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High energy asymptotics of the scattering amplitude for the Schrödinger equation

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Abstract. We find an explicit function approximating at high energies the kernel of the scattering matrix with arbitrary accuracy. Moreover, the same function gives all diagonal singularities of the kernel of the scattering matrix in the angular variables.

Keywords. Scattering matrix; asymptotic expansion; high energy; diagonal singularity.

1. Introduction

High energy asymptotics of the scattering matrix $S(\lambda) : L_2(\mathbb{S}^{d-1}) \to L_2(\mathbb{S}^{d-1})$ for the Schrödinger operator $H = -\Delta + V$ in the space $L_2(\mathbb{R}^d)$ with a short-range potential (bounded and satisfying the condition $V(x) = O(|x|^{-\rho})$, $\rho > 1$, as $|x| \to \infty$) is given by the Born approximation. To describe it, let us introduce the operator $\Gamma_0(\lambda)$,

$$(\Gamma_0(\lambda)f)(\omega) = 2^{-1/2}k^{(d-2)/2}\hat{f}(k\omega),\ \lambda = k^2 \in \mathbb{R}_+ = (0,\infty),\ \omega \in \mathbb{S}^{d-1}, \tag{1.1}$$

of the restriction (up to the numerical factor) of the Fourier transform $\hat{f}$ of f to the sphere of radius k. Set $R_0(z) = (-\Delta - z)^{-1}$. By the Sobolev trace theorem and the limiting absorption principle the operators $\Gamma_0(\lambda)\langle x\rangle^{-r}$ and $\langle x\rangle^{-r}R_0(\lambda + i0)\langle x\rangle^{-r}$ are correctly defined as bounded operators for any $r > 1/2$ and their norms are estimated by $\lambda^{-1/4}$ and $\lambda^{-1/2}$, respectively. Therefore it is easy to deduce (see, e.g. [7, 13]) from the usual stationary representation for the scattering matrix that

$$S(\lambda) = I - 2\pi i \sum_{n=0}^{N} (-1)^n \Gamma_0(\lambda) V (R_0(\lambda + i0)V)^n \Gamma_0^*(\lambda) + \sigma_N(\lambda), \tag{1.2}$$

where $||\sigma_N(\lambda)|| = O(\lambda^{-(N+2)/2})$ as $\lambda \to \infty$. Moreover, the operator σ_N belongs to a suitable Schatten–von Neumann class $\mathfrak{S}_{\alpha(N)}$ and $\alpha(N) \to 0$ as $N \to \infty$. Nevertheless the Born expansion (1.2) is not very convenient because the structure of the nth term is extremely complicated already for relatively small n.

We suppose that the potential $V(x)$ of the Schrödinger operator $H = -\Delta + V$ satisfies the estimates

$$|\partial^\alpha V(x)| \le C_\alpha(1 + |x|)^{-\rho-|\alpha|}, \quad \rho > 1, \tag{1.3}$$

for all multi-indices α. Our goal is to find an explicit function $s_0(\omega, \omega'; \lambda)$ approximating the kernel $s(\omega, \omega'; \lambda)$ of the scattering matrix $S(\lambda)$ with arbitrary accuracy at high energies

This paper is dedicated to Jean–Michel Combes on the occasion of his sixtieth birthday.

(as $\lambda \to \infty$). It turns out that the same function $s_0(\omega, \omega'; \lambda)$ gives all diagonal singularities of the kernel $s(\omega, \omega'; \lambda)$ in the angular variables $\omega, \omega' \in \mathbb{S}^{d-1}$.

Let us formulate our main result. The answer is given in terms of approximate solutions of the Schrödinger equation. To be more precise, we denote by $u(x, \xi) = u^{(N)}(x, \xi)$ explicit functions (see §2, for their construction)

$$u(x, \xi) = \mathrm{e}^{i\langle x, \xi\rangle} a(x, \xi), \quad \xi = |\xi|\hat{\xi} \in \mathbb{R}^d, \tag{1.4}$$

such that

$$r^{(N)}(x, \xi) = \mathrm{e}^{-i\langle x, \xi\rangle}(-\Delta + V(x) - |\xi|^2)u^{(N)}(x, \xi) \tag{1.5}$$

tends to zero faster than $|x|^{-p}$ as $|x| \to \infty$ where $p = p(N) \to \infty$ as $N \to \infty$ and faster than $|\xi|^{-N}$ as $|\xi| \to \infty$ off any conical neighborhood of the direction $\hat{x} = \hat{\xi}$. The amplitude $a(x, \xi)$ is obtained as a solution of the corresponding transport equation.

We note that, off the diagonal $\omega = \omega'$ (see [1]), $s(\omega, \omega'; \lambda)$ is a C^∞-function of $\omega, \omega' \in \mathbb{S}^{d-1}$, and it tends to zero faster than any power of λ^{-1} as $\lambda \to \infty$. Thus, it suffices to describe the structure of $s(\omega, \omega'; \lambda)$ in a neighborhood of the diagonal $\omega = \omega'$. Let $\omega_0 \in \mathbb{S}^{d-1}$ be an arbitrary point, Π_{ω_0} be the plane orthogonal to ω_0 and $\Omega_\pm(\omega_0, \delta) \subset \mathbb{S}^{d-1}$ be determined by the condition $\pm\langle \omega, \omega_0\rangle > \delta > 0$. Set

$$x = \omega_0 z + y, \quad y \in \Pi_{\omega_0},$$

and

$$\begin{aligned} s_0(\omega, \omega'; \lambda) = \pm 2^{-1}\lambda^{(d-1)/2}(2\pi)^{-d+1} \times \int_{\Pi_{\omega_0}} \mathrm{e}^{i\lambda^{1/2}\langle y, \omega' - \omega\rangle} \\ \times \Big[\langle \omega + \omega', \omega_0\rangle a(y, -\lambda^{1/2}\omega) a(y, \lambda^{1/2}\omega') + i\lambda^{-1/2} \\ \times \Big(a(y, \lambda^{1/2}\omega')(\partial_z a)(y, -\lambda^{1/2}\omega) - a(y, -\lambda^{1/2}\omega)(\partial_z a)(y, \lambda^{1/2}\omega')\Big)\Big]\, \mathrm{d}y \end{aligned} \tag{1.6}$$

for $\omega, \omega' \in \Omega_\pm = \Omega_\pm(\omega_0, \delta)$. Then the kernel

$$s(\omega, \omega'; \lambda) - s_0(\omega, \omega'; \lambda), \quad s_0 = s_0^{(N)}, \tag{1.7}$$

belongs to the class $C^p(\Omega \times \Omega)$ where $\Omega = \Omega_+ \cup \Omega_-$ and $p = p(N) \to \infty$ as $N \to \infty$. Moreover, the C^p-norm of this kernel is $O(\lambda^{-p})$ as $\lambda \to \infty$. Thus, all singularities of $s(\omega, \omega'; \lambda)$ both for high energies and in smoothness are described by the explicit formula (1.6). Formula (1.6) shows that we actually consider the singular part $s_0(\omega, \omega'; \lambda)$ of the scattering matrix as a pseudo-differential operator (on the unit sphere) determined by its amplitude. Note that the function $s_0(\omega, \omega'; \lambda)$ satisfies the same symmetry relation

$$s(\omega, \omega'; \lambda) = s(-\omega', -\omega; \lambda)$$

as kernel of the scattering matrix itself. We emphasize that formula (1.6) gives the singular part of the scattering amplitude off any neighborhood of the hyperplane Π_{ω_0}. Since $\omega_0 \in \mathbb{S}^{d-1}$ is arbitrary, this determines the singular part of $s(\omega, \omega'; \lambda)$ for all $\omega, \omega' \in \mathbb{S}^{d-1}$.

A similar procedure of the one described above was used, probably for the first time, in [2] for potentials V from the Schwartz class. The problem is getting substantially more difficult already for short-range potentials V satisfying condition (1.3). In this case the formula for the singular part of the scattering matrix that is similar to (1.6) was given (without proof) in [11]. Our method allows us to also consider long-range electric as well as magnetic potentials. These results will be presented elsewhere.

2. The transport equation

In this section we give a standard construction of an approximate but explicit solution of the Schrödinger equation. This construction relies on a solution of the corresponding transport equation by iterations.

Comparing formulas (1.4) and (1.5), we see that

$$r(x,\xi) = -2i\langle \xi, \nabla a(x,\xi)\rangle - \Delta a(x,\xi) + V(x)a(x,\xi), \quad \nabla = \nabla_x. \tag{2.1}$$

Let us seek the function a in the form

$$a(x,\xi) = a^{(N)}(x,\xi) = \sum_{n=0}^{N} (2i|\xi|)^{-n} b_n(x,\hat{\xi}), \quad b_0(x,\hat{\xi}) = 1. \tag{2.2}$$

Plugging this expression into (2.1) and equating coefficients at the same powers of $(2i|\xi|)^{-n}$, we obtain recurrent equations for the functions b_n:

$$\langle \hat{\xi}, \nabla_x b_{n+1}(x,\hat{\xi})\rangle = -\Delta b_n(x,\hat{\xi}) + V(x) b_n(x,\hat{\xi}). \tag{2.3}$$

Then

$$r^{(N)}(x,\xi) = (2i|\xi|)^{-N}(-\Delta b_N(x,\hat{\xi}) + V(x) b_N(x,\hat{\xi})) = (2i|\xi|)^{-N}\langle \hat{\xi}, \nabla b_{N+1}(x,\hat{\xi})\rangle.$$

Let the domain $\Gamma_\pm(\epsilon, R) \subset \mathbb{R}^d \times \mathbb{R}^d$ be distinguished by the condition: $(x,\xi) \in \Gamma_\pm(\epsilon, R)$ if either $|x| \le R$ or $\pm\langle \hat{x}, \hat{\xi}\rangle \ge -1 + \epsilon$ for some $\epsilon > 0$. We set $\Gamma = \Gamma_-$. The following assertion is almost obvious.

PROPOSITION 2.1

Let assumption 1.3 *hold. Then the functions*

$$b_{n+1}(x,\hat{\xi}) = \int_{-\infty}^{0} \left(-\Delta b_n(x + t\hat{\xi}, \hat{\xi}) + V(x + t\hat{\xi}) b_n(x + t\hat{\xi}, \hat{\xi})\right) \mathrm{d}t$$

satisfy equations (2.3) *and for* $(x,\xi) \in \Gamma(\epsilon, R)$ $(and\ \rho \le 2)$

$$|\partial_x^\alpha \partial_\xi^\beta b_n(x,\hat{\xi})| \le C_{\alpha,\beta}(1 + |x|)^{-(\rho-1)n-|\alpha|}\, |\xi|^{-\beta}. \tag{2.4}$$

In particular, the function (2.2) *and the remainder* (1.5) *satisfy the estimates*

$$|\partial_x^\alpha \partial_\xi^\beta a(x,\xi)| \le C_{\alpha,\beta}(1 + |x|)^{-|\alpha|}\, |\xi|^{-|\beta|} \tag{2.5}$$

and

$$|\partial_x^\alpha \partial_\xi^\beta r^{(N)}(x,\xi)| \le C_{\alpha,\beta}(1 + |x|)^{-1-(\rho-1)(N+1)-|\alpha|}\, |\xi|^{-N-|\beta|}. \tag{2.6}$$

Let us write down explicit expressions for the first two functions b_n:

$$b_1(x,\hat{\xi}) = \int_{-\infty}^{0} V(x + t\hat{\xi})\mathrm{d}t,$$

$$b_2(x,\hat{\xi}) = \int_{-\infty}^{0} t(\Delta V)(x + t\hat{\xi})\mathrm{d}t + \frac{1}{2}\left(\int_{-\infty}^{0} V(x + t\hat{\xi})\mathrm{d}t\right)^2.$$

We put

$$a_-(x,\xi) = a(x,\xi), \quad a_+(x,\xi) = \overline{a(x,-\xi)}$$

and

$$r_-(x,\xi) = r(x,\xi), \quad r_+(x,\xi) = \overline{r(x,-\xi)}.$$

Clearly, the functions $a_+(x,\xi)$ and $r_+(x,\xi)$ satisfy the same assertion as that of Proposition 2.1 but with the region $\Gamma_-(\epsilon, R)$ replaced by $\Gamma_+(\epsilon, R)$.

3. Wave operators and the scattering matrix

1. If $V(x)$ is a bounded function and $V(x) = O(|x|^{-\rho})$, $\rho > 1$, as $|x| \to \infty$, then, for the pair $H_0 = -\Delta$, $H = -\Delta + V(x)$ in the space $\mathcal{H} = L_2(\mathbb{R}^d)$, the wave operators

$$W_\pm(H, H_0) = s - \lim_{t\to\pm\infty} \mathrm{e}^{iHt}\mathrm{e}^{-iH_0t}$$

exist and $W_\pm(H,H_0)H_0 = HW_\pm(H,H_0)$. Moreover, the wave operators are isometric and complete (see, e.g., [10, 13]). Therefore the scattering operator

$$\mathbf{S} = W_+^*(H,H_0)W_-(H,H_0)$$

commutes with the operator H_0 and is unitary in the space $\mathcal{H}$.

Let $\mathfrak{N} = L_2(\mathbb{S}^{d-1})$, let the operator $\Gamma_0(\lambda) : \mathcal{S}(\mathbb{R}^d) \to \mathfrak{N}$ be defined by formula (1.1) and let $(Uf)(\lambda) = \Gamma_0(\lambda)f$. Then $U : \mathcal{H} \to \hat{\mathcal{H}} = L_2(\mathbb{R}_+; \mathfrak{N})$ is a unitary operator, and UH_0U^* acts in the space $\hat{\mathcal{H}}$ as multiplication by the independent variable λ. Since $\mathbf{S}H_0 = H_0\mathbf{S}$, the operator $U\mathbf{S}U^*$ acts in the space $\hat{\mathcal{H}}$ as multiplication by the operator function $S(\lambda) : \mathfrak{N} \to \mathfrak{N}$ known as the scattering matrix.

However our study of the scattering matrix relies on introduction of wave operators with special identifications $J_\pm$ which will be constructed as pseudo-differential operators.

2. Let us recall briefly some basic facts about pseudo-differential operators. Let

$$(Tf)(x) = (2\pi)^{-d/2}\int_{\mathbb{R}^d} \mathrm{e}^{i\langle x,\xi\rangle} t(x,\xi)\hat{f}(\xi)\mathrm{d}\xi,$$

where $\hat{f}$ is the Fourier transform of f, the symbol $t \in C^\infty(\mathbb{R}^d \times \mathbb{R}^d)$ and, for some n and m and for all multi-indices α, β,

$$|(\partial_x^\alpha \partial_\xi^\beta t)(x,\xi)| \le C_{\alpha,\beta}\langle x\rangle^{n-|\alpha|}\langle\xi\rangle^{m-|\beta|}.$$

The class of operators or symbols satisfying this condition will be denoted by $\mathcal{S}^{n,m}$. The operators from these classes send the Schwartz space $\mathcal{S}(\mathbb{R}^d)$ into itself. The proof of the following assertion can be found in [3], ch. 18.

PROPOSITION 3.1

Let $t \in \mathcal{S}^{n,m}$ where $n \le 0$ and $m \le 0$. Then the operator $T\langle x\rangle^{-n}$ is bounded in $L_2(\mathbb{R}^d)$.

We also need a more special class $\mathcal{S}_\pm^{n,m} \subset \mathcal{S}^{n,m}$ of symbols satisfying the additional property

$$t(x,\xi) = 0 \text{ if } \mp\langle\hat{x},\hat{\xi}\rangle \le \varepsilon$$

for some $\varepsilon > 0$. Moreover, we assume that for symbols from this class $t(x,\xi) = 0$ if $|x| \leq \varepsilon_0$ or if $|\xi| \leq \varepsilon_0$ for some $\varepsilon_0 > 0$.

3. Now we are able to define the identifications $J_\pm$. Let $\sigma_+ \in C^\infty(-\gamma,\gamma)$, $\gamma > 1$, be such that $\sigma_+(\tau) = 1$ if $\tau \in (-\varepsilon, 1]$ for some $\varepsilon \in (0,1)$, $\sigma_+(\tau) = 0$ in a neighborhood of the point -1 and $\sigma_-(\tau) = \sigma_+(-\tau)$. Let $\eta \in C^\infty(\mathbb{R}^d)$ be such that $\eta(x) = 0$ in a neighborhood of zero and $\eta(x) = 1$ for large $|x|$. We denote by θ a $C^\infty(\mathbb{R}_+)$-function which equals to zero in a neighborhood of 0 and $\theta(\lambda) = 1$ for, say, $\lambda \geq \lambda_0$ (for some $\lambda_0 > 0$). Set

$$\zeta_\pm(x,\xi) = \sigma_\pm(\eta(x)\langle\hat{x},\hat{\xi}\rangle)\theta(|\xi|^2).$$

We construct $J_\pm$ as a pseudo-differential operator (cf. [4]),

$$(J_\pm f)(x) = (2\pi)^{-d/2}\int_{\mathbb{R}^d} \mathrm{e}^{i\langle x,\xi\rangle} a_\pm(x,\xi)\zeta_\pm(x,\xi)\hat{f}(\xi)\mathrm{d}\xi, \tag{3.1}$$

where $a_\pm$ is the function (it depends on N) defined in the previous section. Due to the cut-off functions $\zeta_\pm$ the symbols $a_\pm\zeta_\pm \in \mathcal{S}^{0,0}$, so that, by Proposition 3.1, the operators $J_\pm$ are bounded.

It is easy to see that

$$s-\lim_{t\to\pm\infty}(J_\pm - \theta(H_0))\mathrm{e}^{-iH_0t} = 0.$$

Therefore the wave operators

$$W_\pm(H,H_0;J_\pm) = s-\lim_{t\to\pm\infty}\mathrm{e}^{iHt}J_\pm\mathrm{e}^{-iH_0t}$$

also exist and

$$W_\pm(H,H_0)\theta(H_0) = W_\pm(H,H_0;J_\pm).$$

It follows that

$$\mathbf{S}\theta^2(H_0) = W_+^*(H,H_0;J_+)W_-(H,H_0;J_-). \tag{3.2}$$

We need a stationary formula (see [4,12,13]) for the scattering matrix $S(\lambda)$ in the case where identifications J_+ and J_- for $t\to+\infty$ and $t\to-\infty$ are different. Let us set

$$T_\pm = HJ_\pm - J_\pm H_0. \tag{3.3}$$

Since auxiliary wave operators

$$s-\lim_{t\to\pm\infty}\mathrm{e}^{iH_0t}J_+^*J_-\mathrm{e}^{-iH_0t} = 0,$$

it can be deduced from (3.2) that the scattering matrix admits for $\lambda \geq \lambda_0$ the representation

$$S(\lambda) = S_0(\lambda) + S_1(\lambda), \tag{3.4}$$

where, at least formally,

$$S_0(\lambda) = -2\pi i\Gamma_0(\lambda)J_+^*T_-\Gamma_0^*(\lambda) \tag{3.5}$$

and

$$S_1(\lambda) = 2\pi i \Gamma_0(\lambda) T_+^* R(\lambda + i0) T_- \Gamma_0^*(\lambda). \tag{3.6}$$

Of course, to give a precise sense to expressions (3.5) and (3.6), we need to discuss restrictions of integral or pseudo-differential operators to the spheres $|\xi|^2 = \lambda$, but we do not dwell upon it here.

Let us choose a function $\psi \in C_0^\infty(\mathbb{R}_+)$ such that $\psi(\lambda) = 1$ in a neighborhood of the point $\lambda = 1$. Then formulas (3.5) and (3.6) remain true if the operators $J_\pm$ and $T_\pm$ are replaced by the operators $J_\pm(\lambda) = J_\pm \psi(H_0/\lambda)$ and $T_\pm(\lambda) = T_\pm \psi(H_0/\lambda)$, respectively.

4. According to (3.4), our proof of formula (1.6) for the singular part of the scattering matrix splits up into two steps. The first is to show that $S_1(\lambda)$ is negligible. To be more precise, we will prove the following.

Theorem 3.2. *The kernel $s_1(\omega, \omega'; \lambda)$ of the operator* (3.6) *belongs to the class $C^p(\mathbb{S}^{d-1} \times \mathbb{S}^{d-1})$ where $p = p(N) \to \infty$ as $N \to \infty$. Moreover, the C^p-norm of this kernel is $O(\lambda^{-q})$ as $\lambda \to \infty$ for some $q = q(N) \to \infty$.*

Set $u_0(x, \omega, \lambda) = \exp(i\lambda^{1/2}\langle \omega, x\rangle)$. Taking into account (1.1), we see that

$$s_1(\omega, \omega'; \lambda) = \pi i \lambda^{(d-2)/2} (2\pi)^{-d} (T_+^*(\lambda) R(\lambda + i0) T_-(\lambda) u_0(\omega', \lambda), u_0(\omega, \lambda)).$$

Thus, for the proof of Theorem 3.2, it suffices to check the following:

PROPOSITION 3.3

Let $u_\pm = u_\pm^{(N)}$ be the functions constructed in Proposition 2.1. *Then, for the operators $J_\pm$ and $T_\pm$ defined by* (3.1) *and* (3.3), *respectively,*

$$||\langle x\rangle^p \psi(H_0/\lambda) T_+^* R(\lambda + i0) T_- \psi(H_0/\lambda) \langle x\rangle^p|| = O(\lambda^{-q})$$

where $p(N) \to \infty$ and $q(N) \to \infty$ as $N \to \infty$.

We use the following elementary:

Lemma 3.4. *For any p and q*

$$||\langle x\rangle^{-p} \langle \xi\rangle^{-q} \psi(H_0/\lambda) \langle x\rangle^p|| = O(\lambda^{-q/2}), \quad \lambda \to \infty.$$

Therefore for the proof of Proposition 3.3 it suffices to verify the following:

PROPOSITION 3.5

Under the assumptions of Proposition 3.3, *the operators*

$$\langle x\rangle^p \langle \xi\rangle^q T_+^* R(\lambda + i0) T_- \langle \xi\rangle^q \langle x\rangle^p$$

are bounded uniformly in $\lambda \geq \lambda_0 > 0$.

This result will be verified in § 4. The second step of the proof is to show that, up to negligible terms, kernel of the operator $S_0(\lambda)$ is given by formula (1.6). This is postponed until § 5.

5. Let us calculate the perturbation (3.3). According to (1.5), we have that

$$\begin{aligned} g_\pm(x,\xi) &:= (-\Delta + V(x) - |\xi|^2)(u_\pm(x,\xi)\zeta_\pm(x,\xi)) = \mathrm{e}^{i\langle x,\xi\rangle} r_\pm(x,\xi)\zeta_\pm(x,\xi) \\ &\quad - 2\langle \nabla u_\pm(x,\xi), \nabla\zeta_\pm(x,\xi)\rangle - u_\pm(x,\xi)\Delta\zeta_\pm(x,\xi). \end{aligned} \tag{3.7}$$

Set also $t_\pm(x,\xi) = \mathrm{e}^{-i\langle x,\xi\rangle} g_\pm(x,\xi)$. Now it follows from (3.1) that

$$\begin{aligned} (T_\pm f)(x) &= (2\pi)^{-d/2} \int_{\mathbb{R}^d} \mathrm{e}^{i\langle x,\xi\rangle} t_\pm(x,\xi) \hat{f}(\xi)\mathrm{d}\xi \\ &= (2\pi)^{-d/2} \int_{\mathbb{R}^d} \mathrm{e}^{i\langle x,\xi\rangle} \left(t_\pm^{(r)}(x,\xi) + t_\pm^{(s)}(x,\xi)\right) \hat{f}(\xi)\mathrm{d}\xi \\ &=: (T_\pm^{(r)} f)(x) + (T_\pm^{(s)} f)(x), \end{aligned} \tag{3.8}$$

where

$$t_\pm^{(r)} = r_\pm \zeta_\pm \quad \text{and} \quad t_\pm^{(s)} = -2\langle i a_\pm \xi + \nabla a_\pm, \nabla\zeta_\pm\rangle - a_\pm \Delta\zeta_\pm.$$

Due to the cut-off functions $\zeta_\pm$, $\nabla\zeta_\pm$ and $\Delta\zeta_\pm$ the next result follows directly from Proposition 2.1.

PROPOSITION 3.6

Let assumption 1.3 *hold. Then*

$$t_\pm^{(r)} \in \mathcal{S}^{-1-(\rho-1)(N+1),-N} \quad \text{and} \quad t_\pm^{(s)} \in \mathcal{S}_\pm^{-1,1}.$$

4. Pseudo-differential operators and resolvent estimates

1. We need some results on the boundedness of combinations of operators from the classes $\mathcal{S}_\pm^{n,m}$ (see subsection 2 of § 3) with functions of the generator of dilations

$$\mathbf{A} = \frac{1}{2}\sum_{j=1}^{d}(x_j D_j + D_j x_j).$$

We denote by $\mathbf{P}_\pm = E_{\mathbf{A}}(\mathbb{R}_\pm)$ the spectral projection of the operator $\mathbf{A}$.

The following two assertions are motivated by the results of [5].

PROPOSITION 4.1

Let $t \in \mathcal{S}_\pm^{0,0}$ for one of the signs, and let $q > 0$ be an arbitrary number. Then the operator

$$\langle\mathbf{A}\rangle^{-q} T \langle\xi\rangle^q \langle x\rangle^q$$

is bounded.

PROPOSITION 4.2

Let $t \in \mathcal{S}_\pm^{n,m}$ for some n and m. Then the operator

$$\langle\mathbf{A}\rangle^p \mathbf{P}_\pm T \langle\xi\rangle^p \langle x\rangle^p$$

is bounded for all p.

2. The following resolvent estimates were deduced for bounded z in [9, 6] from the famous Mourre estimate [9]. Moreover, making the dilation transformation $x \mapsto \lambda^{-1/2}x$ and taking into account that the functions $\lambda^{-1}V(\lambda^{-1/2}x)$ satisfy the assumptions of [6] uniformly in λ, we can obtain estimates for high energies.

PROPOSITION 4.3

Let assumption 1.3 *hold. Then for* $\operatorname{Re} z > 0$, $\operatorname{Im} z \geq 0$ *the operator-functions*

$$\langle \mathbf{A} \rangle^{-p} R(z) \langle \mathbf{A} \rangle^{-p}, \quad p > 1/2, \tag{4.1}$$

$$\langle \mathbf{A} \rangle^{-1+p_2} \mathbf{P}_- R(z) \langle \mathbf{A} \rangle^{-p_1}, \quad \langle \mathbf{A} \rangle^{-p_1} R(z) \mathbf{P}_+ \langle \mathbf{A} \rangle^{-1+p_2} \tag{4.2}$$

for each $p_1 > 1/2$, $p_2 < p_1$ *and*

$$\langle \mathbf{A} \rangle^{p} \mathbf{P}_- R(z) \mathbf{P}_+ \langle \mathbf{A} \rangle^{p} \tag{4.3}$$

for arbitrary p *are continuous in norm with respect to* z. *Moreover, the norms of the operators* (4.1)–(4.3) *at* $z = \lambda + i0$ *are* $O(\lambda^{-1})$ *as* $\lambda \to \infty$.

3. Now we are able to check Proposition 3.5. Let us first show that the operator

$$\langle x \rangle^{p} \langle \xi \rangle^{q} (T_+^{(r)})^* R(\lambda + i0) T_-^{(r)} \langle \xi \rangle^{q} \langle x \rangle^{p}$$

is uniformly bounded. Note that the operators $\langle x \rangle^{\sigma} T_\pm^{(r)} \langle \xi \rangle^{q} \langle x \rangle^{p}$ are bounded by Propositions 3.1 and 3.6 if $(N+1)(\rho - 1) \geq \sigma + p - 1$ and $N \geq q$. Thus, it suffices to use that

$$||\langle x \rangle^{-\sigma} R(\lambda + i0) \langle x \rangle^{-\sigma}|| = O(\lambda^{-1/2}), \quad \sigma > 1/2,$$

which follows, for example, from the first result of Proposition 4.3.

Let us further consider the singular part $T_\pm^{(s)}$ of $T_\pm$. Recall that, according to Proposition 3.6, $T_\pm^{(s)} \in \mathcal{S}_\pm^{-1,1}$. We need to prove the boundedness of four operators

$$\langle x \rangle^{p} \langle \xi \rangle^{q} (T_+^{(s)})^* \mathbf{P}_- R(\lambda + i0) \mathbf{P}_+ T_-^{(s)} \langle \xi \rangle^{q} \langle x \rangle^{p}, \tag{4.4}$$

$$\langle x \rangle^{p} \langle \xi \rangle^{q} (T_+^{(s)})^* \mathbf{P}_+ R(\lambda + i0) \mathbf{P}_- T_-^{(s)} \langle \xi \rangle^{q} \langle x \rangle^{p} \tag{4.5}$$

and

$$\langle x \rangle^{p} \langle \xi \rangle^{q} (T_+^{(s)})^* \mathbf{P}_\pm R(\lambda + i0) \mathbf{P}_\pm T_-^{(s)} \langle \xi \rangle^{q} \langle x \rangle^{p}. \tag{4.6}$$

The result about the operator (4.4) is a combination of Proposition 4.1 and the result of Proposition 4.3 about the operator (4.3). Similarly, the result about the operator (4.5) is a combination of Proposition 4.2 and the result of Proposition 4.3 about the operator (4.1). Finally, to consider the operator (4.6) we have to combine Propositions 4.1 and 4.2 with the result of Proposition 4.3 about the operator (4.2).

The cross-terms containing

$$(T_+^{(r)})^* R(\lambda + i0) T_-^{(s)}, \quad (T_+^{(s)})^* R(\lambda + i0) T_-^{(r)}$$

can be considered quite similarly. This concludes our sketch of the proof of Proposition 3.5 and hence of Theorem 3.2.

5. Main theorem

According to Theorem 3.2 the operator (3.5) contains all power terms of the high-energy expansion of the scattering matrix as well as its diagonal singularity. The obvious drawback of the expression (3.5) is that it depends on the cut-off functions $\zeta_\pm$. So our goal is to show that, up to negligible terms, it can be transformed to the invariant expression (1.6).

Let us consider first the operator $J_+^* T_-$. We set $\zeta = \zeta_-$, $u = u_-$, then $\zeta_+(x,\xi) = \zeta(x,-\xi)$ and $u_+(x,\xi) = \overline{u(x,-\xi)}$. It follows from (3.1), (3.7) and (3.8) that $J_+^* T_-$ is the integral operator with kernel $(2\pi)^{-d} G(\xi,\xi')$ where

$$G(\xi,\xi') = \int_{\mathbb{R}^d} u(x,-\xi)\zeta(x,-\xi)g_-(x,\xi')\mathrm{d}x. \tag{5.1}$$

By (1.1), kernel of the singular part (3.5) of the scattering matrix is given by the formal relation

$$s_0(\omega,\omega';\lambda) = -\pi i \lambda^{(d-2)/2}(2\pi)^{-d} G(\lambda^{1/2}\omega, \lambda^{1/2}\omega'). \tag{5.2}$$

Let us plug (3.7) into (5.1) and denote by G_j, $j = 1,2,3$, the integrals corresponding to the three functions in the right-hand side of (3.7):

$$\begin{aligned} G_1(\xi,\xi') &= \int_{\mathbb{R}^d} \mathrm{e}^{i\langle x,\xi'-\xi\rangle} a(x,-\xi)\zeta(x,-\xi)r(x,\xi')\zeta(x,\xi')\mathrm{d}x, \\ G_2(\xi,\xi') &= -2\int_{\mathbb{R}^d} u(x,-\xi)\zeta(x,-\xi)\langle(\nabla u)(x,\xi'), (\nabla\zeta)(x,\xi')\rangle \mathrm{d}x, \\ G_3(\xi,\xi') &= -\int_{\mathbb{R}^d} u(x,-\xi)\zeta(x,-\xi)u(x,\xi')(\Delta\zeta)(x,\xi')\mathrm{d}x. \end{aligned}$$

Then $G = G_1 + G_2 + G_3$.

By virtue of Proposition 2.1 the function $a(x,-\xi)\zeta(x,-\xi)$ satisfies estimates (2.5) for all $x,\xi \in \mathbb{R}^d$ and the function $r(x,\xi')\zeta(x,\xi')$ satisfies estimates (2.6) for all $x,\xi' \in \mathbb{R}^d$. It follows that

$$\begin{aligned} &\left|\partial_x^\alpha \partial_\xi^\beta \partial_{\xi'}^{\beta'} \left(a(x,-\xi)\zeta(x,-\xi)r(x,\xi')\zeta(x,\xi')\right)\right| \\ &\leq C_{\alpha,\beta,\beta'}(1+|x|)^{-1-(\rho-1)N-|\alpha|}\,|\xi|^{-|\beta|}\,|\xi'|^{-N-|\beta'|}, \end{aligned}$$

and hence $G_1(\xi,\xi')$ is a smooth function of ξ,ξ' rapidly decreasing as $|\xi| = |\xi'| \to \infty$.

Let ω and ω' belong to some conical neighborhood of a point $\omega_1 \in \mathbb{S}^{d-1}$. Then

$$\zeta(x,-\xi)(\nabla\zeta)(x,\xi') = (\nabla\zeta)(x,\xi')$$

so that the function $\zeta(x,-\xi)$ in the integrals $G_j(\xi,\xi')$, $j = 2,3$, can be omitted. Integrating in the integral $G_3(\xi,\xi')$ by parts, we find that

$$\begin{aligned} G_2(\xi,\xi') + G_3(\xi,\xi') = \int_{\mathbb{R}^d} &\langle(\nabla u)(x,-\xi)u(x,\xi') \\ &- u(x,-\xi)(\nabla u)(x,\xi'), (\nabla\zeta)(x,\xi')\rangle \mathrm{d}x. \end{aligned} \tag{5.3}$$

If, for example, $\langle\omega_1,\omega_0\rangle > 0$, then due to the function $(\nabla\zeta)(x,\xi')$, the integral (5.3) is actually taken over the half-space $z \geq 0$ only. Therefore integrating once more by parts, we obtain that

$$G_2(\xi,\xi') + G_3(\xi,\xi') = -\int_{z\geq 0} \big((\Delta u)(x,-\xi)u(x,\xi') \\ -u(x,-\xi)(\Delta u)(x,\xi')\big)\,\zeta(x,\xi')\mathrm{d}x \\ +\int_{\Pi_{\omega_0}} \big(u(y,-\xi)(\partial_z u)(y,\xi') - u(y,\xi')(\partial_z u)(y,-\xi)\big)\,\mathrm{d}y. \tag{5.4}$$

Substituting the integral (5.4) over Π_{ω_0} into (5.2), we obtain the expression (1.6).

It remains to show that the first integral over the half-space $z \geq 0$ in (5.4) is negligible. Let us take into account relation (1.5). Then

$$-(\Delta u)(x,-\xi)u(x,\xi') + u(x,-\xi)(\Delta u)(x,\xi') = \mathrm{e}^{i\langle x,\xi'-\xi\rangle}\big(r(x,-\xi)a(x,\xi') \\ -r(x,\xi')a(x,-\xi) + (|\xi|^2 - |\xi'|^2)a(x,-\xi)a(x,\xi')\big) \tag{5.5}$$

To consider the integral

$$\int_{z\geq 0} \mathrm{e}^{i\langle x,\xi'-\xi\rangle}\big(r(x,-\xi)a(x,\xi') - r(x,\xi')a(x,-\xi)\big)\,\zeta(x,\xi')\mathrm{d}x \tag{5.6}$$

we use again that, by Proposition 2.1, the functions

$$a(x,\xi')\zeta(x,\xi') \quad \text{and} \quad r(x,\xi')\zeta(x,\xi')$$

satisfy estimates (2.5) and (2.6), respectively, for all $x,\xi' \in \mathbb{R}^d$. The same result for the functions $a(x,-\xi)$ and $r(x,-\xi)$ holds true in the half-space $z \geq 0$ which does not contain the 'bad' direction $\hat{x} = -\hat{\xi}$. Therefore, similarly to the function $G_1(\xi,\xi')$, the integral (5.6) is a smooth function of ξ,ξ' rapidly decreasing as $|\xi| = |\xi'| \to \infty$.

Let us, finally, consider the integral

$$\mathcal{K}(\mu,\nu;\omega,\omega') = \int_{z\geq 0} \mathrm{e}^{i\langle x,\xi'-\xi\rangle}a(x,-\xi)a(x,\xi')\zeta(x,\xi')\mathrm{d}x, \tag{5.7}$$

where $\xi = \mu^{1/2}\omega$, $\xi' = \nu^{1/2}\omega'$. We regard (5.7) as kernel of the operator $K(\mu,\nu)$ acting in the space $L_2(\mathbb{S}^{d-1})$. According to the results of [8,14] the family $K(\mu,\nu)$ is continuous in $\mu,\nu > 0$ in a suitable topology of operators. Actually in [8,14] only the integrals taken over the whole space (that is pseudo-differential operators defined by their amplitudes) were considered but the restriction $z \geq 0$ is inessential. The crucial point of the proof is that due to the function $\zeta(x,\xi')$ the integrand in (5.7) equals zero in a neighborhood of the direction $\hat{x} = \hat{\xi}'$. Therefore the operator $(\mu-\nu)K(\mu,\nu)$ equals zero on the diagonal $\mu = \nu$.

Now we can formulate our main result.

Theorem 5.1. *Let assumption* (1.3) *hold. Let p be an arbitrary number and $N = N(p)$ be sufficiently large. Let functions $a(x,\xi) = a^{(N)}(x,\xi)$ be constructed in Proposition* 2.1. *Define, for $\omega,\omega' \in \Omega$, the singular part $s_0(\lambda)$ of the scattering amplitude $s(\lambda)$ by formula* (1.6). *Then the remainder* (1.7) *belongs to the class $C^p(\Omega\times\Omega)$ and the C^p-norm of this kernel is $O(\lambda^{-p})$ as $\lambda \to \infty$.*

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