{d}\tau}\hat{x} = \bar{c}, \\ \frac{\mathrm{d}}{\mathrm{d}\tau}\bar{c} = -(1 - \frac{\mu}{2})b\bar{c} - \bar{c}^2\hat{x}, \\ \frac{\mathrm{d}}{\mathrm{d}\tau}b = (1 - \frac{\mu}{2})\bar{c}^2 + \frac{\mu}{2}(b^2 + \bar{c}^2 - 1). \end{cases} \tag{9.2}$$

(Notice that the last equation follows from (4.29).) The maximal solution of (9.2) that passes $z = (\hat{x}, b, \bar{c}) \in \mathbb{T}^*$ at $\tau = 0$ is denoted by $\gamma(\tau, z)$.

Beside (9.2), we shall consider a related dynamics given by the equations

$$\begin{cases} \frac{\mathrm{d}}{\mathrm{d}\tau}\hat{x} = \bar{c}, \\ \frac{\mathrm{d}}{\mathrm{d}\tau}\bar{c} = -(1 - \frac{\mu}{2})b\bar{c} - \bar{c}^2\hat{x}, \\ \frac{\mathrm{d}}{\mathrm{d}\tau}b = (1 - \frac{\mu}{2})\bar{c}^2. \end{cases} \tag{9.3}$$

The (maximal) solution of the system (9.3) that passes $z = (\hat{x}, b, \bar{c}) \in \mathbb{T}^*$ at $\tau = 0$ will be denoted by $\gamma_0(\tau, z)$. Clearly the equation $\bar{c} = 0$ defines the fixed points, and the system is complete.

Notice that the surface $h_1^{-1}(0)$ in the coordinates $(\hat{x}, b, \bar{c})$ corresponds to the condition $b^2 + \bar{c}^2 = 1$. This surface is preserved both by the flow γ and γ_0, and on this surface both flows coincide.

Note that the flow γ_0 is exactly solvable. The variable b is always increasing and $k = b^2 + \bar{c}^2$ is a conserved quantity; of course the relevant value is $k = 1$. For non-fixed points we can compute its dependence on the modified time

$$b(\tau) = \sqrt{k}\tanh\sqrt{k}\left(1 - \frac{\mu}{2}\right)(\tau - \tau_0). \tag{9.4}$$

Values $k \neq 1$ correspond in this picture to replacing the coupling constant $\gamma \to k\gamma$. More precisely, if $k = b^2 + \bar{c}^2$ for a solution to (9.3), we can define $r(\tau) = r_0 \exp(\int_0^\tau b\,\mathrm{d}\tau')$, introduce $t = \int_0^\tau \frac{r}{g(r)}\,\mathrm{d}\tau'$ and check that indeed

$$\begin{cases} x(t) = r\hat{x}, \\ \xi(t) = g(r)(b\hat{x} + \bar{c}), \end{cases} \tag{9.5}$$

defines a zero energy solution to Hamilton's equations with $V \to kV$. The equation $b = 0$ corresponds to a turning point (at which $|x(t)|$ has the smallest value).

Clearly, it follows from (9.4) that $\lim_{\tau\to\infty} b = \sqrt{k}$, $\lim_{\tau\to-\infty} b = -\sqrt{k}$. Upon writing $\hat{x}(\tau) \cdot \hat{x}(\infty) = \cos\theta(\tau)$ for some monotone continuous function $\theta(\cdot)$, we obtain from (1.27) that

$$\left|\theta(\infty) - \theta(-\infty)\right| = \frac{2}{2 - \mu}\pi. \tag{9.6}$$

9.2. *Propagation of singularities*

We will use the scattering wave front set at zero energy, introduced in Section 4.2. The following proposition is somewhat similar to Hörmander's theorem about propagation of singularities adapted to scattering at the zero energy. It is a "local" version of Proposition 4.5 which takes into account the fact that in the case of a homogeneous potential we can use the dynamics in the reduced phase space. Again the proof is a modification of that of [12, Proposition 3.5.1], see also [21] and [11].

Proposition 9.1. *Suppose $u, v \in L^{2,-\infty}$, $Hu = v$, $s \in \mathbb{R}$, $z \in \mathbb{T}^*$ and $z \notin WF^s_{\mathrm{sc}}(u)$. Define*

$$\tau^+ := \sup\{\tau \geqslant 0 \mid \gamma_0(\tilde\tau, z) \notin WF^s_{\mathrm{sc}}(u) \text{ for all } \tilde\tau \in [0,\tau]\},$$
$$\tau^- := \inf\{\tau \leqslant 0 \mid \gamma_0(\tilde\tau, z) \notin WF^s_{\mathrm{sc}}(u) \text{ for all } \tilde\tau \in [\tau,0]\}.$$

If $\tau^+ < \infty$, then $\gamma_0(\tau^+, z) \in WF^{s+2s_0}_{\mathrm{sc}}(v)$. If $\tau^- > -\infty$, then $\gamma_0(\tau^-, z) \in WF^{s+2s_0}_{\mathrm{sc}}(v)$.

Proof. The proof is similar to the one of Proposition 4.5. We shall only deal with the case of forward flow; the case of superscript "−" is similar (actually it follows from the case of "+" by time reversal invariance). For convenience, we shall assume that $\epsilon_2 \leqslant 2 - \mu$.

Step I. We will first show the following weaker statement: Suppose $u \in L^{2,s-\frac{\epsilon_2}{2}}$, $v \in L^{2,s+2s_0}$ and $Hu = v$. Then

$$\gamma_0(\tau, z) \notin WF^s_{\mathrm{sc}}(u) \quad \text{for all } \tau \geqslant 0. \tag{9.7}$$

Suppose on the contrary that (9.7) is false. Then we obtain from Proposition 4.3 that the flows of (9.2) and (9.3), starting at z, coincide. Letting $\gamma(\tau) = \gamma(\tau, z)$, it thus needs to be shown that

$$\tau^+ := \sup\{\tau \geqslant 0 \mid \gamma(\tilde\tau) \notin WF^s_{\mathrm{sc}}(u) \text{ for all } \tilde\tau \in [0,\tau]\} = \infty. \tag{9.8}$$

Suppose on the contrary that τ^+ is finite. Then $\gamma(\tau^+)$ is not a fixed point. Consequently, we can pick a slightly smaller $\tilde\tau^+ < \tau^+$ and a transversal $(2d-2)$-dimensional submanifold at $\gamma(\tilde\tau^+)$, say $\mathcal{M}$, such that with $J =]-\epsilon + \tilde\tau^+, \tau^+ + \epsilon[$, for some small $\epsilon > 0$, the map

$$J \times \mathcal{M} \ni (\tau, m) \to \Psi(\tau, m) = \gamma(\tau - \tilde\tau^+, m) \in \mathbb{T}^*$$

is a diffeomorphism onto its range.

We pick $\chi \in C_c^\infty(\mathcal{M})$ supported in a small neighbourhood of $\gamma(\tilde\tau^+)$ such that $\chi(\gamma(\tilde\tau^+)) = 1$ and

$$\Psi(]-\epsilon + \tilde\tau^+, \tilde\tau^+] \times \operatorname{supp}\chi) \cap WF^s(u) = \emptyset. \tag{9.9}$$

We pick a non-positive function $f \in C_c^\infty(J)$ such that $f' \geqslant 0$ on a neighbourhood of $[\tilde\tau^+, \tau^+ + \epsilon)$ and $f(\tau^+) < 0$.

Let $f_K(\tau) = \exp(-K\tau) f(\tau)$ for $K > 0$, and $X_\kappa = (1 + \kappa r^2)^{1/2}$ for $\kappa \in]0,1]$. We consider the symbol

$$b_\kappa = g^{-1/2} X^{1/2} a_\kappa; \qquad a_\kappa = X^s X_\kappa^{-\epsilon_2/2} F(r > 2)(f_K \otimes \chi) \circ \Psi^{-1}. \tag{9.10}$$

First we fix K. A part of the Poisson bracket with b_κ^2 is

$$\{h_2, g^{-1} X^{2s+1} X_\kappa^{-\epsilon_2}\} = r^{-1} Y_\kappa b X^{2s+1} X_\kappa^{-\epsilon_2}, \tag{9.11}$$

where $Y_\kappa = Y_\kappa(r)$ is uniformly bounded in κ. We fix K such that $2K \geqslant |Y_\kappa b| + 2$ on $\operatorname{supp} b_\kappa$.

We compute

$$\{h_1, (f_K \otimes \chi) \circ \Psi^{-1}\} = \frac{g}{r}\left(\left[\frac{\mathrm{d}}{\mathrm{d}\tau} f_K\right] \otimes \chi\right) \circ \Psi^{-1}. \tag{9.12}$$

From (9.11) and (9.12), and by the choice of f and K, we conclude that

$$\{h_2, b_\kappa^2\} \leqslant -2a_\kappa^2 + O\big(r^{2s-\epsilon_2}\big) \quad \text{at } \mathcal{P} \subseteq \mathbb{T}^* \tag{9.13}$$

given by

$$\mathcal{P} = \Psi\big(\{\tau \in J \mid f'(\tau) \geqslant 0\} \times \operatorname{supp} \chi\big).$$

Introducing $A_\kappa = \mathrm{Op}^{\mathrm{w}}(a_\kappa)$ and $B_\kappa = \mathrm{Op}^{\mathrm{w}}(b_\kappa)$, we have

$$\big\langle \mathrm{i}\big[H, B_\kappa^2\big]\big\rangle_u = -2\,\mathrm{Im}\langle v, B_\kappa^2 u\rangle, \tag{9.14}$$

and we estimate the right-hand side using the calculus of pseudodifferential operators, cf. [14, Theorems 18.5.4, 18.6.3, 18.6.8], to obtain the uniform bound

$$\big|\big\langle \mathrm{i}\big[H, B_\kappa^2\big]\big\rangle_u\big| \leqslant C_1 \|v\|_{s+2s_0} \|A_\kappa u\| + C_2 \leqslant \|A_\kappa u\|^2 + C_3. \tag{9.15}$$

On the other hand, using (9.9) and (9.13), we infer that

$$\big\langle \mathrm{i}\big[H - V_3, B_\kappa^2\big]\big\rangle_u \leqslant -2\|A_\kappa u\|^2 + C_4. \tag{9.16}$$

An application of (4.12a) yields

$$\big\langle \mathrm{i}\big[V_3, B_\kappa^2\big]\big\rangle_u \leqslant C_5. \tag{9.17}$$

Combining (9.15)–(9.17) yields

$$\|A_\kappa u\|^2 \leqslant C_6 = C_3 + C_4 + C_5,$$

which in turn gives a uniform bound

$$\big\| X_\kappa^{-\epsilon_2/2} \mathrm{Op}^{\mathrm{w}}\big(\chi_{\gamma(\tau^+)} F(r > 2)\big) u \big\|_s^2 \leqslant C_7. \tag{9.18}$$

Here $\chi_{\gamma(\tau^+)}$ signifies a phase-space localization factor of the form entering in (4.8) supported in a sufficiently small neighbourhood of the point $\gamma(\tau^+)$.

We let $\kappa \to 0$ in (9.18) and infer that $\tau^+ \notin WF_{\mathrm{sc}}^s(u)$, which is a contradiction. We have proved (9.8) and hence (9.7).

Step II. To relax the assumptions on u and v used in Step I, we modify the above proof (using localization) in an iterative procedure very similar to Step II of the proof of Proposition 4.5.

Pick $t < s$ such that $u \in L^{2,t}$ and define $s_m = \min(s, t + m\epsilon_2/2)$ for $m \in \mathbb{N}$. Let correspondingly τ_m^+ be given as τ^+, upon replacing $s \to s_m$. Clearly,

$$\tau_m^+ \leqslant \tau_{m-1}^+; \quad m = 2, 3, \ldots. \tag{9.19}$$

We shall show that

$$\tau_m^+ < \infty \quad \Rightarrow \quad \gamma_0\big(\tau_m^+, z\big) \in WF_{\mathrm{sc}}^{s_m+2s_0}(v). \tag{9.20}$$

We are done by using (9.20) for an m taken so large that $s_m = s$.

Let us consider the start of induction given by $m = 1$, in which case obviously $u \in L^{2,s_m-\epsilon_2/2}$. Suppose on the contrary that (9.20) is false. Then we consider the following case:

$$\tau_m^+ < \infty \quad \text{and} \quad \gamma_0\big(\tau_m^+, z\big) \notin WF_{\mathrm{sc}}^{s_m+2s_0}(v). \tag{9.21}$$

It follows from (9.21) and an ellipticity argument that $b^2 + \bar{c}^2 = 1$ at $\gamma_0(\tau_m^+, z)$ (using that $\gamma_0(\tau_m^+, z) \notin WF_{\mathrm{sc}}^{s_m+\mu}(Hu)$). Consequently we can henceforth use the flow of (9.2), $\gamma(\tau) = \gamma(\tau, \cdot)$, exactly as in Step I.

We let $\epsilon > 0$, J, f, f_K, χ and Ψ be chosen as in Step I with $\tau^+ \to \tau_m^+$ and $\tilde{\tau}^+ \to \tilde{\tau}_m^+$. Let $\tilde{f} \in C_c^\infty(]\tilde{\tau}_m^+ - 2\epsilon, \tau_m^+ + 2\epsilon[)$ with $\tilde{f} = 1$ on J. Similarly, let $\tilde{\chi} \in C_c^\infty(\mathcal{M})$ be supported in a small neighbourhood of $\gamma(\tilde{\tau}_m^+)$ such that $\tilde{\chi}(\gamma(\tilde{\tau}_m^+)) = 1$ in a neighbourhood of supp χ.

It follows from (9.21), possibly by shrinking the supports of $\tilde{f}$ and $\tilde{\chi}$, that

$$I_\epsilon v \in L^{2,s_m+2s_0}, \qquad I_\epsilon = \mathrm{Op}^{\mathrm{w}}\big(F(r > 2)(\tilde{f}_K \otimes \tilde{\chi}) \circ \Psi^{-1}\big). \tag{9.22}$$

Next, we introduce the symbol b_κ by (9.10) (with $s \to s_m$) and proceed as in Step I. As for the bounds (9.15), we can replace v by $I_\epsilon v$ up to addition of a term that is bounded uniformly in κ. Clearly, we can verify (9.16) and (9.17). So again we obtain (9.18) (with $s \to s_m$), and therefore a contradiction as in Step I. We have shown (9.20) for $m = 1$.

Now suppose $m \geqslant 2$ and that (9.20) is verified for $m - 1$. We need to show the statement for the given m. Due to (9.19) and the induction hypothesis, we can assume that

$$\tau_m^+ < \tau_{m-1}^+. \tag{9.23}$$

Again we argue by contradiction assuming (9.21). We proceed as above noticing that it follows from (9.23) that in addition to (9.22) we have

$$I_\epsilon u \in L^{2,s_{m-1}}; \tag{9.24}$$

at this point we possibly need to shrink the supports of $\tilde{f}$ and $\tilde{\chi}$ even more (viz. taking $\epsilon < (\tau_{m-1}^+ - \tau_m^+)/2$). By replacing v by $I_\epsilon v$ and u by $I_\epsilon u$ at various points in the procedure of Step I (using (9.22) and (9.24), respectively) we obtain again a contradiction. Whence (9.20) follows. □

Remark 9.2. Suppose $u \in L^{2,t_1}$, $v \in L^{2,t_2}$ and $Hu = v$. Suppose $z_0 \notin WF_{\mathrm{sc}}^s(u)$ for some $s > t_1$. Fix $\tilde{\tau}^+ \in]0, \infty[$ and suppose that $\gamma_0(\tau, z_0) \notin WF_{\mathrm{sc}}^{s+2s_0}(v)$ for all $\tau \in [0, \tilde{\tau}^+]$. Write $\gamma_0(\tilde{\tau}^+, z_0) = (\omega_1, \bar{c}_1, b_1) = (\omega_1, \eta_1)$. Then there exist neighbourhoods $\mathcal{N}_{\omega_1} \ni \omega_1$ and $\mathcal{N}_{\eta_1} \ni \eta_1$ such that for all $\chi_{\omega_1} \in C_c^\infty(\mathcal{N}_{\omega_1})$ and $\chi_{\eta_1} \in C_c^\infty(\mathcal{N}_{\eta_1})$ we have $\mathrm{Op}^{\mathrm{w}}\big(\chi_{z_1} F(r > 2)\big)u \in L^{2,s}$. Here $\chi_{z_1}(x, \xi) = \chi_{\omega_1}(\hat{x})\chi_{\eta_1}(\xi/g)$. Notice that this conclusion is already contained in Proposition 9.1; however the above proof yields an additional bound:

First, writing $z_0 = (\omega_0, \eta_0)$, we can pick any similarly defined localization factor, say denoted by χ_{z_0}, with $\chi_{\omega_0} = 1$ and $\chi_{\eta_0} = 1$ around the points ω_0 and η_0, respectively, and such that

$\mathrm{Op}^{\mathrm{w}}(\chi_{z_0}F(r>2))u \in L^{2,s}$ (this is by assumption). Next we pick a small neighbourhood U of $\gamma_0([0,\tilde{\tau}^+], z_0) \subset \mathbb{T}^*$ and $\chi \in C_c^\infty(U)$ with $\chi = 1$ around this orbit segment. If U is small enough we have (again by assumption) that $\mathrm{Op}^{\mathrm{w}}(\chi_{\gamma_0}F(r>2))v \in L^{s+2s_0}$, $\chi_{\gamma_0}(x,\xi) := \chi(\hat{x}, \xi/g)$. Now, there are neighbourhoods $\mathcal{N}_{\omega_1} \ni \omega_1$ and $\mathcal{N}_{\eta_1} \ni \eta_1$ depending only on χ_{z_0} and χ_{γ_0} such that for all $\chi_{\omega_1} \in C_c^\infty(\mathcal{N}_{\omega_1})$ and $\chi_{\eta_1} \in C_c^\infty(\mathcal{N}_{\eta_1})$ we have

$$\begin{aligned}&\left\|\mathrm{Op}^{\mathrm{w}}\left(\chi_{z_1}F(r>2)\right)u\right\|_s \\ &\quad\leqslant C\left(\left\|\mathrm{Op}^{\mathrm{w}}\left(\chi_{z_0}F(r>2)\right)u\right\|_s + \|u\|_{t_1} + \left\|\mathrm{Op}^{\mathrm{w}}\left(\chi_{\gamma_0}F(r>2)\right)v\right\|_{s+2s_0} + \|v\|_{t_2}\right),\end{aligned}$$

where the constant C only depends on the various localization factors.

9.3. *Location of singularities of the kernel of the scattering matrix*

In this subsection we describe the location of the singularities of the scattering matrix at zero energy.

Theorem 9.3. *Suppose that $V_1(r) = -\gamma r^{-\mu}$ for $r \geqslant 1$. Then the kernel $S(0)(\omega,\omega')$ is smooth outside the set $\{(\omega,\omega') \mid \omega\cdot\omega' = \cos\frac{\mu}{2-\mu}\pi\}$.*

To analyse $S(0)(\omega,\omega')$ we shall use the representation (7.3a), which we write (formally) as

$$S(0)(\omega,\omega') = -2\pi\left\langle j^+(\cdot,\omega), v^-(\cdot,\omega')\right\rangle + 2\pi\mathrm{i}\left\langle v^+(\cdot,\omega), R(+\mathrm{i}0)v^-(\cdot,\omega')\right\rangle,$$

where

$$\begin{aligned} j^\pm(x,\omega) &= (2\pi)^{-d/2}\left(\mathrm{e}^{\mathrm{i}\phi^\pm}\tilde{a}^\pm\right)(x,\omega,0), \\ v^\pm(x,\omega) &= (2\pi)^{-d/2}\left(\mathrm{e}^{\mathrm{i}\phi^\pm}\tilde{t}^\pm\right)(x,\omega,0). \end{aligned}$$

Let ϕ^+_{sph} denote the solution of the eikonal equation for the potential V_1 at zero energy, cf. (3.9). It is given by

$$\phi^+_{\mathrm{sph}}(x,\omega) = \frac{\sqrt{2\gamma}}{1-\mu/2}\left(r^{1-\mu/2}\cos(1-\mu/2)\theta - R_0^{1-\mu/2}\right), \tag{9.25}$$

where $\cos\theta = \hat{x}\cdot\omega$. Using $x^\perp = \frac{\omega-\hat{x}\cos\theta}{\sin\theta}$ and $\nabla_x\theta = -\frac{x^\perp}{r}$, we can also compute

$$\begin{aligned} F^+_{\mathrm{sph}}(x,\omega) &= \nabla_x\phi^+_{\mathrm{sph}}(x,\omega) \\ &= \sqrt{2\gamma}\,r^{-\mu/2}\left(\hat{x}\cos(1-\mu/2)\theta + x^\perp\sin(1-\mu/2)\theta\right). \end{aligned}$$

Lemma 9.4. *For all $s \in \mathbb{R}$, $\omega \in S^{d-1}$ and multiindices δ,*

$$\begin{aligned} &WF_{\mathrm{sc}}^{s}\big(\partial_\omega^\delta v^\pm(\cdot,\omega)\big) \\ &\quad\subseteq \left\{ z = (\hat{x}, \bar{c}, b) \in \mathbb{T}^* \;\middle|\; 1-\sigma' \leqslant \pm\hat{x}\cdot\omega \leqslant 1-\sigma,\ b\hat{x} + \bar{c} = \pm \frac{F_{\mathrm{sph}}^{+}(\hat{x}, \pm\omega)}{(2\gamma)^{1/2}} \right\}, \quad (9.26) \\ &WF_{\mathrm{sc}}^{s}\big(\partial_\omega^\delta j^\pm(\cdot,\omega)\big) \\ &\quad\subseteq \left\{ z = (\hat{x}, \bar{c}, b) \in \mathbb{T}^* \;\middle|\; 1-\sigma' \leqslant \pm\hat{x}\cdot\omega,\ b\hat{x} + \bar{c} = \pm \frac{F_{\mathrm{sph}}^{+}(\hat{x}, \pm\omega)}{(2\gamma)^{1/2}} \right\}. \quad (9.27) \end{aligned}$$

Suppose in addition that $\chi_+ \in C^\infty(\mathbb{R})$, $\chi_+' \in C_c^\infty(\mathbb{R})$ and $\operatorname{supp}\chi_+ \subset]1,\infty[$. *Then*

$$\operatorname{Op}^{\mathrm{w}}\big(\chi_+(a)\big)\partial_\omega^\delta v^\pm(\cdot,\omega),\ \operatorname{Op}^{\mathrm{w}}\big(\chi_+(a)\big)\partial_\omega^\delta j^\pm(\cdot,\omega) \in L^{2,s}. \quad (9.28)$$

Proof. Only the "+" case needs to be considered (can be seen by complex conjugation). Upon multiplying by a localization operator supported outside of the right-hand side of (9.26), we need to demonstrate that the result is in $L^{2,s}$, cf. the definition (4.8). Using the right Kohn–Nirenberg quantization (instead of the Weyl quantization) this can be done by integrating by parts in explicit integrals, exactly as in the proofs of Lemma 6.8(iii) and Theorem 6.11. The arguments for (9.27) and (9.28) are the same, in particular, (9.28) follows from the proof of Theorem 6.11. □

Proof of Theorem 9.3. Due to Proposition 4.8 and Lemma 9.4 we are allowed to act by $R(+\mathrm{i}0)$ on $\partial_{\omega'}^{\delta'} v^-(\cdot,\omega')$). In fact, for all $\tau \in C^\infty(S^{d-1})$

$$R(+\mathrm{i}0)T^-(0)\tau = \int_{S^{d-1}} R(+\mathrm{i}0)v^-(\cdot,\omega')\tau(\omega')\,\mathrm{d}\omega'. \quad (9.29)$$

Using the representation (7.3a) interpreted as a form on $C^\infty(S^{d-1})$, and (9.29), we have $S_\kappa(0) \to S(0)$ as $\kappa \searrow 0$, where the kernel of $S_\kappa(0)$ is the well-defined smooth expression

$$\begin{aligned} &S_\kappa(0)(\omega,\omega') \\ &\quad= -2\pi\big\langle j^+(\cdot,\omega), F\big(\kappa|\cdot|<1\big)v^-(\cdot,\omega')\big\rangle + 2\pi\imath\big\langle v^+(\cdot,\omega), F\big(\kappa|\cdot|<1\big)R(+\mathrm{i}0)v^-(\cdot,\omega')\big\rangle. \end{aligned}$$

It remains to be shown that $S_\kappa(0)(\cdot,\cdot)$ has a limit in $C^\infty(\{\omega\cdot\omega' \neq \cos\frac{\mu\pi}{2-\mu}\})$.

By integration by parts, it follows that the first term has a limit, in fact in $C^\infty(S^{d-1}\times S^{d-1})$, cf. the proof of Lemma 9.4. Whence we only look at the second term.

By Lemma 9.4 and Proposition 3.3, for all s

$$\begin{aligned} WF_{\mathrm{sc}}^{s}\big(\partial_\omega^\delta v^+(\cdot,\omega)\big) &\subseteq \big\{\bar{c} \neq 0,\ b^2 + \bar{c}^2 = 1\big\} \cap \Big\{ z \;\Big|\; \lim_{\tau\to+\infty} \hat{x}(\tau) = \omega, \\ &\quad \text{where } \gamma_0(\tau,z) = \big(\hat{x}(\tau), b(\tau), \bar{c}(\tau)\big) \Big\}. \quad (9.30) \end{aligned}$$

Here $\gamma_0(\tau,z)$ refers to the flow defined by (9.3).

By Propositions 4.8 and 9.1, for all s,

$$\begin{aligned} &WF^s_{\mathrm{sc}}\big(R(+\mathrm{i}0)\partial^{\delta'}_{\omega'}v^-(\cdot,\omega')\big) \\ &\quad\subseteq \big\{\gamma_0(\tau,z)\ \big|\ \tau\geqslant 0,\ z\in WF^s_{\mathrm{sc}}\big(\partial^{\delta'}_{\omega'}v^-(\cdot,\omega')\big)\big\}\cup\{\bar c=0,\ b>0\} \\ &\quad\subseteq \Big\{z\ \Big|\ \lim_{\tau\to-\infty}\hat x(\tau)=-\omega'\Big\}\cup\{\bar c=0,\ b>0\}. \end{aligned} \tag{9.31}$$

By invoking (9.6), we see that the sets on the right-hand side of (9.30) and (9.31) are disjoint away from $\{\omega\cdot\omega'\neq\cos\frac{\mu\pi}{2-\mu}\}$. Hence also

$$WF^s_{\mathrm{sc}}\big(\partial^{\delta}_{\omega}v^+(\cdot,\omega)\big)\cap WF^s_{\mathrm{sc}}\big(R(+\mathrm{i}0)\partial^{\delta'}_{\omega'}v^-(\cdot,\omega')\big)=\emptyset,$$

which implies, upon taking $s=0$ and using (9.28) and a suitable partition of unity, that

$$\big\langle\partial^{\delta}_{\omega}v^+(\cdot,\omega,0),\,R(+\mathrm{i}0)\partial^{\delta'}_{\omega'}v^-(\cdot,\omega',0)\big\rangle$$

is well defined.

By the same arguments

$$\begin{aligned} &\partial^{\delta}_{\omega}\partial^{\delta'}_{\omega'}\big\langle v^+(\cdot,\omega,0),\,F\big(\kappa|\cdot|<1\big)R(+\mathrm{i}0)v^-(\cdot,\omega',0)\big\rangle \\ &\quad\to\big\langle\partial^{\delta}_{\omega}v^+(\cdot,\omega,0),\,R(+\mathrm{i}0)\partial^{\delta'}_{\omega'}v^-(\cdot,\omega',0)\big\rangle \end{aligned}$$

locally uniformly in $\{\omega\cdot\omega'\neq\cos\frac{\mu\pi}{2-\mu}\}$. Notice that the bound (9.28) is uniform in ω; a similar statement is valid for the bounds underlying (9.26), and we also need at this point to invoke Remark 9.2. □

Remarks 9.5.

(1) The somewhat abstract procedure of the proof of Theorem 9.3 does not provide information about the nature of the singularities at the cone $\omega\cdot\omega'=\cos\frac{\mu}{2-\mu}\pi$. In the study of the singularities at the diagonal of the kernel of scattering matrices for positive energies (see [19] and [31]) it is important that the eikonal and transport equations can be solved in sufficiently big sectors. In combination with resolvent estimates this allows one to put the singularities in a rather explicit term similar to the first one on the right-hand side of (7.2a). A very similar procedure can be used (at least for $V_2=0$) for $S(0)(\omega,\omega')$ provided $\mu<1$. However, for $\mu\in[1,2[$ there is a "glueing problem" due to the fact that in order to apply resolvent estimates in this case the constructed solutions to the eikonal equations $\phi^\pm$ need to be extended, viz. as to including some $\theta>\frac{\pi}{2-\mu}$. Therefore, multivalued $\phi^\pm$ are needed. We devote Section 9.4 to a discussion of this question.

(2) Under Condition 1.1, it follows essentially by the same method of proof that, for $\lambda>0$, the kernel $S(\lambda)(\omega,\omega')$ is smooth outside the set $\{(\omega,\omega')\mid\omega=\omega'\}$; for that we use (9.3) with $\mu=0$. See [27, Chapter 19] for a related result and procedure.

(3) There is a discrepancy between our results and the main result of [20]. The idea of [20] is to use a partial wave analysis to obtain an asymptotic expression of the scattering amplitude for $\lambda\to0$ (with the assumption of radial symmetry and under the short-range condition $\mu>1$). Unfortunately [20, (17)] is incompatible with Theorems 7.2, 7.3 and 9.3.

9.4. Distributional kernel of $S(0)$ as an oscillatory integral

In addition to the previous assumption $V_1(r) = -\gamma r^{-\mu}$ for $r \geqslant 1$, we shall here assume that $V_2 = 0$, see though Remark 9.6(1). We shall explain a procedure which in principle allows us to calculate the singularities of the kernel $S(0)(\omega, \omega')$; a fairly explicit *oscillatory integral* will be specified. Using this integral we derive below the location of the singularities of $S(0)$ by the method of non-stationary phase, which gives an alternative proof of Theorem 9.3 (under the condition that $V_2 = 0$).

We shall improve on the representation (7.3a) for $S(0)$. Notice that the functions $\tilde{a}^+$ and ϕ^+ used up to now are supported near the forward region $\cos\theta = \hat{x} \cdot \omega \approx 1$ only. Now we shall take advantage of the fact that the expression (9.25) defines a solution to the eikonal equation for all values of θ. We shall consider a cut-off at larger values of θ, in fact slightly to the left of the critical angle $\theta = (1 - \mu/2)^{-1}\pi$. The basic idea is similar to the one applied in the study of the kernel of scattering matrices for positive energies, cf. Remark 9.5(1). If we can extend the construction of the phase and amplitude as indicated above, then we can apply a "two-sided" resolvent estimate to deal with the second term on the right-hand side of (7.3a), i.e. to show that it contributes by a smooth kernel; in our case the appropriate "two-sided" estimate is given by (4.3f).

Now besides the problem of extending the phase up to $\theta = (1 - \mu/2)^{-1}\pi$, there is obviously the issue of well-definedness, since θ as a function of x is multi-valued; for the case of positive energies this problem does not occur since the cut-off in this case occurs before the angle $\theta = \pi$. We have

$$\bigl(J^+\tau\bigr)(x) = (2\pi)^{-d/2} \int_{S^{d-1}} \bigl(e^{i\phi^+}\tilde{a}^+\bigr)(x, \omega, 0)\tau(\omega)\,d\omega. \tag{9.32}$$

In fact, in the present spherically symmetric case the dependence of the variables x and ω is through $r = |x|$ and $\hat{x} \cdot \omega$ only. Writing

$$\omega = \cos\theta\hat{x} + \sin\theta\widetilde{\omega},$$

where $\widetilde{\omega} \cdot \hat{x} = 0$, (9.32) can be written as

$$(2\pi)^{-d/2} \int_{S^{d-2}} d\widetilde{\omega} \int_0^{\pi} \bigl(e^{i\phi}\tilde{a}\bigr)(r, \theta)\tau(\cos\theta\hat{x} + \sin\theta\widetilde{\omega}) \sin^{d-2}\theta\,d\theta; \tag{9.33}$$

for convenience we dropped the superscript. The phase ϕ is given by (9.25), and using this expression and the orbit (1.27), we can extend the support of $\tilde{a}$ by solving transport equations as in Section 5.3; the cut-off is now taken slightly to the left of $\theta = (1 - \mu/2)^{-1}\pi$. More precisely, the cut-off is defined as follows: First pick $L \in \mathbb{N}$ such that $(1 - \mu/2)L < 1$ while $(1 - \mu/2) \times (L + 1) \geqslant 1$. We shall assume that the analogue of σ' for the construction of J^-, entering in (5.2) for the construction of J^+, is so small that

$$(1 - \mu/2)\bigl(L\pi + \cos^{-1}(1 - \sigma')\bigr) < \pi. \tag{9.34}$$

Next the version of (5.2) that we need is given in terms of the σ of the construction of J^- as follows: Choose angles $\pi L < \theta_0 < \theta_0' < \pi(L+1)$ such that $(1-\mu/2)\theta_0' < \pi$ and $(1-\mu/2)(\theta_0 + \cos^{-1}(1-\sigma)) > \pi$. Introduce a smoothed out characteristic function

$$\chi_2(s) = \begin{cases} 1, & \text{for } s \leqslant \theta_0, \\ 0, & \text{for } s \geqslant \theta_0'; \end{cases} \tag{9.35}$$

and with this choice the new cut-off function takes the (essentially same) form $\chi = \chi_1(r)\chi_2(\theta)$.

The extended $\tilde{a}$ has similar properties as before due to the cut-off. Whence we are lead to consider the following modification of the expression (9.33):

$$\int_{S^{d-2}} \mathrm{d}\widetilde{\omega} \int_0^\infty f(r,\theta)\tau(\cos\theta\hat{x} + \sin\theta\widetilde{\omega})\left|\sin^{d-2}\theta\right| \mathrm{d}\theta; \qquad f = (2\pi)^{-d/2}\mathrm{e}^{\mathrm{i}\phi}\tilde{a},$$

where the θ-integration (due to the cut-off) effectively takes place on the interval $[0, (1-\mu/2)^{-1}\pi]$. The next step is to change variable, writing for θ in intervals of the form $(2k\pi, (2k+1)\pi]$,

$$\cos\theta\hat{x} + \sin\theta\widetilde{\omega} = \cos\psi\hat{x} + \sin\psi\widetilde{\omega}; \quad \psi = \theta - 2k\pi,$$

while on intervals of the form $((2k+1)\pi, (2k+2)\pi]$,

$$\cos\theta\hat{x} + \sin\theta\widetilde{\omega} = \cos\psi\hat{x} + \sin\psi(-\widetilde{\omega}); \qquad \psi = (2k+2)\pi - \theta,$$

respectively; here $k \in \mathbb{N} \cup \{0\}$. Whence we consider the expression

$$\int_{S^{d-1}} F(r,\psi)\tau(\omega)\,\mathrm{d}\omega,$$

where

$$F(r,\psi) = \sum_{k=0}^{\infty} \big\{ f(r, \psi + 2k\pi) + f\big(r, (2k+2)\pi - \psi\big) \big\},$$

and as above

$$\omega = \cos\psi\hat{x} + \sin\psi\widetilde{\omega} \quad \text{with } \widetilde{\omega}\cdot\hat{x} = 0 \text{ and } \psi \in [0,\pi],$$

i.e. $\psi = \cos^{-1}\hat{x}\cdot\omega$.

We claim that $F(r,\psi)$ is smooth in x and ω. Notice that this is not an obvious fact, since although the function $\psi = \cos^{-1}\hat{x}\cdot\omega$ is continuous, it has a cusp singularity at $\hat{x}\cdot\omega = \pm 1$. However, as can easily verified, ψ^2 is smooth at $\hat{x}\cdot\omega = 1$ and $(\pi-\psi)^2$ is smooth at $\hat{x}\cdot\omega = -1$, respectively. Moreover, $f(r,\psi)$ and $f(r, \psi + 2(k+1)\pi) + f(r, (2k+2)\pi - \psi)$ are in fact smooth functions of ψ^2 near $\hat{x}\cdot\omega = 1$, and similarly $f(r, \psi + 2k\pi) + f(r, (2k+2)\pi - \psi) = f(r, (2k+1)\pi - (\pi - \psi)) + f(r, (2k+1)\pi + (\pi - \psi))$ is a smooth function of $(\pi-\psi)^2$ at $\hat{x}\cdot\omega = -1$.

Recall that we have the representation (7.3b)

$$S(0)(\omega,\omega') = -2\pi\big\langle w^+(\omega,0), \mathrm{e}^{\mathrm{i}\phi^-}\tilde{t}^-(\cdot,\omega',0)\big\rangle, \tag{9.36}$$

where $w^+(\omega,0)$ is the generalized eigenfunction of Theorem 6.5.

Define $w = w(x,\omega) = F(r,\psi) - R(-\mathrm{i}0)HF$. Due to Proposition 4.10, Proposition 4.1(iii) and Lemma 6.8(iii), this w agrees with the eigenfunction $w^+(\omega,0)$, cf. the proof of Lemma 6.10. Therefore, our (extended) version of (7.3a) reads

$$S(0)(\omega,\omega') = -2\pi\big\langle F, \mathrm{e}^{\mathrm{i}\phi^-}\tilde{t}^-(\cdot,\omega',0)\big\rangle + 2\pi\big\langle R(-\mathrm{i}0)HF, \mathrm{e}^{\mathrm{i}\phi^-}\tilde{t}^-(\cdot,\omega',0)\big\rangle. \tag{9.37}$$

As indicated above, the contribution to $S(0)(\omega,\omega')$ from the second term on the right-hand side of (9.37) is smooth in ω and ω', if we use a cut-off sufficiently close (but to the left of) the critical angle $\theta = (1-\mu/2)^{-1}\pi$; this is indeed accomplished by using (9.35) as cut-off function.

We conclude that the singularities of the kernel of $S(0)$ are the same as those of the kernel of the operator $\widetilde{S}(0)$ given by

$$\big\langle\tau_1, \widetilde{S}(0)\tau_2\big\rangle = -2\pi\bigg\langle\int F(r,\psi)\tau_1(\omega)\,\mathrm{d}\omega, \int\big(\mathrm{e}^{\mathrm{i}\phi^-}\tilde{t}^-\big)(\cdot,\omega',0)\tau_2(\omega')\,\mathrm{d}\omega'\bigg\rangle.$$

Whence (formally)

$$\widetilde{S}(0)(\omega,\omega') = -2\pi\int\overline{F(r,\psi)}\big(\mathrm{e}^{\mathrm{i}\phi^-}\tilde{t}^-\big)(\cdot,\omega',0)\,\mathrm{d}x. \tag{9.38}$$

Next we introduce the variable $\theta' = \cos^{-1}\hat{x}\cdot(-\omega') \in [0,\pi/2)$; we can represent $\phi^-(x,\omega',0) = -\phi(r,\theta')$, cf. (3.6). The integrand on the right-hand side of (9.38) is given as $\sum_{k=0}^{\infty} f_k$, where f_k has the form

$$\begin{aligned}&\mathrm{e}^{-\mathrm{i}(\phi(r,\psi+2k\pi)+\phi(r,\theta'))}g(r,\psi+2k\pi,\theta')\\&\quad+\mathrm{e}^{-\mathrm{i}(\phi(r,(2k+2)\pi-\psi)+\phi(r,\theta'))}g\big(r,(2k+2)\pi-\psi,\theta'\big).\end{aligned} \tag{9.39}$$

Let us argue that the integral (9.38) is well-defined in $\{\omega\cdot\omega' \neq \cos\frac{\mu}{2-\mu}\pi\}$, in agreement with Theorem 9.3. The argument is based on the method of non-stationary phase. First we notice that the cusp singularities at $\psi = 0$ and $\psi = \pi$ correspond to non-stationary points. More precisely, we can write

$$x = r(\cos\psi\,\omega + \sin\psi\,\tilde{\hat{x}}),$$

and perform the x-integration as

$$\int\cdots\mathrm{d}x = \int_0^{\pi}\sin^{d-2}\psi\,\mathrm{d}\psi\int_{S^{d-2}}\mathrm{d}\tilde{\hat{x}}\int_0^{\infty}\cdots r^{d-1}\,\mathrm{d}r. \tag{9.40}$$

Now on the support of g the factor $\cos(1-\mu/2)\theta' \geqslant \cos\theta' \geqslant 1-\sigma'$, while the factors $\cos(1-\mu/2)(\psi+2k\pi)$ and $\cos(1-\mu/2)((2k+2)\pi-\psi)$ stay sufficiently away from -1

(given that $\psi \approx 0$ or $\psi \approx \pi$) to ensure that the sum of phases does not vanish; here we use (9.34). Thus the phases of f_k are nonzero near the ψ-endpoints of integration, and consequently integration by parts with respect to r regularizes the integral (9.38) (upon first substituting (9.40) and localizing near the ψ-endpoints).

By the same reasoning as above, depending on whether L is even or odd (viz. $L = 2l$ or $L = 2l + 1$), only the integral of one term of (9.39) (and only with $k = l$) carries singularities. We first look at the case for which only $\mathrm{e}^{-\mathrm{i}(\phi(r,\psi+2l\pi)+\phi(r,\theta'))} g(r, \psi + 2l\pi, \theta')$ contributes by singularities. Clearly, for a stationary point

$$\cos\big((1-\mu/2)(\psi + 2l\pi)\big) + \cos\big((1-\mu/2)\theta'\big) = 0, \tag{9.41}$$

which leads to the condition

$$\cos(\psi + \theta') = \cos\left(\frac{2}{2-\mu}\pi\right). \tag{9.42}$$

There are three cases to consider.

Case I. $\omega = -\omega'$. In this case $\theta' = \psi$, so that

$$\begin{aligned} &\frac{\mathrm{d}}{\mathrm{d}\psi}\big(\phi(r, \psi + 2l\pi) + \phi(r, \theta')\big) \\ &\quad = -\sqrt{2\gamma}\, r^{1-\mu/2}\big(\sin(1-\mu/2)(\psi + 2l\pi) + \sin(1-\mu/2)\psi\big) < 0. \end{aligned} \tag{9.43}$$

Whence there are no stationary points.

Case II. $\omega = \omega'$. In this case $\theta' = \pi - \psi$ so that (9.42) reads

$$\omega \cdot \omega' = 1 = -\cos\left(\frac{2}{2-\mu}\pi\right) = \cos\left(\frac{\mu}{2-\mu}\pi\right).$$

This agrees with the "rule" of Theorem 9.3.

Case III. $\omega \neq C\omega'$. In dimension $d \geqslant 3$ the vectors $\tilde{\hat{x}} = \pm y/|y|$ where $y = \omega' - \omega' \cdot \omega\omega$ are the only possible critical points of the map

$$S^{d-2} \ni \tilde{\hat{x}} \to \theta' = \cos^{-1}\big(-(\cos\psi\omega + \sin\psi\tilde{\hat{x}}) \cdot \omega'\big) \in \mathbb{R}.$$

Consequently, for any stationary point, $\hat{x}$ must belong to the plane spanned by ω and ω' (like for $d = 2$). Let us introduce the angle $\gamma = \cos^{-1}\omega \cdot (-\omega')$. There are three possible relationships to be considered (a) $\gamma = |\psi - \theta'|$, (b) $\gamma = \psi + \theta'$ and (c) $\gamma = 2\pi - (\psi + \theta')$. For (a), $\theta' = \psi \mp \gamma$ can be substituted into the sum of phases and we compute as in (9.43). Again there will not be any stationary point. For (b) we can use (9.42) to compute

$$\omega \cdot \omega' = -\cos\gamma = -\cos\left(\frac{2}{2-\mu}\pi\right) = \cos\left(\frac{\mu}{2-\mu}\pi\right),$$

which agrees with the "rule" of Theorem 9.3. Similarly, for (c) we compute

$$\omega \cdot \omega' = -\cos\gamma = -\cos(\psi + \theta') = -\cos\left(\frac{2}{2-\mu}\pi\right) = \cos\left(\frac{\mu}{2-\mu}\pi\right).$$

Next we look at the case for which only $\mathrm{e}^{-\mathrm{i}(\phi(r,2(l+1)\pi-\psi)+\phi(r,\theta'))}g(r, 2(l+1)\pi - \psi, \theta')$ contributes to singularities. The stationary point is given by

$$\cos\bigl((1-\mu/2)\bigl(2(l+1)\pi\bigr) - \psi\bigr) + \cos\bigl((1-\mu/2)\theta'\bigr) = 0, \tag{9.44}$$

which leads to the condition

$$\cos(\psi - \theta') = \cos\left(\frac{2}{2-\mu}\pi\right). \tag{9.45}$$

Again there are three cases to consider.

Case I. $\omega = -\omega'$. In this case $\theta' = \psi$, so that

$$\omega \cdot \omega' = -1 = -\cos\left(\frac{2}{2-\mu}\pi\right) = \cos\left(\frac{\mu}{2-\mu}\pi\right),$$

which agrees with Theorem 9.3.

Case II. $\omega = \omega'$. We have $\theta' = \pi - \psi$, so that

$$\begin{aligned}&\frac{\mathrm{d}}{\mathrm{d}\psi}\bigl(\phi\bigl(r, 2(l+1)\pi - \psi\bigr) + \phi(r, \theta')\bigr)\\ &\quad = \sqrt{2\gamma}\, r^{1-\mu/2}\bigl(\sin(1-\mu/2)\bigl(2(l+1)\pi - \psi\bigr) + \sin(1-\mu/2)(\pi - \psi)\bigr) > 0;\end{aligned} \tag{9.46}$$

whence there are no stationary points.

Case III. $\omega \neq C\omega'$. As in the previous "Case III", for any stationary point the vector $\hat{x}$ must belong to the plane spanned by ω and ω'. Again we define $\gamma = \cos^{-1}\omega \cdot (-\omega')$, and there are three possible relationships to be considered: (a) $\gamma = |\psi - \theta'|$, (b) $\gamma = \psi + \theta'$ and (c) $\gamma = 2\pi - (\psi + \theta')$. For (a),

$$\omega \cdot \omega' = -\cos\gamma = -\cos(\psi - \theta') = -\cos\left(\frac{2}{2-\mu}\pi\right) = \cos\left(\frac{\mu}{2-\mu}\pi\right),$$

which agrees with Theorem 9.3. For (b) and (c) we compute as in (9.46); there are no stationary points.

Remarks 9.6.

(1) For the above considerations (on the location of singularities), it is not strictly needed that $V_2 = 0$. In fact we can include a V_2 as in Condition 2.1 with $\epsilon_2 > 1 - \frac{1}{2}\mu$ and solve transport equations as before using the same phase function (the one determined by V_1 only).

(2) Suppose in addition to (1) that V_2 is spherically symmetric. Then the operators $T = S(0)$, as well as $T = \tilde{S}(0)$, obey that $RTR^{-1} = T$ for all d-dimensional rotations R. This means that the kernel $T(\omega, \omega')$ of these operators is a function of $\omega \cdot \omega'$ only. Using the stationary phase method it is feasible for $\frac{\mu}{2-\mu} \notin \mathbb{Z}$ to write (as a possible continuation of the above analysis) the singular part of the kernel of $\tilde{S}(0)$ as a sum of terms of the form $(\omega \cdot \omega' - \nu \pm \mathrm{i}0)^{-\frac{s}{2}} a(\omega \cdot \omega')$ (at least for poly-homogeneous V_2); we shall not elaborate. Our recent paper [7] is devoted to an alternative approach that we find more elementary, and besides, by that method we can extract the singular part in the exceptional cases $\frac{\mu}{2-\mu} \in \mathbb{Z}$ too.

Appendix A. Elements of abstract scattering theory

Various versions of stationary scattering theory can be found in the literature. In this appendix we give, in an abstract setting, a self-contained presentation of its elements used in our paper. It is a version of the standard approach contained e.g. in [29], adapted to our paper. In our stationary formulas for the scattering operator we use in addition ideas due to Isozaki–Kitada, see the proof of [19, Theorem 3.3].

A.1. Wave operators

Let H_0 and H be two self-adjoint operators on a Hilbert space $\mathcal{H}$. We assume that H_0 has only continuous spectrum. Throughout this appendix, let Λ_n, $n \in \mathbb{N}$, be a sequence of compact subsets of $\sigma(H_0)$ such that Λ_n is a subset of the interior of Λ_{n+1}, and such that $\sigma(H_0) \setminus \bigcup_n \Lambda_n$ has the Lebesgue measure zero. Pick a sequence $h_n \in C_c^\infty(\Lambda_{n+1})$ with $h_n = 1$ on Λ_n. Let $\mathcal{D} := \bigcup_n \operatorname{Ran} 1_{\Lambda_n}(H_0)$; it is dense in $\mathcal{H}$.

We will write $R(\zeta) = (H - \zeta)^{-1}$ and $R_0(\zeta) = (H_0 - \zeta)^{-1}$ for $\zeta \notin \sigma(H_0)$, and

$$\delta_\epsilon(\lambda) = \frac{\epsilon}{\pi((H_0 - \lambda)^2 + \epsilon^2)} = \frac{\epsilon}{\pi} R_0(\lambda - \mathrm{i}\epsilon) R_0(\lambda + \mathrm{i}\epsilon), \quad \epsilon > 0.$$

Note that if I is an interval and $f \in \mathcal{H}$, then

$$\left\| \int_I \frac{\epsilon}{\pi} R_0(\lambda - \mathrm{i}\epsilon) R_0(\lambda + \mathrm{i}\epsilon) f \, \mathrm{d}\lambda \right\| \leqslant \|f\|, \tag{A.1}$$

$$\lim_{\epsilon \searrow 0} \int_I \frac{\epsilon}{\pi} R_0(\lambda - \mathrm{i}\epsilon) R_0(\lambda + \mathrm{i}\epsilon) f \, \mathrm{d}\lambda = 1_I(H_0) f. \tag{A.2}$$

Theorem A.1. *Suppose $J^\pm$ is a densely defined operator whose domain contains $\mathcal{D}$ such that $J_n^\pm := J^\pm h_n(H_0)$ is bounded for any n, and*

$$\lim_{t \to \pm\infty} \left\| J^\pm \mathrm{e}^{\mathrm{i}tH_0} f \right\|^2 = \|f\|^2, \quad f \in \mathcal{D}.$$

We also suppose that there exists the wave operator

$$W^\pm f := \lim_{t \to \pm\infty} \mathrm{e}^{\mathrm{i}tH} J^\pm \mathrm{e}^{-\mathrm{i}tH_0} f, \quad f \in \mathcal{D}. \tag{A.3}$$

Then

(i) $W^{\pm}$ *extends to an isometric operator and* $W^{\pm}H_0 = HW^{\pm}$.

(ii) *For any interval* I *and* $f \in \mathcal{D}$,

$$W^{\pm}1_I(H_0)f = \lim_{\epsilon \searrow 0} \int_I \frac{\epsilon}{\pi} R(\lambda \mp \mathrm{i}\epsilon) J^{\pm} R_0(\lambda \pm \mathrm{i}\epsilon) f \, \mathrm{d}\lambda. \tag{A.4}$$

(iii) *For any continuous function* $g : \mathbb{R} \to \mathbb{C}$ *vanishing at infinity, interval* I *and* $f \in \mathcal{D}$,

$$W^{\pm}g(H_0)1_I(H_0)f = \lim_{\epsilon \searrow 0} \int_I \frac{\epsilon}{\pi} g(\lambda) R(\lambda \mp \mathrm{i}\epsilon) J^{\pm} R_0(\lambda \pm \mathrm{i}\epsilon) f \, \mathrm{d}\lambda. \tag{A.5}$$

(iv) *Suppose in addition that* $J^{\pm}$ *maps* $\mathcal{D}$ *into* $\operatorname{Dom} H$. *Suppose that* $T^{\pm}$ *is a densely defined operator such that* $T_n^{\pm} := T^{\pm}h_n(H_0)$ *is bounded for any* n *and that* $T^{\pm}f = \mathrm{i}(HJ^{\pm} - J^{\pm}H_0)f$ *for any* $f \in \mathcal{D}$. *Then we have the following modifications of* (A.4) *and* (A.5):

$$W^{\pm}1_I(H_0)f = \lim_{\epsilon \searrow 0} \int_I \big(J^{\pm} + \mathrm{i}\, R(\lambda \mp \mathrm{i}\epsilon) T^{\pm}\big) \delta_{\epsilon}(\lambda) f \, \mathrm{d}\lambda, \tag{A.6}$$

$$W^{\pm}g(H_0)1_I(H_0)f = \lim_{\epsilon \searrow 0} \int_I g(\lambda) \big(J^{\pm} + \mathrm{i}\, R(\lambda \mp \mathrm{i}\epsilon) T^{\pm}\big) \delta_{\epsilon}(\lambda) f \, \mathrm{d}\lambda. \tag{A.7}$$

Proof. (i) is well known.

Let us prove (ii): By (A.3),

$$W^{\pm}f = \lim_{\epsilon \searrow 0} 2\epsilon \int_0^{\infty} \mathrm{e}^{-2\epsilon t} \mathrm{e}^{\pm \mathrm{i} t H} J^{\pm} \mathrm{e}^{\mp \mathrm{i} t H_0} f \, \mathrm{d}t.$$

By the vector-valued Plancherel formula, we obtain

$$W^{\pm}f = \lim_{\epsilon \searrow 0} \int \frac{\epsilon}{\pi} R(\lambda \mp \mathrm{i}\epsilon) J^{\pm} R_0(\lambda \pm \mathrm{i}\epsilon) f \, \mathrm{d}\lambda. \tag{A.8}$$

Therefore,

$$\begin{aligned} W^{\pm}1_I(H_0)f = {} & \lim_{\epsilon \searrow 0} \int_I \frac{\epsilon}{\pi} R(\lambda \mp \mathrm{i}\epsilon) J^{\pm} R_0(\lambda \pm \mathrm{i}\epsilon) f \, \mathrm{d}\lambda \\ & - \lim_{\epsilon \searrow 0} \int_I \frac{\epsilon}{\pi} R(\lambda \mp \mathrm{i}\epsilon) J^{\pm} R_0(\lambda \pm \mathrm{i}\epsilon) 1_{\mathbb{R} \setminus I}(H_0) f \, \mathrm{d}\lambda \\ & + \lim_{\epsilon \searrow 0} \int_{\mathbb{R} \setminus I} \frac{\epsilon}{\pi} R(\lambda \mp \mathrm{i}\epsilon) J^{\pm} R_0(\lambda \pm \mathrm{i}\epsilon) 1_I(H_0) f \, \mathrm{d}\lambda. \end{aligned}$$

We need to show that the last two terms vanish. The proof for both terms is identical. Consider the last one term. Let $f_1 \in \mathcal{H}$ and pick an n so that $f = 1_{\Lambda_n}(H_0)f$. Then (using (A.1) in the last estimation)

$$\left| \int\limits_{\mathbb{R}\setminus I} \frac{\epsilon}{\pi} \langle f_1, R(\lambda \mp \mathrm{i}\epsilon) J^{\pm} R_0(\lambda \pm \mathrm{i}\epsilon) 1_I(H_0) f \rangle \,\mathrm{d}\lambda \right|$$

$$\leqslant \| J_n^{\pm} \| \Bigl(\int\limits_{\mathbb{R}\setminus I} \frac{\epsilon}{\pi} \| R(\lambda \pm \mathrm{i}\epsilon) f_1 \|^2 \,\mathrm{d}\lambda \Bigr)^{\frac{1}{2}} \Bigl(\int\limits_{\mathbb{R}\setminus I} \frac{\epsilon}{\pi} \| R_0(\lambda \pm \mathrm{i}\epsilon) 1_I(H_0) f \|^2 \,\mathrm{d}\lambda \Bigr)^{\frac{1}{2}}$$

$$\leqslant C_\epsilon \| f_1 \|; \qquad C_\epsilon := \| J_n^{\pm} \| \Bigl(\int\limits_{\mathbb{R}\setminus I} \frac{\epsilon}{\pi} \| R_0(\lambda \pm \mathrm{i}\epsilon) 1_I(H_0) f \|^2 \,\mathrm{d}\lambda \Bigr)^{\frac{1}{2}}.$$

Due to (A.2), $C_\epsilon \to 0$ as $\epsilon \to 0$. Whence (ii) follows.

Let us prove (iii): Let $f_1 \in \mathcal{H}$ and pick an n so that $f = 1_{\Lambda_n}(H_0)f$. Any continuous function g vanishing at infinity can be uniformly approximated by g_m, finite linear combinations of characteristic functions of intervals. By (ii) and (A.1),

$$W^{\pm} g_m(H_0) 1_I(H_0) f = \lim_{\epsilon \searrow 0} \int\limits_I \frac{\epsilon}{\pi} g_m(\lambda) R(\lambda \mp \mathrm{i}\epsilon) J^{\pm} R_0(\lambda \pm \mathrm{i}\epsilon) f \,\mathrm{d}\lambda.$$

Now

$$\left| \int\limits_I \frac{\epsilon}{\pi} \bigl(g_m(\lambda) - g(\lambda)\bigr) \langle f_1, R(\lambda \mp \mathrm{i}\epsilon) J^{\pm} R_0(\lambda \pm \mathrm{i}\epsilon) f \rangle \,\mathrm{d}\lambda \right|$$

$$\leqslant \| J_n^{\pm} \| \Bigl(\int \frac{\epsilon}{\pi} \| R(\lambda \pm \mathrm{i}\epsilon) f_1 \|^2 \,\mathrm{d}\lambda \Bigr)^{\frac{1}{2}} \Bigl(\int \frac{\epsilon}{\pi} \| R_0(\lambda \pm \mathrm{i}\epsilon) f \|^2 \,\mathrm{d}\lambda \Bigr)^{\frac{1}{2}} \sup |g_m - g|$$

$$\leqslant C_m \| f_1 \|; \qquad C_m := \| J_n^{\pm} \| \| f \| \sup |g_m - g|.$$

Since $C_m \to 0$ we are done.

To prove (iv), we use (iii) and the identity

$$R(\lambda \mp \mathrm{i}\epsilon) J^{\pm} = \bigl(J^{\pm} + \mathrm{i} R(\lambda \mp \mathrm{i}\epsilon) T^{\pm} \bigr) R_0(\lambda \mp \mathrm{i}\epsilon). \qquad \square$$

Remark. In the context of our paper, we can take $\Lambda_n = [\frac{1}{n}, n]$.

A.2. Scattering operator

Define the scattering operator by $S := W^{+*} W^{-}$. Clearly, $H_0 S = S H_0$.

Theorem A.2. *Suppose that the conditions of Theorem* A.1 *hold. Let the operator J^- satisfy*

$$\lim_{t \to +\infty} \mathrm{e}^{\mathrm{i}tH} J^{-} \mathrm{e}^{-\mathrm{i}tH_0} f = 0, \quad f \in \mathcal{D}. \tag{A.9}$$

Then for all $f \in \mathcal{D}$

$$Sf = -\lim_{\epsilon \searrow 0} 2\pi \int \delta_\epsilon(\lambda) W^{+*} T^- \delta_\epsilon(\lambda) f \, \mathrm{d}\lambda. \tag{A.10}$$

Proof.

$$\begin{aligned} W^- f &= -\lim_{t \to +\infty} \left(\mathrm{e}^{\mathrm{i}tH} J^- \mathrm{e}^{-\mathrm{i}tH_0} - \mathrm{e}^{-\mathrm{i}tH} J^- \mathrm{e}^{\mathrm{i}tH_0} \right) f \\ &= -\lim_{t \to +\infty} \int_{-t}^{t} \mathrm{e}^{\mathrm{i}sH} T^- \mathrm{e}^{-\mathrm{i}sH_0} f \, \mathrm{d}s \\ &= -\lim_{\epsilon \searrow 0} \epsilon \int_0^\infty \mathrm{e}^{-\epsilon t} \, \mathrm{d}t \int_{-t}^{t} \mathrm{e}^{\mathrm{i}sH} T^- \mathrm{e}^{-\mathrm{i}sH_0} f \, \mathrm{d}s \\ &= -\lim_{\epsilon \searrow 0} \int \mathrm{e}^{-\epsilon|s|} \mathrm{e}^{\mathrm{i}sH} T^- \mathrm{e}^{-\mathrm{i}sH_0} f \, \mathrm{d}s. \end{aligned}$$

Then we use the definition of S and the intertwining property of W^{+*} to obtain

$$Sf = -\lim_{\epsilon \searrow 0} \int \mathrm{e}^{-\epsilon|s|} \mathrm{e}^{\mathrm{i}sH_0} W^{+*} T^- \mathrm{e}^{-\mathrm{i}sH_0} f \, \mathrm{d}s.$$

Finally, we use the vector-valued Plancherel theorem. □

A.3. Method of rigged Hilbert spaces applied to wave operators

Consider a family of separable Hilbert spaces $\mathcal{H}$ and $\mathcal{V}_s$, $s > \frac{1}{2}$, such that $\mathcal{V}_s$ is densely and continuously embedded in $\mathcal{H}$, and similarly, $\mathcal{V}_s$ is densely and continuously embedded in $\mathcal{V}_t$ if $s > t$. Let $\mathcal{V}_s^*$ be the space dual to $\mathcal{V}_s$, so that we have nested Hilbert spaces

$$\mathcal{V}_s \subseteq \mathcal{V}_t \subseteq \mathcal{H} \subseteq \mathcal{V}_t^* \subseteq \mathcal{V}_s^*; \quad s > t.$$

We remark that $\mathcal{H}$ equipped with such a structure is sometimes called a *rigged Hilbert space*.

The following theorem allows us to introduce wave matrices:

Theorem A.3. *Fix* $s > t > \frac{1}{2}$. *Suppose that there exists for almost all* λ *the limit*

$$\text{s-}\lim_{\epsilon \to 0} \delta_\epsilon(\lambda) =: \delta_0(\lambda) \in \mathcal{B}\big(\mathcal{V}_t, \mathcal{V}_t^*\big).$$

Suppose the conditions of Theorem A.1 and that the operators $J_n^\pm$ *and* $R(\lambda \mp \mathrm{i}\epsilon) T_n^\pm$ *with* $\lambda \in \Lambda_n$ *and* $\epsilon > 0$ *extend to elements of* $\mathcal{B}(\mathcal{V}_t^*, \mathcal{V}_s^*)$. *Suppose that for fixed* n *and almost everywhere in* Λ_n *there exists*

$$R(\lambda \mp \mathrm{i}0) T_n^\pm := \text{s-}\lim_{\epsilon \searrow 0} R(\lambda \mp \mathrm{i}\epsilon) T_n^\pm \in \mathcal{B}\big(\mathcal{V}_t^*, \mathcal{V}_s^*\big).$$

Suppose furthermore that for any n there exists $\epsilon_n > 0$ *such that*

$$\sup_{\lambda\in\Lambda_n}\sup_{\epsilon<\epsilon_n}\big\|\delta_\epsilon(\lambda)\big\|_{\mathcal{V}_t\to\mathcal{V}_t^*},\ \sup_{\lambda\in\Lambda_n}\sup_{\epsilon<\epsilon_n}\big\|R(\lambda\mp\mathrm{i}\epsilon)T_n^\pm\big\|_{\mathcal{V}_t^*\to\mathcal{V}_s^*}<\infty. \tag{A.11}$$

Let I *be an interval with* $I\subseteq\Lambda_n$ *for some n, and let* $f\in\mathcal{V}_t$ *be given such that* $f=h_n(H_0)f$ (*in particular this means that* $f\in\mathcal{D}\cap\mathcal{V}_t$). *Then* (*in terms of an integral of a* $\mathcal{V}_s^*$*-valued function*), *for all* $g\in C(\mathbb{R})$,

$$W^\pm g(H_0)1_I(H_0)f=\int_I g(\lambda)\big(J_n^\pm+\mathrm{i}\,R(\lambda\mp\mathrm{i}\,0)T_n^\pm\big)\delta_0(\lambda)f\,\mathrm{d}\lambda. \tag{A.12}$$

Proof. We can replace $T^\pm\to T_n^\pm$, $J^\pm\to J_n^\pm$ in the integrand of (A.7). Then, by the assumptions, it has a pointwise limit as an element of $\mathcal{V}_s^*$. Due to (A.11), we can apply the dominated convergence theorem. □

Remark. In the context of our paper, we take $\mathcal{V}_s:=L^{2,s}$.

A.4. Method of rigged Hilbert spaces applied to the scattering operator

The method of rigged Hilbert spaces allows us to introduce scattering matrices:

Theorem A.4. *Suppose that the conditions of Theorem* A.3 *hold for some* $s>t>\frac{1}{2}$. *Suppose* (A.9). *Fix* $r>s$. *Suppose that for all* $n\in\mathbb{R}$ *and* $\epsilon>0$ *the operators* $T_n^-\delta_\epsilon(\lambda)\in\mathcal{B}(\mathcal{V}_r,\mathcal{V}_s)$ *with a measurable dependence on* $\lambda\in\mathbb{R}$. *Suppose that for fixed n and almost everywhere in* Λ_n *there exists the limit*

$$\text{s-}\lim_{\epsilon\to 0}T_n^-\delta_\epsilon(\lambda)=:T_n^-\delta_0(\lambda)\in\mathcal{B}(\mathcal{V}_r,\mathcal{V}_s).$$

Suppose furthermore that for any n there exists $\epsilon_n>0$ *such that*

$$\sup_{\lambda\in\mathbb{R}}\sup_{\epsilon<\epsilon_n}\big\|T_n^-\delta_\epsilon(\lambda)\big\|_{\mathcal{V}_r\to\mathcal{V}_s}<\infty. \tag{A.13}$$

Let I *be an interval with* $I\subseteq\Lambda_n$ *for some n, and let* $f_1\in\mathcal{D}\cap\mathcal{V}_t$ *and* $f_2\in\mathcal{D}\cap\mathcal{V}_r$ *be given such that* $f_1=1_I(H_0)f_1$ *and* $f_2=h_n(H_0)f_2$. *Then*

$$\langle f_1,Sf_2\rangle=-2\pi\int_I\big\langle f_1,\delta_0(\lambda)J_n^{+*}T_n^-\delta_0(\lambda)f_2\big\rangle\,\mathrm{d}\lambda$$
$$+2\pi\mathrm{i}\int_I\big\langle f_1,\delta_0(\lambda)T_n^{+*}R(\lambda+\mathrm{i}\,0)T_n^-\delta_0(\lambda)f_2\big\rangle\,\mathrm{d}\lambda.$$

Proof. Set $r_\epsilon(\lambda):=\frac{\epsilon}{\pi(\lambda^2+\epsilon^2)}$. We insert (A.12) with $g(\lambda)=r_\epsilon(\lambda-\lambda_1)$ into (A.10):

$$
\begin{aligned}
\langle f_1, S f_2\rangle &= -\lim_{\epsilon\searrow 0} 2\pi \int \big\langle f_1, \delta_\epsilon(\lambda_1) W^{+*} T^- \delta_\epsilon(\lambda_1) f_2\big\rangle\, \mathrm{d}\lambda_1 \\
&= -\lim_{\epsilon\searrow 0} 2\pi \iint_I r_\epsilon(\lambda-\lambda_1)\big\langle f_1, \delta_0(\lambda)\big(J_n^{+*} - \mathrm{i}\, T_n^{+*} R(\lambda+\mathrm{i}0)\big) T_n^- \delta_\epsilon(\lambda_1) f_2\big\rangle \\
&= -\lim_{\epsilon\searrow 0} 2\pi \int_I \big\langle f_1, \delta_0(\lambda)\big(J_n^{+*} - \mathrm{i}\, T_n^{+*} R(\lambda+\mathrm{i}0)\big) T_n^- \delta_{2\epsilon}(\lambda) f_2\big\rangle\, \mathrm{d}\lambda.
\end{aligned}
$$

In the last step we interchanged integrals using (A.13) and the Fubini theorem, and we used that

$$
\int \delta_\epsilon(\lambda_1) r_\epsilon(\lambda-\lambda_1)\, \mathrm{d}\lambda_1 = \delta_{2\epsilon}(\lambda).
$$

Then we pass with $\epsilon \to 0$ using (A.13) and the dominated convergence theorem. □

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