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On the mathematical theory of the Aharonov–Bohm effect

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Abstract
We consider the Schrödinger operator $H = (\mathrm{i}\nabla + A)^2$ in the space $L_2(\mathbb{R}^2)$ with a magnetic potential $A(x) = a(\hat{x})(-x_2, x_1)|x|^{-2}$, where a is an arbitrary function on the unit circle. Our goal is to study spectral properties of the corresponding scattering matrix $S(\lambda)$, $\lambda > 0$. We obtain its stationary representation and show that its singular part (up to compact terms) is a pseudodifferential operator of zero order whose symbol is an explicit function of a. We deduce from this result that the essential spectrum of $S(\lambda)$ does not depend on λ and consists of two complex conjugated and perhaps overlapping closed intervals of the unit circle. Finally, we calculate the diagonal singularity of the scattering amplitude (kernel of $S(\lambda)$ considered as an integral operator). In particular, we show that for all these properties only the behaviour of a potential at infinity is essential. The preceding papers on this subject treated the case $a(\hat{x}) = \text{const}$ and used the separation of variables in the Schrödinger equation in the polar coordinates. This technique does not, of course, work for arbitrary a. From an analytical point of view, our paper relies on some modern tools of scattering theory and well-known properties of pseudodifferential operators.

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1. Introduction

From a mathematical point of view, the famous Aharonov–Bohm effect [1, 3, 13] consists of unusual spectral properties of the scattering matrix (SM) $S_\alpha(\lambda)$, $\lambda > 0$, for the Schrödinger operator H_α with magnetic potential $A_\alpha(x) = \alpha(-x_2, x_1)|x|^{-2}$, $\alpha \in \mathbb{R}$, $x = (x_1, x_2)$, in the space $L_2(\mathbb{R}^2)$. For such potentials the Schrödinger equation admits separation of variables in polar coordinates (r, θ), and for every fixed angular momentum $m = 0, \pm 1, \pm 2, \ldots$ the radial equation

$$-u_m'' + ((m - \alpha)^2 - 1/4)r^{-2}u_m = \lambda u_m \qquad \lambda > 0$$

can be solved in terms of the Bessel functions $u_m(r) = r^{1/2}\mathcal{I}_{|m-\alpha|}(\lambda^{1/2}r)$. Using the asymptotics of these functions as $r \to \infty$, we see that $S_\alpha(\lambda)$ has two eigenvalues $\mathrm{e}^{\mathrm{i}\alpha\pi}$ and $\mathrm{e}^{-\mathrm{i}\alpha\pi}$ with corresponding eigenfunctions $\mathrm{e}^{\mathrm{i}m\theta}$ for $m \leqslant \alpha$ and $m \geqslant \alpha$, respectively. This is qualitatively different both from the case of short-range (satisfying the condition $O(|x|^{-1-\varepsilon})$, $\varepsilon > 0$, at infinity) electric and magnetic potentials and from the electric (Coulomb) potential decaying as $|x|^{-1}$. In the first case, the essential spectrum of the SM consists of only point 1 and in the second it covers the whole unit circle (see, e.g., [16]).

Since eigenvalues and eigenfunctions of $S_\alpha(\lambda)$ are known, the spectral theorem yields directly an explicit expression (see [13]) for the kernel of $S_\alpha(\lambda)$ considered as an integral operator. As usual, it is singular only on the diagonal, but its singularity is quite different from the case of short-range magnetic and electric potentials (as well as from the electric Coulomb potential). Indeed, in the short-range case the leading singularity is given by the Dirac function whereas for the Aharonov–Bohm potential it is a linear combination (with coefficients depending on α) of the Dirac function and of the singular denominator understood as the principal value.

Note also that if H_α is considered for $|x| \geqslant r_0$ with the Dirichlet boundary condition at $|x| = r_0$ (see [13]), then the corresponding SM has infinitely many eigenvalues which however accumulate at the points $\mathrm{e}^{\mathrm{i}\alpha\pi}$ and $\mathrm{e}^{-\mathrm{i}\alpha\pi}$ only. To put it differently, the essential spectrum of such a SM consists again of the points $\mathrm{e}^{\mathrm{i}\alpha\pi}$ and $\mathrm{e}^{-\mathrm{i}\alpha\pi}$.

In the present paper, we study the spectral properties of the SM and the diagonal singularity of its kernel in a more general context. Actually, we suppose that, for sufficiently large $|x|$,

$$A(x) = a(\hat{x})(-x_2, x_1)|x|^{-2} \qquad \hat{x} = x/|x| \tag{1.1}$$

where a is an arbitrary real C^∞-function on the unit circle. For such potentials $A(x) = (A_1(x), A_2(x))$, the magnetic field $B(x) = \partial A_1(x)/\partial x_2 - \partial A_2(x)/\partial x_1$ vanishes (for large $|x|$). An arbitrary short-range potential can be added to $A(x)$ without changing our results significantly. In particular, only the behaviour of a potential at infinity is essential. Of course, except for the case $a(\hat{x}) = \text{const}$, for potentials (1.1) the variables in the two-dimensional Schrödinger equation cannot be separated. Therefore, to solve the problem, we use modern tools of scattering theory (a stationary formula for the SM in a general framework, different resolvent estimates, etc) and some well-known properties of pseudodifferential operators (PDO). Note that we consider the SM as a PDO on the unit circle. We try here to single out the main ideas and to keep the presentation as simple as possible, so that technical details are usually omitted.

In fact, we follow rather closely paper [15] where electric long-range potentials were considered. The technique of this paper applies automatically to magnetic potentials, but the concrete expressions for symbols of the SM and for diagonal singularities of their kernels (if the SM are considered as integral operators) are qualitatively different for electric and magnetic potentials decaying as $|x|^{-1}$ at infinity. This also leads to a qualitative difference in the spectral properties of the corresponding SM.

2. Main results

We consider the pair of self-adjoint operators $H_0 = -\Delta$,

$$H = (\mathrm{i}\nabla + A(x))^2 \qquad x \in \mathbb{R}^2$$

with a magnetic potential (1.1) in the space $\mathcal{H} = L_2(\mathbb{R}^2)$. As was noted in [10], although the potential $A(x)$ decays only as $|x|^{-1}$ at infinity, due to the transversal gauge

$$\langle A(x), x\rangle = 0 \tag{2.1}$$

the usual wave operators $W_\pm(H, H_0)$ exist. The scattering operator $\mathbf{S}$ and the SM $S(\lambda)$, $\lambda > 0$ are defined in terms of these operators. Recall that, for general short- and long-range electric and magnetic potentials, the SM is a unitary operator in the space $L_2(\mathbb{S})$. It is usually considered as an integral operator, that is

$$(S(\lambda)u)(\omega) = \int_{\mathbb{S}} s(\omega, \omega'; \lambda)u(\omega')\,\mathrm{d}\omega'.$$

The kernel $s(\omega, \omega', \lambda)$ of the SM (the scattering amplitude) is a smooth function of $\omega, \omega' \in \mathbb{S}$ for $\omega \neq \omega'$ but can be very singular on the diagonal $\omega = \omega'$ (see, e.g., [16]). In particular, this is true in the case considered.

Let us formulate our main result on the essential spectrum σ_{ess} of $S(\lambda)$. Set

$$f(\omega) = \int_{\mathbb{S}(-\omega,\omega)} a(\theta)\,\mathrm{d}\theta \tag{2.2}$$

where the integral is taken in the positive (counterclockwise) direction over the half-circle between the points $-\omega$ and ω. Note that

$$f(\omega) + f(-\omega) = \int_{\mathbb{S}} a(\theta)\,\mathrm{d}\theta =: \phi \tag{2.3}$$

is the total magnetic flux.

Theorem 2.1. *For all* $\lambda > 0$

$$\sigma_{\mathrm{ess}}(S(\lambda)) = \mathrm{e}^{\mathrm{i}f(\mathbb{S})} \cup \mathrm{e}^{-\mathrm{i}f(\mathbb{S})} \tag{2.4}$$

that is, $\sigma_{\mathrm{ess}}(S(\lambda))$ *consists of the two complex conjugated and perhaps overlapping closed intervals of the unit circle.*

We do not have any information on the detailed structure of the essential spectrum of the SM. For example, it is an open question whether it might contain the absolutely or singularly continuous parts.

We emphasize that the essential spectrum of $S(\lambda)$ does not depend on λ. For concrete functions a in (1.1), one can compute integral (2.2) and find $\sigma_{\mathrm{ess}}(S(\lambda))$ explicitly. We give only one example.

Corollary 2.2. *Let*

$$a(\hat{x}) = \alpha + \langle p, \hat{x}\rangle \qquad \alpha \in \mathbb{R} \qquad p \in \mathbb{R}^2. \tag{2.5}$$

Then relation (2.4) holds with

$$f(\mathbb{S}) = [\pi\alpha - 2|p|, \pi\alpha + 2|p|]. \tag{2.6}$$

In particular, if $a(\hat{x}) = \alpha$*, then* $\sigma_{\mathrm{ess}}(S(\lambda))$ *consists of the two points* $\exp(\pm\mathrm{i}\pi\alpha)$ *which equal* $(-1)^n$ *for* $\alpha = n \in \mathbb{Z}$.

Indeed, for function (2.5), we have that $f(\omega) = \pi\alpha \pm 2|\omega \times p|$ if $\pm\omega$ can be obtained from $\hat{p}$ by rotation in the positive direction at an angle smaller than π. This yields formula (2.6).

Next, we can describe the diagonal singularity of the scattering amplitude.

Theorem 2.3. *Let* S_0 *be the integral operator on* $L_2(\mathbb{S})$ *with kernel*

$$s_0(\omega, \omega') = \mathrm{e}^{\mathrm{i}f(\omega)-\mathrm{i}\phi/2}\left(\cos(\phi/2)\delta(\omega, \omega') + (2\pi)^{-1}\sin(\phi/2)\,\mathrm{PV}\frac{1}{\sin(\{\omega, \omega'\}/2)}\right) \tag{2.7}$$

where $\delta(\omega, \omega')$ is the Dirac function on the unit circle, PV *is the principal value and $\{\omega, \omega'\}$ is the oriented angle between an initial vector ω and a final vector ω'. Then*

$$|s(\omega, \omega'; \lambda) - s_0(\omega, \omega')| = O(|\ln|\omega - \omega'||) \qquad \omega - \omega' \to 0.$$

In particular, the operator $S(\lambda) - S_0$ belongs to the Hilbert–Schmidt class.

It follows from (2.2) and (2.3) that if the function a is even, then $f(\omega) = \phi/2$ for all $\omega \in \mathbb{S}$ and hence the first factor in the right-hand side of (2.7) equals 1. Thus, for an arbitrary even a, formula (2.7) for the singular part of the SM is the same as for a constant $a(\hat{x}) = \alpha$ but the role of α is played by $(2\pi)^{-1}\phi$. If a is odd, then $\phi = 0$ and f is also odd. In this case $s_0(\omega, \omega') = \mathrm{e}^{\mathrm{i}f(\omega)}\delta(\omega, \omega')$, so that S_0 is the operator of multiplication by $\mathrm{e}^{\mathrm{i}f(\omega)}$. Note that $s_0(\omega, \omega')$ is a real function if a is even, but this is of course wrong in the general case.

Theorem 2.3 implies

Corollary 2.4. *Let $\omega \neq \omega'$ and $\omega - \omega' \to 0$. Then*

$$s(\omega, \omega'; \lambda) = \frac{\exp(\mathrm{i}f(\omega) - \mathrm{i}\phi/2)\sin(\phi/2)}{2\pi\sin(\{\omega, \omega'\}/2)} + O(|\ln|\omega - \omega'||).$$

Now we can give an explicit asymptotics of the scattering cross section

$$\Sigma_{\mathrm{diff}}(\omega; \omega_0, \lambda) = \frac{2\pi}{\sqrt{\lambda}}|s(\omega, \omega_0; \lambda)|^2 \qquad \omega \neq \omega_0$$

for incident direction ω_0 of a beam of particles and direction of observation ω.

Corollary 2.5. *Let $\omega \to \omega_0$. Then*

$$\Sigma_{\mathrm{diff}}(\omega; \omega_0, \lambda) = \frac{1}{2\pi\sqrt{\lambda}}\frac{\sin^2(\phi/2)}{\sin^2(\{\omega, \omega_0\}/2)} + O\left(\frac{|\ln|\omega - \omega_0||}{|\omega - \omega_0|}\right). \tag{2.8}$$

The total cross section

$$\Sigma_{\mathrm{tot}}(\omega_0, \lambda) = \int_{\mathbb{S}} \Sigma_{\mathrm{diff}}(\omega; \omega_0, \lambda)\,\mathrm{d}\omega$$

is finite (for all ω_0 at the same time) if and only if $\phi \in 2\pi\mathbb{Z}$. In this case

$$\Sigma_{\mathrm{diff}}(\omega; \omega_0, \lambda) = O(\ln^2|\omega - \omega_0|).$$

We emphasize that formula (2.8) depends on the total magnetic flux ϕ only. It looks quite natural from the physics point of view. Indeed, the potential (1.1) with $a(\hat{x}) = \alpha$ was chosen in the original paper [1] essentially for phenomenological reasons. It was required that the magnetic flux take the given value ϕ (determined by the current) and the magnetic field be zero. In the general case the potential (1.1) also satisfies both these conditions. So it is not astonishing that for potentials with asymptotics (1.1), the leading singularity of $\Sigma_{\mathrm{diff}}(\omega; \omega_0, \lambda)$, which is the main quantum-mechanical observable, depends on ϕ only.

Note that $\sin(\{\omega, \omega'\}/2)$ and $\sin(\{\omega, \omega_0\}/2)$ in the formulae above can be replaced by $\{\omega, \omega'\}/2$ and $\{\omega, \omega_0\}/2$, respectively. The results of theorem 2.3 and its corollaries generalize the well-known formulae (see, e.g., [13]) for scattering on the Aharonov–Bohm potential to the case where the function $a(\hat{x})$ is not constant. Of course, in the case $a(\hat{x}) = \alpha$ (then $f(\omega) = \pi\alpha$) they reduce to these formulae.

This paper is organized as follows. In section 3, we give precise definitions of basic objects. The structure of the SM is studied in section 4. Theorem 2.1 is proved in section 5. Finally, in section 6 we find the diagonal singularity of the scattering amplitude (theorem 2.3).

3. Scattering theory

Although for the pair $H_0 = -\Delta$, $H = (\mathrm{i}\nabla + A(x))^2$ the usual wave operators exist, we first treat $A(x)$ as a long-range potential and consider wave operators

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

with non-trivial 'identifications' $J_\pm$ (depending on the sign of t). This idea first appeared in [5]. The operators $J_\pm$ emerge naturally as PDO with symbols $j_\pm(x,\xi)$ constructed in terms of approximate eigenfunctions $\Psi_\pm(x,\xi) = \mathrm{e}^{\mathrm{i}\varphi_\pm(x,\xi)}$ of the operator H. Substituting $\Psi = \mathrm{e}^{\mathrm{i}\varphi}$ in the Schrödinger equation $H\Psi = |\xi|^2\Psi$, we obtain the eikonal equation

$$|\nabla\varphi|^2 - 2\langle A, \nabla\varphi\rangle = |\xi|^2 \qquad \nabla = \nabla_x$$

for the phase function $\varphi = \varphi_\pm$. Following [15], we construct approximate solutions of this equation by explicit formulae

$$\varphi_\pm(x,\xi) = \langle x,\xi\rangle + \Phi_\pm(x,\xi) \tag{3.1}$$

and

$$\Phi_\pm(x,\xi) = \mp\int_0^\infty (\langle A(x\pm t\xi) - A(\pm t\xi), \xi\rangle)\,\mathrm{d}t = \mp\int_0^\infty \langle A(x\pm t\xi),\xi\rangle\,\mathrm{d}t. \tag{3.2}$$

Note that the last equality is a consequence of the transversal gauge condition (2.1). Then the Schrödinger equation for $\Psi_\pm = \mathrm{e}^{\mathrm{i}\varphi_\pm}$ is satisfied up to a short-range term off any neighbourhood of the direction $\hat{x} = \mp\hat{\xi}$. To be more precise,

$$((\mathrm{i}\nabla + A)^2 - |\xi|^2)\Psi_\pm = \mathrm{e}^{\mathrm{i}\varphi_\pm} q_\pm \tag{3.3}$$

where

$$q_\pm = |\nabla\Phi_\pm|^2 - \mathrm{i}\Delta\Phi_\pm - 2\langle A, \nabla\Phi_\pm\rangle + |A|^2 + \mathrm{i}\,\mathrm{div}\,A. \tag{3.4}$$

It follows from (1.1) and (3.2) that

$$\left|\partial_x^\alpha\partial_\xi^\beta \Phi_\pm(x,\xi)\right| \leqslant C_{\alpha,\beta}(\kappa)(1+|x|)^{-|\alpha|} \tag{3.5}$$

and hence

$$\left|\partial_x^\alpha\partial_\xi^\beta q_\pm(x,\xi)\right| \leqslant C_{\alpha,\beta}(\kappa)(1+|x|)^{-m-|\alpha|} \tag{3.6}$$

where $m = 2$, for all multi-indices α, β in the region $\pm\langle\hat{x},\hat{\xi}\rangle \geqslant \kappa$ for any $\kappa > -1$. Here and below we suppose that $|\xi|$ belongs to a compact and disjoint from zero interval of $\mathbb{R}_+$. This is possible due to the conservation of energy.

Let Σ be an open set in the space $\mathbb{R}^d$. Recall that a PDO $P : C_0^\infty(\Sigma) \to C^\infty(\Sigma)$ with symbol $p(\zeta, y)$ is defined by the formula

$$(Pf)(\zeta) = (2\pi)^{-\mathrm{d}/2}\int_{\mathbb{R}^d} \mathrm{e}^{\mathrm{i}\langle\zeta,y\rangle} p(\zeta,y)\hat{f}(y)\,\mathrm{d}y \tag{3.7}$$

where $\hat{f} = \mathcal{F}f$ is the Fourier transform of f. Here ζ plays the role of the space variable and y is the dual one. A symbol $p(\zeta, y)$ (or a PDO P) belongs to the Hörmander class $\mathcal{S}^n$ if, for all α and β,

$$\left|\partial_y^\alpha\partial_\zeta^\beta p(\zeta,y)\right| \leqslant C_{\alpha,\beta}(1+|y|)^{n-|\alpha|}.$$

We construct $J_\pm$ as a PDO by the formula

$$(J_\pm f)(x) = (2\pi)^{-1}\int_{\mathbb{R}^2} \mathrm{e}^{\mathrm{i}\langle x,\xi\rangle + \mathrm{i}\Phi_\pm(x,\xi)}\sigma_\pm(\langle\hat{x},\hat{\xi}\rangle)\hat{f}(\xi)\,\mathrm{d}\xi \tag{3.8}$$

where the cut-off function $\sigma_\pm \in C^\infty$ is such that $\sigma_\pm(\tau) = 1$ near ± 1 and $\sigma_\pm(\tau) = 0$ near ∓ 1. We deliberately ignore here some technical details which can be found in [15]. For example, strictly speaking, additional cut-offs of low and high energies by a function of $|\xi|^2$ and that of a neighbourhood of $x = 0$ by a function of x should be added in (3.8) to the symbol

$$j_\pm(x, \xi) = e^{i\Phi_\pm(x,\xi)}\sigma_\pm(\langle \hat{x}, \hat{\xi}\rangle) \tag{3.9}$$

of the PDO $J_\pm$. Compared to (3.7), ξ and x play in (3.8) the roles of ζ and y, respectively. Thus, only the operator $P_\pm = \mathcal{F} J_\pm^* \mathcal{F}^*$ is a PDO with symbol $p_\pm(\xi, x) = \overline{j_\pm(-x, \xi)}$ in the sense of definition (3.7). Nevertheless, all usual definitions and results of the PDO theory can be directly applied to the operators (3.8). In particular, according to (3.5), the PDO $J_\pm$ belongs to the class $\mathcal{S}^0$. Below all PDO acting on functions of $x \in \mathbb{R}^2$ are understood in the same sense as $J_\pm$.

We note that both wave operators $W_\pm(H, H_0; J_\pm)$ and $W_\pm(H, H_0)$ exist and

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

(see [10, 16]). However, introduction of the auxiliary identifications $J_\pm$ is necessary to obtain a representation of the SM in terms of the resolvent $R(z) = (H - z)^{-1}$ of the operator H. Since the scattering operator $\mathbf{S} = W_+^* W_-$ commutes with H_0, it reduces in the spectral representation of H_0 to the multiplication by the operator-function $S(\lambda)$, $\lambda > 0$, acting in the space $L_2(\mathbb{S})$ and known as the SM. Let us construct the standard spectral representation of the operator H_0. Let

$$(\Gamma_0(\lambda) f)(\omega) = 2^{-1/2}\hat{f}(\lambda^{1/2}\omega) = 2^{-1/2}(2\pi)^{-1}\int_{\mathbb{R}^2} e^{-i\lambda^{1/2}\langle x,\omega\rangle} f(x)\,dx \qquad \omega \in \mathbb{S} \tag{3.10}$$

be, up to the numerical factor, the restriction of $\hat{f}$ to the circle of radius $\lambda^{1/2}$ and $(\mathcal{U} f)(\lambda) = \Gamma_0(\lambda) f$, $f \in C_0^\infty(\mathbb{R}^2)$, $\lambda > 0$. Then the operator $\mathcal{U}$ extends by continuity to a unitary operator $\mathcal{U} : L_2(\mathbb{R}^2) \to L_2(\mathbb{R}_+; L_2(\mathbb{S}))$, and the operator H_0 is diagonalized by $\mathcal{U}$, i.e., $(\mathcal{U} H_0 f)(\lambda) = \lambda\, (\mathcal{U} f)(\lambda)$. This implies that $(\mathcal{U}\mathbf{S} f)(\lambda) = S(\lambda)(\mathcal{U} f)(\lambda)$.

Let

$$T_\pm = H J_\pm - J_\pm H_0 \tag{3.11}$$

be the 'effective perturbation' for the triple $\{H_0, H, J_\pm\}$. We proceed from the following (see [6, 15, 16]) stationary representation

$$S(\lambda) = -2\pi i \Gamma_0(\lambda)(J_+^* T_- - T_+^* R(\lambda + i0) T_-)\Gamma_0^*(\lambda) \tag{3.12}$$

for the SM $S(\lambda)$.

To justify it, we need the following two analytical results. The first of them (the limiting absorption principle; see, e.g., [2, 11]) can easily be obtained by the Mourre method. We use the notation $\langle x\rangle$ for the operator of multiplication by the function $\langle x\rangle = (1 + |x|^2)^{1/2}$.

Proposition 3.1. *For any $\gamma > 1/2$ the operator-function $\langle x\rangle^{-\gamma} R(z)\langle x\rangle^{-\gamma}$ is continuous in norm with respect to the parameter z in the closed complex plane cut along $[0, \infty)$ with the exception of the point 0. In particular, the positive spectrum of H is absolutely continuous.*

We also need more delicate resolvent estimates usually called propagation estimates. The following assertion was proven in [7, 8, 12] using again the Mourre estimate [11].

Proposition 3.2. *Let $P_\pm$ be the PDO with symbol $p_\pm(x, \xi) \in \mathcal{S}^n$. Suppose that the support of $p_\pm(x, \xi)$ is contained in the cone $\mp\langle \hat{x}, \hat{\xi}\rangle \geqslant \varepsilon$ for some $\varepsilon > 0$. Then the operator-functions*

$$\langle x\rangle^{\gamma-\beta} P_+^* R(z)\langle x\rangle^{-\gamma}, \qquad \langle x\rangle^{-\gamma} R(z) P_- \langle x\rangle^{\gamma-\beta} \qquad \gamma > 1/2 \qquad \beta > n + 1 \tag{3.13}$$

and

$$\langle x\rangle^{\gamma} P_+^* R(z) P_- \langle x\rangle^{\gamma} \qquad \forall\gamma \tag{3.14}$$

are bounded and continuous in norm with respect to the parameter z in the region $\operatorname{Re} z \in (\lambda_0, \infty)$, $\lambda_0 > 0$, $\operatorname{Im} z \geqslant 0$.

We also recall the Sobolev trace theorem.

Proposition 3.3. *The operator $\Gamma_0(\lambda)\langle x\rangle^{-\gamma} : L_2(\mathbb{R}^2) \to L_2(\mathbb{S})$ is compact for any $\gamma > 1/2$.*

4. The structure of the scattering matrix

Let us first find a convenient representation for operator (3.11). The following result follows directly from definition (3.8), equation (3.3) and estimates (3.5), (3.6).

Proposition 4.1. *The operator $T_\pm$ admits the decomposition $T_\pm = T_\pm^{(s)} + T_\pm^{(r)}$ where $T_\pm^{(s)}$, $T_\pm^{(r)}$ are, respectively, PDO with symbols*

$$\begin{aligned} t_\pm^{(s)}(x,\xi) &= -2\mathrm{i}\mathrm{e}^{\mathrm{i}\Phi_\pm(x,\xi)}\langle \xi, \nabla\sigma_\pm(\langle \hat{x}, \hat{\xi}\rangle)\rangle \\ &= -2\mathrm{i}\mathrm{e}^{\mathrm{i}\Phi_\pm(x,\xi)}|x|^{-1}|\xi|(1-\langle \hat{x},\hat{\xi}\rangle^2)\sigma_\pm'(\langle \hat{x},\hat{\xi}\rangle) \in \mathcal{S}^{-1} \end{aligned} \tag{4.1}$$

and $t_\pm^{(r)} \in \mathcal{S}^{-2}$.

We always suppose that the functions $\sigma_\pm$ in (3.8) satisfy, for some $\varepsilon \in (0, 1/2)$, the relations

$$\sigma_+(\tau) = 1 \quad \text{for} \quad \tau \in [-\varepsilon, 1] \qquad \sigma_+(\tau) = 0 \quad \text{for} \quad \tau \in [-1, -2\varepsilon] \tag{4.2}$$

and $\sigma_-(\tau) = \sigma_+(-\tau)$. Then the operators $T_\pm^{(s)}$ satisfy the assumptions of proposition 3.2. It follows from its assertion about the operators (3.13) that the operators $\langle x\rangle^{\gamma}\big(T_+^{(s)}\big)^* R(\lambda + \mathrm{i}0) T_-^{(r)}\langle x\rangle^{\gamma}$ and $\langle x\rangle^{\gamma}\big(T_+^{(r)}\big)^* R(\lambda+\mathrm{i}0)T_-^{(s)}\langle x\rangle^{\gamma}$ are bounded for $\gamma < 1$. The boundedness of the operator (3.14) implies that $\langle x\rangle^{\gamma}\big(T_+^{(s)}\big)^* R(\lambda + \mathrm{i}0)T_-^{(s)}\langle x\rangle^{\gamma}$ is bounded for any γ. Finally, the operator $\langle x\rangle^{\gamma}\big(T_+^{(r)}\big)^* R(\lambda+\mathrm{i}0)T_-^{(r)}\langle x\rangle^{\gamma}$ is bounded for $\gamma < 3/2$ by proposition 3.1. Therefore, the operator

$$B_\gamma(\lambda) = \langle x\rangle^{\gamma} T_+^* R(\lambda + \mathrm{i}0) T_- \langle x\rangle^{\gamma} \tag{4.3}$$

is bounded for any $\gamma < 1$. Hence, by proposition 3.3, the operator

$$\Gamma_0(\lambda)T_+^* R(\lambda+\mathrm{i}0)T_-\Gamma_0^*(\lambda) = (\Gamma_0(\lambda)\langle x\rangle^{-\gamma})B_\gamma(\lambda)(\Gamma_0(\lambda)\langle x\rangle^{-\gamma})^* \qquad \gamma \in (1/2, 1) \tag{4.4}$$

is compact. Since the operator $\langle x\rangle J_+^* T_-^{(r)}\langle x\rangle$ is bounded, the operator $\Gamma_0(\lambda)J_+^*T_-^{(r)}\Gamma_0^*(\lambda)$ is also compact by proposition 3.3. Thus, we obtain

Proposition 4.2. *Let*

$$S_1(\lambda) = -2\pi\mathrm{i}\Gamma_0(\lambda)J_+^* T_-^{(s)}\Gamma_0^*(\lambda). \tag{4.5}$$

Then for all $\lambda > 0$ the operator $S(\lambda) - S_1(\lambda)$ is compact.

Corollary 4.3. *The essential spectra of the operators $S(\lambda)$ and $S_1(\lambda)$ are the same.*

It follows (see, e.g., [16]) from definition (4.5) that, considered as an integral operator, $S_1(\lambda)$ (as well as the SM $S(\lambda)$ itself) has a smooth kernel $s_1(\omega, \omega'; \lambda)$, $\omega, \omega' \in \mathbb{S}$, off the diagonal $\omega = \omega'$. Therefore its essential spectrum is determined by the diagonal singularity of $s_1(\omega, \omega'; \lambda)$. Actually, it is more convenient to treat $S_1(\lambda)$ as a PDO on the unit circle. We fix an arbitrary point $\omega_0 \in \mathbb{S}$ and consider standard chart coordinates in its neighbourhood $\Omega \subset \mathbb{S}$. Let Λ_{ω_0} be the line (identified with $\mathbb{R}$) orthogonal to ω_0, and let $\zeta = \kappa(\omega)$ be the orthogonal projection of $\omega \in \Omega$ on Λ_{ω_0}. In particular, we assume that $\kappa(\omega_0) = 0$. We denote by $\Sigma \subset \Lambda_{\omega_0}$ the orthogonal projection of Ω and identify points $\omega \in \Omega$ and $\zeta = \kappa(\omega) \in \Sigma$. Let us also consider the unitary mapping $Z_\kappa : L_2(\Omega) \to L_2(\Sigma)$ defined by

$$(Z_\kappa u)(\zeta) = (1 - |\zeta|^2)^{-1/4} u(\omega). \tag{4.6}$$

We shall see that the operator $S_1^\kappa(\lambda) = Z_\kappa S_1(\lambda) Z_\kappa^*$ is a PDO defined by formula (3.7) for $d = 1$ and, up to terms from the class $\mathcal{S}^{-1}$, its symbol $p_1^\kappa(\zeta, y)$ is an asymptotically homogeneous function $p_0^\kappa(\zeta, y)$ of y of order zero. The function $p_0^\kappa(\zeta, y)$ is called the principal symbol of the PDO $S_1^\kappa(\lambda)$. It is invariant with respect to diffeomorphisms, which allows one to define the principal symbol of the PDO $S_1(\lambda)$ on the cotangent bundle of $\mathbb{S}$ by the equality

$$p_0(\omega, b) = p_0^\kappa(\zeta, y) \qquad |\omega| = 1 \qquad \langle \omega, b\rangle = 0 \tag{4.7}$$

where $\zeta = \kappa(\omega)$ and b is the orthogonal projection of y on the line Λ_ω. Alternatively, one can say that, for a PDO from the class $\mathcal{S}^n$, the principal symbol is the full symbol, considered modulo functions from $\mathcal{S}^{n-1}$.

In the rest of this section, we shall find an explicit expression for the principal symbol of $S_1(\lambda)$. According to definition (4.5), we have to consider first the operator $\mathbf{G} = J_+^* T_-^{(s)}$. Recall that J_+ and $T_-^{(s)}$ are PDO with symbols (3.8) and (4.1), respectively. Let us use the fact (see, e.g., [4, 14]) that J_+^* is also a PDO with the principal symbol $\overline{j_+(x, \xi)}$ and $\mathbf{G} = J_+^* T_-^{(s)}$ is a PDO with the principal symbol $\mathbf{g}_0(x, \xi)$ which equals the product of the symbols of PDO J_+^* and $T_-^{(s)}$. It follows that

$$(\mathbf{G}f)(x) = (2\pi)^{-1} \int_{\mathbb{R}^2} \mathrm{e}^{\mathrm{i}\langle x, \xi\rangle} \mathbf{g}(x, \xi) \hat{f}(\xi)\, \mathrm{d}\xi \tag{4.8}$$

where $\mathbf{g} \in \mathcal{S}^{-1}$ and the principal symbol

$$\mathbf{g}_0(x, \xi) = \overline{j_+(x, \xi)} t_-^{(s)}(x, \xi) = -2\mathrm{i}\mathrm{e}^{\mathrm{i}\Theta(x,\xi)} \sigma_+(\langle \hat{x}, \hat{\xi}\rangle) \langle \xi, \nabla \sigma_-(\langle \hat{x}, \hat{\xi}\rangle)\rangle. \tag{4.9}$$

Here

$$\Theta(x, \xi) = \Phi_-(x, \xi) - \Phi_+(x, \xi) = \int_{-\infty}^{\infty} \langle A(x + t\xi), \xi\rangle\, \mathrm{d}t = \int_{-\infty}^{\infty} \langle A(\hat{x} + t\hat{\xi}), \hat{\xi}\rangle\, \mathrm{d}t \tag{4.10}$$

according to (3.2). At the last step we have used that $A(x)$ is a homogeneous function of order -1, so that the function $\Theta(x, \xi)$ is homogeneous of order 0 in both variables. Note also that

$$\Theta(x, \xi) = -\Theta(x, -\xi). \tag{4.11}$$

Remark now that, due to the function $\nabla\sigma_-(\langle \hat{x}, \hat{\xi}\rangle)$, the symbol (4.9) equals zero on the conormal bundle to every circle $|\xi|^2 = \lambda$, i.e., $\mathbf{g}_0(x, \xi) = 0$ if $x = t\xi$ for some $t \in \mathbb{R}$. Therefore, we can use the following general result of [9] guaranteeing the existence of the operators $\Gamma_0(\lambda)\mathbf{G}\Gamma_0^*(\lambda)$.

Proposition 4.4. *Let $\mathbf{G} \in \mathcal{S}^{-1}$ be a PDO defined by formula (4.8), and let $\mathbf{g}_0$ be its principal symbol. Suppose that $\mathbf{g}_0(t\omega, \lambda^{1/2}\omega) = 0$ for all $\omega \in \mathbb{S}$ and $t \in \mathbb{R}$. Then the operator $G(\lambda) = \Gamma_0(\lambda)\mathbf{G}\Gamma_0^*(\lambda)$ is well defined as a bounded operator in the space $L_2(\mathbb{S})$. Moreover, $G(\lambda)$ is a PDO on the unit sphere from the class $\mathcal{S}^0$ with the principal symbol given by the absolutely convergent integral*

$$g_0(\omega, b; \lambda) = (4\pi)^{-1}\lambda^{-1/2} \int_{-\infty}^{\infty} \mathbf{g}_0(t\omega - \lambda^{-1/2} b, \lambda^{1/2}\omega)\, \mathrm{d}t \qquad |\omega| = 1 \qquad \langle \omega, b\rangle = 0. \tag{4.12}$$

Let us apply this result to the operator (4.5) and calculate integral (4.12) for the function (4.9). Under assumption (4.2) $\sigma_+(\langle\hat{x},\hat{\xi}\rangle) = 1$ on the support of $\nabla\sigma_-(\langle\hat{x},\hat{\xi}\rangle)$, so that the function $\sigma_+(\langle\hat{x},\hat{\xi}\rangle)$ can be omitted in (4.9). Next we take into account that, by definition (4.10),

$$\Theta(t\omega - \lambda^{-1/2}b, \lambda^{1/2}\omega) = \Theta(-b, \omega).$$

Since

$$\int_{-\infty}^{\infty} \left\langle \omega, \nabla\sigma_- \left(\left\langle \frac{t\omega - \lambda^{-1/2}b}{|t\omega - \lambda^{-1/2}b|}, \omega \right\rangle \right) \right\rangle \mathrm{d}t = \int_{-\infty}^{\infty} \frac{\partial}{\partial t}\sigma_- \left(\frac{t}{(t^2+\lambda^{-1}b^2)^{1/2}} \right) \mathrm{d}t$$
$$= \sigma_-(1) - \sigma_-(-1) = -1$$

we arrive at the following conclusion.

Proposition 4.5. *The operator $S_1(\lambda)$ is a PDO on the unit sphere with the principal symbol*

$$p_0(\omega, b) = \mathrm{e}^{\mathrm{i}\Theta(-b,\omega)} \qquad |\omega| = 1 \qquad \langle\omega, b\rangle = 0.$$

We emphasize that $p_0(\omega, b)$ does not depend on λ. Let us calculate the integral (4.10). Recall that the function f was defined by formula (2.2).

Lemma 4.6. *Suppose that $\hat{b}$ is obtained from ω by rotation at angle $\mp\pi/2$. Then*

$$\Theta(b, \omega) = \pm f(\pm\omega). \tag{4.13}$$

Proof. By virtue of (4.11), it suffices to consider the case of the upper sign. Let $\omega = (\omega_1, \omega_2)$, $\hat{b} = (\hat{b}_1, \hat{b}_2)$ and $\theta_t = (\hat{b} + t\omega)|\hat{b} + t\omega|^{-1}$. Below we identify the points θ on the unit circle with the angle between θ and $\hat{b}$. Then $\tan\theta_t = t$. Since $-\omega_1\hat{b}_2 + \omega_2\hat{b}_1 = 1$, we have that for the potential (1.1)

$$\langle A(\hat{b} + t\omega), \omega\rangle = a(\theta_t)(t^2+1)^{-1}.$$

Plugging this expression into (4.10) and making the change of variables $t = \tan\theta$, we get formula (4.13). □

Thus, we arrive at

Theorem 4.7. *The operator $S_1(\lambda)$ is a PDO on the unit sphere with the principal symbol*

$$p_0(\omega, b) = \mathrm{e}^{\pm\mathrm{i}f(\pm\omega)} \qquad |\omega| = 1 \qquad \langle\omega, b\rangle = 0 \tag{4.14}$$

if $\hat{b}$ is obtained from ω by rotation at angle $\pm\pi/2$.

5. The proof of theorem 1.1

We can now describe the essential spectrum of the SM. Below we need the following result which can be checked by a direct calculation.

Lemma 5.1. *Let P be a PDO on $L_2(\mathbb{R})$ with an asymptotically homogeneous symbol $p(\zeta, y)$ of order zero such that $p(\zeta, y) = p_\pm(\zeta)$ for sufficiently large $\pm y$. Set*

$$v_{\varepsilon,\tau}^{(\pm)}(\zeta) = \varepsilon^{-1/2} g(\zeta/\varepsilon)\,\mathrm{e}^{\pm\mathrm{i}\tau\zeta} \qquad \hat{g} \in C_0^\infty(\mathbb{R}). \tag{5.1}$$

Then

$$\left(Pv_{\varepsilon,\tau}^{(\pm)}\right)(\zeta) = p_\pm(\zeta)v_{\varepsilon,\tau}^{(\pm)}(\zeta)$$

if $\varepsilon \in (0, 1)$ and $\varepsilon\tau$ is large enough.

It follows from (4.7) and (4.14) that the principal symbol of the PDO $S_1^\kappa(\lambda) = Z_\kappa S_1(\lambda) Z_\kappa^*$ is given by

$$p_0^\kappa(\zeta, y) = \mathrm{e}^{-\mathrm{i} f(-\omega)} h_0(y) + \mathrm{e}^{\mathrm{i} f(\omega)} h_0(-y) \tag{5.2}$$

where $h_0 \in C^\infty(\mathbb{R})$, $h_0(y) = 1$ for sufficiently large y and $h_0(y) = 0$ for sufficiently large $-y$. Note that $S_1^\kappa(\lambda)$ differs from the PDO S_0^κ with full symbol (5.2) by a compact term.

Let $\mu^{(\pm)} = \mathrm{e}^{\mp \mathrm{i} f(\mp\omega_0)}$ for some $\omega_0 \in \mathbb{S}$. We shall first construct a Weyl sequence for the point $\mu^{(\pm)}$ and the operator S_0^κ. Clearly, the functions (5.1) tend weakly to zero as $\varepsilon \to 0$ uniformly in $\tau \in \mathbb{R}$ and $\|v_{\varepsilon,\tau}^{(\pm)}\| = \|g\|$. Let us set

$$u_\varepsilon^{(\pm)}(\zeta) = \varphi(\zeta) v_{\varepsilon,\varepsilon^{-2}}^{(\pm)}(\zeta)$$

where $\varphi \in C_0^\infty(\Sigma)$ and $\varphi(0) = 1$. It can be easily deduced from lemma 5.1 that

$$\lim_{\varepsilon\to 0} \left\| S_0^\kappa u_\varepsilon^{(\pm)} - \mu^{(\pm)} u_\varepsilon^{(\pm)} \right\| = 0. \tag{5.3}$$

The same relation is of course true also for the operator $S_1^\kappa(\lambda)$. Since $s_1(\omega, \omega'; \lambda)$ is a smooth function for $\omega \neq \omega'$, we have that

$$\lim_{\varepsilon\to 0} (I - \chi_\Omega) S_1(\lambda) Z_\kappa^* u_\varepsilon^{(\pm)} = 0 \tag{5.4}$$

(χ_Ω is the characteristic function of Ω). Therefore, comparing (5.3) and (5.4), we see that $Z_\kappa^* u_\varepsilon^{(\pm)}$ is the Weyl sequence for the point $\mu^{(\pm)}$ and the operator $S_1(\lambda)$. This implies that $\mu^{(\pm)} \in \sigma_{\mathrm{ess}}(S_1(\lambda))$ and hence, by corollary 4.3, $\mu^{(\pm)} \in \sigma_{\mathrm{ess}}(S(\lambda))$.

Let us prove, on the contrary, that $\sigma_{\mathrm{ess}}(S_1(\lambda))$ is contained in the right-hand side of (2.4). Suppose that $\mu_0 \neq \mathrm{e}^{\pm \mathrm{i} f(\pm\omega)}$ for all $\omega \in \mathbb{S}$ (and both signs '$\pm$'). Let $\mathcal{R}(\mu_0)$ be a PDO on the unit circle with the principal symbol

$$\rho(\omega, b) = (\mathrm{e}^{\pm \mathrm{i} f(\pm\omega)} - \mu_0)^{-1} \qquad |\omega| = 1 \qquad \langle \omega, b\rangle = 0 \tag{5.5}$$

if $\hat{b}$ is obtained from ω by rotation at angle $\pm\pi/2$. Since $\rho \in \mathcal{S}^0$, the operator $\mathcal{R}(\mu_0)$ is bounded in $L_2(\mathbb{S})$. Comparing (4.14) and (5.5), we see that the principal symbol of the product $\mathcal{R}(\mu_0)(S_1(\lambda) - \mu_0 I)$ equals 1. It follows that

$$\mathcal{R}(\mu_0)(S_1(\lambda) - \mu_0 I) = I + K \tag{5.6}$$

where K is a compact operator on $L_2(\mathbb{S})$. Now suppose that there exists a sequence u_n such that

$$\|u_n\| = 1 \qquad w - \lim_{n\to\infty} u_n = 0 \qquad \lim_{n\to\infty} \|S_1(\lambda) u_n - \mu_0 u_n\| = 0. \tag{5.7}$$

Using (5.6), we get the estimate

$$\|u_n\| \leqslant \|\mathcal{R}(\mu_0)\| \|S_1(\lambda) u_n - \mu_0 u_n\| + \|K u_n\|$$

which contradicts (5.7). This concludes the proof of theorem 2.1.

6. The diagonal singularity of the scattering amplitude

Our final goal is to find explicitly the leading diagonal singularity of the kernel $s(\omega, \omega'; \lambda)$ of the SM $S(\lambda)$. To this end, we need to construct better approximate solutions of the Schrödinger equation than those of section 3, using additionally (see [15, 16]) the transport equation. Let the functions $\varphi_\pm$, $\Phi_\pm$ and $q_\pm$ be defined by equalities (3.1), (3.2) and (3.4), respectively. Set

$$g_\pm(x, \xi) = 1 \mp 2^{-1} \mathrm{i} \int_0^\infty q_\pm(x \pm t\xi, \xi)\, \mathrm{d}t$$

and $\Psi_\pm(x,\xi) = \mathrm{e}^{\mathrm{i}\varphi_\pm(x,\xi)} g_\pm(x,\xi)$. Then equation (3.3) is satisfied with the corresponding functions $q_\pm$ obeying estimates (3.6) for $m = 3$. Let now $J_\pm$ be the PDO with symbol (cf (3.9))

$$j_\pm(x,\xi) = \mathrm{e}^{\mathrm{i}\Phi_\pm(x,\xi)} g_\pm(x,\xi)\sigma_\pm(\langle \hat{x}, \hat{\xi}\rangle) \qquad (6.1)$$

and let $T_\pm$ be the operator (3.11). Then proposition 4.1 is true with $t_\pm^{(r)} \in \mathcal{S}^{-3}$. Of course, representation (3.12) for the SM $S(\lambda)$ remains valid for this choice of $J_\pm$. Using propositions 3.1 and 3.2, we can show that now the operator (4.3) is bounded for any $\gamma < 3/2$. It follows from (3.10) that the kernel of the operator (4.4) equals

$$\tilde{s}(\omega,\omega';\lambda) = 2^{-1}(2\pi)^{-2}(B_\gamma(\lambda)u_{\omega'}(\lambda), u_\omega(\lambda)) \qquad \gamma \in (1, 3/2)$$

where $u_\omega(x;\lambda) = \langle x\rangle^{-\gamma}\mathrm{e}^{\mathrm{i}\lambda^{1/2}\langle x,\omega\rangle}$. Since, for $\gamma > 1$, these functions are continuous in the space $L_2(\mathbb{R}^2)$ with respect to $\omega \in \mathbb{S}$, the kernel $\tilde{s}(\omega,\omega';\lambda)$ is a continuous function of ω and ω'. Quite similarly, the continuity of the kernel of the operator $\Gamma_0(\lambda)J_+^*T_-^{(r)}\Gamma_0^*(\lambda)$ follows directly from the boundedness of the operator $\langle x\rangle^{3/2}J_+^*T_-^{(r)}\langle x\rangle^{3/2}$. Thus, we obtain

Proposition 6.1. *Let $J_\pm$ be the PDO with symbol (6.1), and let $S_1(\lambda)$ be the operator (4.5). Then for all $\lambda > 0$ the operator $S(\lambda) - S_1(\lambda)$ has continuous kernel.*

Hence, to prove theorem 2.3, it remains to find the diagonal singularity of the operator $S_1(\lambda)$. As in the previous section, we consider first the operator $S_1^\kappa(\lambda) = Z_\kappa S_1(\lambda) Z_\kappa^*$ acting on functions from the class $C_0^\infty(\Sigma)$, $\Sigma \subset \mathbb{R}$. Since

$$\int_0^\infty \mathrm{e}^{\mathrm{i}y\zeta}\,\mathrm{d}y = \pi\delta(\zeta) + \mathrm{i}\mathrm{PV}\zeta^{-1}$$

the kernel of the operator S_0^κ with symbol (5.2) equals (up to smooth terms)

$$\begin{aligned} s_0^\kappa(\zeta,\zeta') &= (2\pi)^{-1}\int_{-\infty}^\infty \mathrm{e}^{\mathrm{i}(\zeta-\zeta')y} p_0^\kappa(\zeta,y)\,\mathrm{d}y = 2^{-1}\big(\mathrm{e}^{\mathrm{i}f(\omega)} + \mathrm{e}^{-\mathrm{i}f(-\omega)}\big)\delta(\zeta-\zeta') \\ &\quad + (2\pi\mathrm{i})^{-1}\big(\mathrm{e}^{\mathrm{i}f(\omega)} - \mathrm{e}^{-\mathrm{i}f(-\omega)}\big)\,\mathrm{PV}(\zeta-\zeta')^{-1}. \end{aligned} \qquad (6.2)$$

The symbol $p_1^\kappa(\zeta,y) - p_0^\kappa(\zeta,y)$ of the operator $S_1^\kappa(\lambda) - S_0^\kappa$ belongs to the class $\mathcal{S}^{-1}$ and therefore its kernel is bounded by $|\ln|\zeta-\zeta'||$. This implies that

$$s_1^\kappa(\zeta,\zeta';\lambda) = s_0^\kappa(\zeta,\zeta') + O(|\ln|\zeta-\zeta'||). \qquad (6.3)$$

Next, we remark that, according to (4.6), the kernels of the operators $S_1(\lambda)$ and $S_1^\kappa(\lambda)$ are related by the equality

$$s_1(\omega,\omega';\lambda) = s_1^\kappa(\zeta,\zeta';\lambda)(1-|\zeta|^2)^{1/4}(1-|\zeta'|^2)^{1/4} \qquad \omega,\omega' \in \Omega.$$

Making this change of variables in (6.2) and using (2.3), we obtain the kernel (2.7). Finally, we take into account estimate (6.3) and proposition 6.1. This proves theorem 2.3.

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