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On dynamical justification of quantum scattering cross section

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ABSTRACT

We suggest a dynamical justification of quantum differential cross section in the context of long-time transition to stationary regime for the Schrödinger equation. The problem has been stated by Reed and Simon. Our approach is based on spherical incident waves produced by a harmonic source and the long-range asymptotics for the corresponding spherical limiting amplitudes. The main results are as follows: i) the convergence of spherical limiting amplitudes to the limit as the source goes away to infinity, and ii) the proof of the coincidence of the corresponding limit scattering cross section with the universally recognized formula. The main technical ingredients are the Agmon–Jensen–Kato's analytical theory of the Green function, Ikebe's uniqueness theorem for the Lippmann–Schwinger equation, and some refinement of classical long-range asymptotics for the Coulomb potentials.

1. Introduction

The differential cross section is the main observable in quantum scattering experiments. This concept was first introduced to describe the Rayleigh scattering of sunlight and the Rutherford alpha-particle scattering as the quotient

$$\sigma(\theta) = j_a^{\rm sc}(\theta)/|j^{\rm in}|. \tag{1.1}$$

Here, $j^{\rm in}$ is the incident stationary flux, and $j_a^{\rm sc}(\theta)$ is the angular density of the scattered stationary flux $j^{\rm sc}(x)$ in the direction $\theta \in \mathbb{R}^3$, $|\theta| = 1$ (see Fig. 1):

$$j_a^{\rm sc}(\theta) = \lim_{R\to\infty} R^2 j^{\rm sc}(R\theta)\theta. \tag{1.2}$$

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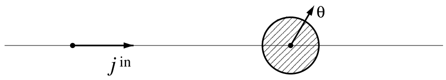

Fig. 1. Incident flux and scatterer.

In both scattering processes studied by Rayleigh and Rutherford the concept of differential cross section is well-established in the framework of the corresponding dynamical equations: the Maxwell equations in the case of Rayleigh scattering and the Newton equations in the case of Rutherford scattering.

On the other hand, a satisfactory dynamical justification of quantum scattering cross section is still missing in the framework of the Schrödinger equation

$$i\dot{\psi}(x,t) = H\psi(x,t) := -\frac{1}{2}\Delta\psi(x,t) + V(x)\psi(x,t), \qquad x \in \mathbb{R}^3. \tag{1.3}$$

The problem has been stated and discussed by Reed and Simon in [19, pp. 355–357]. We suggest the solution for the first time, as far as we are aware. The corresponding charge and flux densities are defined as

$$\rho(x,t) = |\psi(x,t)|^2, \qquad j(x,t) = \mathrm{Im}[\overline{\psi(x,t)}\nabla\psi(x,t)]. \tag{1.4}$$

These densities satisfy the charge continuity equation

$$\dot{\rho}(x,t) + \operatorname{div} j(x,t) = 0, \qquad (x,t) \in \mathbb{R}^4. \tag{1.5}$$

Let us denote by $k \in \mathbb{R}^3 \setminus 0$ the 'wave vector' of the incident plane wave

$$\psi^{\mathrm{in}}(x,t) = e^{i(kx - E_k t)}, \qquad E_k := \frac{1}{2}k^2. \tag{1.6}$$

Our main goal is a dynamical justification of the formula for the differential cross section

$$\sigma(k,\theta) = 16\pi^4 |T(|k|\theta, k)|^2, \qquad \theta \neq \pm n := \pm k/|k|, \tag{1.7}$$

which is universally recognized in physical and mathematical literature (see, for example, [11,17,19,22,25]).

Let the brackets $(\cdot,\cdot)$ denote the Hermitian scalar product in the complex Hilbert space $\mathcal{L}^2 := L^2(\mathbb{R}^3)$, as well as its extension to the duality between the weighted Agmon–Sobolev spaces, see (2.2) and (7.11). The *T-matrix* is given by

$$T(k',k) := \frac{1}{(2\pi)^3}(T(E_k + i0)e^{ikx}, e^{ik'x}), \qquad k', k \in \mathbb{R}^3, \tag{1.8}$$

which is the integral kernel of the operator $T(E_k + i0) := V - VR(E_k + i0)V$ (see Section 25 of [15]) in the Fourier transform

$$\hat{\psi}(k) = \int e^{-ikx}\psi(x)dx, \qquad \psi \in C_0^\infty(\mathbb{R}^3). \tag{1.9}$$

Here, $R(E) := (H - E)^{-1}$ is the resolvent of the Schrödinger operator H.

It is well known that the integral kernel $S(k',k)$ of the scattering operator S in the Fourier transform reads as

$$S(k',k) = \delta(k'-k) - i\pi\delta(E_{k'} - E_k)T(k',k), \quad k', k \in \mathbb{R}^3 \tag{1.10}$$

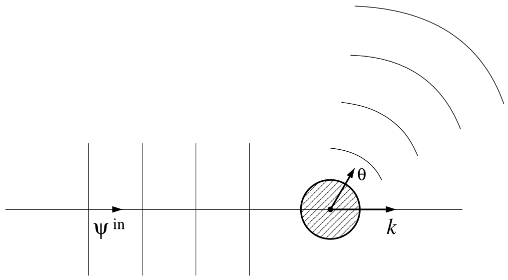

Fig. 2. Incident plane wave and outgoing spherical wave.

(see [3,17,19,22]). The commonly used 'naive scattering theory' consists of the following statements [19,21,22].

I. The incident wave is identified with the plane wave (1.6), which propagates in the direction of the wave vector k and is a solution to the free Schrödinger equation (1.3) with $V(x) = 0$.

II. The corresponding 'scattered' solution to (1.3) is identified by its long-time asymptotics on any bounded region $|x| < R$ (see Lemma 6.1),

$$\psi(x,t) \sim A(x)e^{-iE_k t}, \qquad t \to \infty. \tag{1.11}$$

The amplitude $A(x)$ is expressed by

$$A(x) = e^{ikx} - R(E_k + i0)[V(x)e^{ikx}], \tag{1.12}$$

and admits the following long-range asymptotics of type [3, (3.58) of Ch. 4]:

$$A(x) \sim e^{ikx} + a(k,\theta)\frac{e^{i|k||x|}}{|x|}, \qquad |x| \to \infty, \qquad \theta := x/|x|; \tag{1.13}$$

see Fig. 2.

III. By (1.4), asymptotics (1.13) give

$$j^{\text{in}} = k, \qquad j_a^{\text{sc}}(\theta) = |a(k,\theta)|^2|k|. \tag{1.14}$$

Hence, the differential cross section reads

$$\sigma(k,\theta) = |a(k,\theta)|^2 \tag{1.15}$$

since $k \neq 0$. It is well known that $a(k,\theta)$ is proportional to the T-matrix (formula (97a) of [19]):

$$a(k,\theta) = -4\pi^2 T(|k|\theta, k). \tag{1.16}$$

Hence, (1.15) reads as (1.7).

A *heuristic derivation* of relations (1.11), (1.12) can be found in [19, pp. 355–357]. However, a mathematically consistent justification of the relations in a *time dependent picture* was not suggested until now. Moreover, relation (1.7) was considered up to now as the *definition* of the differential cross section: see formulas (1.2) and (A.1.6) of [11], formula (96) of [19], and Definition 7.9 on p. 254 of [26].

The main problem in mathematical justification of (1.11) and (1.12) is related to the lack of a consistent model for the incident wave $\psi^{\text{in}}(x,t)$, securing convergence (1.11) to a stationary regime, and at the same time satisfies the '*adiabatic condition*'

$$\psi^{\rm in}(x,t)\to 0, \qquad t\to-\infty, \quad x\in\mathbb{R}^3, \tag{1.17}$$

which is in the spirit of the scattering theory. The plane incident wave (1.6) in the 'naive scattering theory' does not satisfy (1.17), since the wave occupies the entire space. The plane wave is a solution to the free Schrödinger equation

$$i\dot\psi(x,t)=-\frac{1}{2}\Delta\psi(x,t), \qquad x\in\mathbb{R}^3. \tag{1.18}$$

The adiabatic condition (1.17) in *acoustic scattering* is provided by the 'semi-infinite' incident plane wave

$$\psi^{\rm in}(x,t)=\Theta(|k|t-kx)e^{i(kx-|k|t)}$$

for $t<0$, where Θ is the Heaviside function. This incident wave is a solution to the acoustic equation

$$\ddot\psi(x,t)=\Delta\psi(x,t), \qquad |x|>R \tag{1.19}$$

for $t<-R$ if the scatterer is located in the region $|x|\le R$. The similar incident plane wave can be constructed for the Maxwell equations, which makes apparent the meaning of the differential cross section in the Rayleigh scattering.

On the other hand, a similar semi-infinite incident plane wave does not exist in the case of the Schrödinger equation. Indeed, we may fix $R\gg|k|B$ if the scatterer is contained in a ball $|x|\le B$ and take the semi-infinite plane wave

$$\psi^{\rm in}(x)=\Theta(-R-kx)e^{ikx}$$

as the initial condition at $t=0$. However, the corresponding solution does not satisfy the adiabatic condition for $t\to-\infty$. The problem is of great importance also in the context of the quantum field theory, where the incident and outgoing plane waves play the fundamental role [17,20,21,25].

In the traditional approach, the incident wave is a specific initial field, which is a solution to the corresponding free wave equation in the entire space. On the other hand, in practice, the incident wave is a beam of particles or light produced by a macroscopic source and satisfies the free wave equation only outside the source. One could expect that, for a large time, the incident wave near the scatterer will asymptotically be a free plane wave if the source is 'monochromatic' and its distance from the scatterer, D, tends to infinity. This model obviously corresponds to *spherical incident waves*, which are standard devices in optical and acoustic scattering [4].

We justify formula (1.7) in the following steps:

A. First, we prove *the limiting amplitude principle* for the Schrödinger equation (1.3) with harmonic source; i.e., the long-time convergence to a stationary harmonic regime with a 'spherical limiting amplitude', which does not depend on initial state.

B. Second, we prove the convergence of the spherical limiting amplitudes to the plane limiting amplitude when the source goes off to infinity: $D\to\infty$.

C. We deduce from A and B that relations (1.11)–(1.13) hold true up to a factor in this double limit: first, as $t\to\infty$, and then, as $D\to\infty$.

D. Finally, we establish (1.14) up to a factor for $\theta\ne\pm n$. The incident and scattered fluxes are defined by

$$j^{\rm in}:=\lim_{|x|\to\infty}j_\infty(x,t), \qquad j^{\rm sc}(x,t):=j_\infty(x,t)-j^{\rm in}, \tag{1.20}$$

where $j_\infty(x,t)$ is the double limit of the flux (1.4). The definitions of $j^{\rm in}$ and $j_a^{\rm sc}$ will be adjusted in Section 8. Now formula (1.7) follows from (1.15) and (1.16).

Our strategy is as follows. We prove the limiting amplitude principle A, relying on our development [15] of the Agmon–Jensen–Kato's theory of the resolvent of the Schrödinger operator [1,14]. The proof of the convergence B relies on a novel application of Ikebe's uniqueness theorem for the Lippmann–Schwinger equation [3,12] and on uniform bounds for the Coulomb potentials (4.6), (4.14), (4.26). These bounds are due to novel asymptotics for the Coulomb potentials (4.4), which are regularized at the zero point (the corresponding bound (3.51) of [3, Ch. 4], is correct only for $|x| \ge \delta > 0$ due to the singularity of the main term).

We have developed similar approach in [15, Chapter 9] for the case of empty discrete spectrum of the Schrödinger operator (1.3). In present paper we get rid of this restriction and adjust our basic assumptions and references.

Moreover, we have improved significantly our arguments in derivation of (1.14) from (1.13). Our main novelties here are as follows.

I. Traditionally, the scattered flux (1.14) is defined by the second term on the right-hand side of (1.13). The separation of these terms is possible experimentally by suitable screens due to different directions of propagation.

In present paper we get rid of this separation problem defining the scattered flux by (1.20) where the flux $j_\infty(x)$ corresponds to the total sum (1.13). Surprisingly, we obtain the same result (1.14). This coincidence is not obvious a priori since *the magnitude* of the corresponding "cross terms" at the points $x = R\theta$ with $|\theta| = 1$ are of order $\sim 1/R$ and $\sim 1/R^2$ which are not negligible in the limit (1.2) (see (8.7), (8.9)).

Namely, we prove that, the cross terms cancel on the sphere $|\theta| = 1$ as $R \to \infty$ in the sense of distributions of $\theta \ne \pm n$ since the terms contain the oscillatory factors $e^{iRk\theta}$. It is instructive to note that the stationary points of the phase $k\theta$ on the sphere are exactly $\theta = \pm n$. Respectively, the limit (1.2) converges in the sense of the distributions (see Definition 8.1) that we prove in our novel Theorem 8.2.

II. The proof of Theorem 8.2 relies on oscillatory integral representation (8.6) for the limiting flux $j_\infty(x)$ and on the long-range asymptotics of $j_\infty(x)$. This asymptotic analysis required novel estimates (7.4) and (7.9) for the remainders in classical long-range asymptotics of the Coulomb potentials. These estimates refine the corresponding estimates from Lemma 3.2 and Theorem 3.2 of [3, Ch. 4], which dates back to the results of Povzner and Ikebe [12,18].

Let us comment on previously known arguments for formula (1.7). The traditional physical approach [22] is based on random incident wave packets $\psi^{\rm in}(x,0)$, which are asymptotically proportional to the plane waves e^{ikx}:

$$|\hat\psi^{\rm in}(k',0)|^2 \to \delta(k'-k). \tag{1.21}$$

The known mathematical justifications reside in Dollard's fundamental result [6] on *scattering into cones*. This result is used in [23] for a clarifying treatment of formula (1.7). Namely, the normalized angular distribution of a finite charge, scattered for infinite time, converges to the *normalized function* (1.7) in the limit (1.21).

Dollard's result was refined in [5,13] and in Section 3-3 of [2], where *the flux across the surface theorem* is proved. This result was later developed in [7–9,24] and applied for justification of formula (1.7) in the context of the *Bohmian particle mechanics* and incident stationary random processes constructed of normalized wave packets (1.7) in the limit (1.21). For a survey, see [10]. It is worth noting that we do not exclude the discrete spectrum of the Schrödinger operator H, in contrast to [7].

We point out that all the previous results give the same expression (1.7) for the differential cross section, though these results were not concerned with the long-time transition to a stationary regime.

Our paper is organized as follows. The main results are stated in Section 2. The limiting amplitude principle is established in Section 3. In Section 4 we obtain long-range asymptotics and uniform bounds for the spherical limiting amplitudes. Next, in Sections 5 and 6 we prove convergence B and the corresponding convergence for the flux. Finally, in Sections 7 and 8 we verify formulas (1.16) and (1.14), which justify (1.15) and (1.7).

2. Main results

We consider the Schrödinger equation with harmonic source:

$$\left\{\begin{array}{ll} i\dot\psi(x,t) = H\psi(x,t) + \rho_q(x)\, e^{-iE_k t}, & t>0 \\ \psi(x,0)=\psi^0(x) & \end{array}\right| \qquad x\in\mathbb{R}^3. \tag{2.1}$$

Here, $H=-\frac{1}{2}\Delta+V(x)$, $k\in\mathbb{R}^3\setminus 0$, and $\rho_q(x):=|q|\rho(x-q)$ is the form factor of the source.

We mean that our model suits the physics of quantum scattering. Namely, the incident wave is produced by time periodic source, like a heated cathode in an electron gun. The source is not at infinity, though its distance from the scatterer is sufficiently large.

The solution $\psi(x,t)$ describes the spherical waves produced by the source with the density $|q|\rho(x-q)$ which is located asymptotically near q (for large $|q|$). The factor $|q|$ is introduced for a suitable normalization. Namely, this factor provides that the spherical waves look like plane waves (for bounded x) in the limit $|q|\to\infty$, see (2.13) below.

The weighted Agmon–Sobolev spaces $\mathcal{H}^s_\sigma=\mathcal{H}^s_\sigma(\mathbb{R}^3)$, $s,\sigma\in\mathbb{R}$, are defined as follows. Let $\mathcal{L}^2_\sigma=\mathcal{L}^2_\sigma(\mathbb{R}^3)$ be the Hilbert space of measurable functions in $\mathbb{R}^3$ with norm

$$\|\psi\|^2_{\mathcal{L}^2_\sigma}=\int\langle x\rangle^{2\sigma}|\psi(x)|^2dx, \qquad \langle x\rangle:=\sqrt{x^2+1}. \tag{2.2}$$

Definition 2.1. $\mathcal{H}^s_\sigma=\mathcal{H}^s_\sigma(\mathbb{R}^3)$ denotes the Hilbert space of tempered distributions $\psi(x)$ with finite norm

$$\|\psi\|_{\mathcal{H}^s_\sigma}:=\|\langle\nabla\rangle^s\psi\|_{\mathcal{L}^2_\sigma}<\infty. \tag{2.3}$$

We will assume the following conditions.

H0. The initial state ψ^0 is a function from the space $\mathcal{H}^2_{\sigma_0}$ with some $\sigma_0>5/2$.
H1. For some $\varepsilon_1>0$,

$$\sup_{x\in\mathbb{R}^3}\langle x\rangle^{4+\varepsilon_1}|\partial^\alpha\rho(x)|<\infty, \qquad |\alpha|\le 2. \tag{2.4}$$

H2. The following Wiener condition holds:

$$\hat\rho(|k|\theta):=\int e^{i|k|\theta x}\rho(x)dx\ne 0, \qquad \theta\in\mathbb{R}^3, \quad |\theta|=1. \tag{2.5}$$

H3. The potential $V(x)$ is a real C^2-function satisfying the condition

$$\sup_{x\in\mathbb{R}^3}\langle x\rangle^{5+\varepsilon_2}|\partial^\alpha V(x)|<\infty, \qquad |\alpha|\le 2, \tag{2.6}$$

with some $\varepsilon_2>0$.

Finally, we introduce our key spectral assumption. Denote

$$\mathcal{M}_\sigma := \{\psi \in \mathcal{L}^2_{-\sigma} : \psi + R_0(0)V\psi = 0\},$$

where $R_0(E) := (-\frac{1}{2}\Delta - E)^{-1}$ is the free resolvent. The space $\mathcal{M}_\sigma = \mathcal{M}$ does not depend on $\sigma \in (1/2, (5+\varepsilon_2)/2)$ by the arguments preceding Lemma 3.1 of [14].

H4. We assume:

$$\textbf{The Spectral Condition:} \quad \mathcal{M} = 0. \tag{2.7}$$

This condition holds for *generic* potentials, see the discussion preceding Lemma 3.1 in [14].

Let us outline our plan.

I. First, we will prove the *limiting amplitude principle*:

$$\psi(x,t) \sim \varphi_q(x,t) = B_q(x)e^{-iE_k t} + \sum_1^N C_q^l \psi_l(x) e^{-iE^l t}, \quad t \to \infty, \tag{2.8}$$

where $\psi_l(x)$ are the eigenfunctions of H corresponding to the eigenvalues $E^l < 0$. The asymptotics hold in $\mathcal{H}^2_{-\sigma}$ with any $\sigma > 5/2$, and the *limiting amplitude* $B_q(x)$ is given by

$$B_q(x) = R(E_k + i0)\rho_q. \tag{2.9}$$

The coefficients C_q^l depend on the initial state $\psi(x,0)$. On the other hand, it is crucially important that the coefficients C_q^l converge as $|q| \to \infty$, while the eigenfunctions $\psi_l(x)$ decay rapidly at infinity by Agmon's theorem [1, Theorem 3.3] (see also Theorem 20.7 of [15]). Respectively, the sum over the discrete spectrum on the right-hand side of (2.8) does not contribute to the scattering cross section.

II. Second, let us denote $n := k/|k|$, $B_D(x) := B_{q_D}(x)$ where $q_D := -nD$ and $D > 0$. We will establish the following *'spherical version'* of long-range asymptotics (1.13):

$$B_D(x) \sim b_D(n)\Big[\frac{|q_D|}{|x-q_D|}e^{i|k|(|x-q_D|-|q_D|)} + a_D(k,\theta)\frac{e^{i|k||x|}}{|x|}\Big]$$
$$\text{as} \quad |x-q_D| \to \infty, \quad |x| \to \infty, \tag{2.10}$$

where $\theta := x/|x|$ and $b_D(n) := b(n)e^{i|k|D}$ with $b(n) \neq 0$; see Fig. 3. The asymptotics (2.10) mean that the difference between the left-hand side and the right-hand side converges to zero.

III. Further, we prove the convergence of the spherical limiting amplitudes, which is our central result: for $k \neq 0$

$$A_D(x) := B_D(x)/b_D(n) \to A(x), \qquad D \to \infty, \tag{2.11}$$

where $A(x)$ is expressed by (1.12).

IV. At last, (2.11) implies the convergence of the flux (1.4) corresponding to the limiting amplitudes $B_D(x)$:

$$J_D(x) := |b(n)|^2 \operatorname{Im}[\overline{A_D(x)}\nabla A_D(x)] \longrightarrow J_\infty(x) := |b(n)|^2 \operatorname{Im}[\overline{A(x)}\nabla A(x)], \qquad D \to \infty. \tag{2.12}$$

V. Finally, we calculate the long-range asymptotics of $A(x)$ as $|x| \to \infty$ and show that the convergence (2.12) and formula (1.12) justify (1.7).

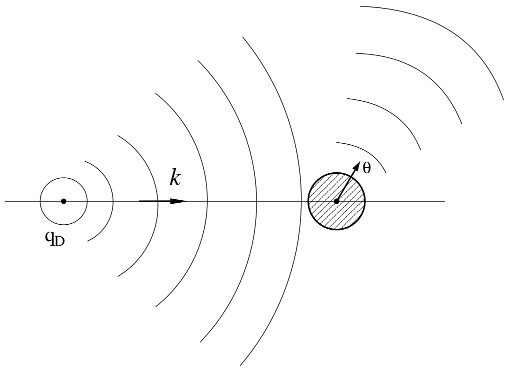

Fig. 3. Incident and outgoing spherical waves.

Let us comment on our methods. We derive the limiting amplitude principle (2.8) from the dispersion decay in weighted energy norms by a suitable development of Agmon–Jensen–Kato's methods [1,14,15]. The long-range asymptotics (2.10) is deduced from the 'spherical version' (4.1) of the Lippmann–Schwinger equation and a refinement of Lemma 3.2 from [3, Ch. 4]. One of our key observations is that *the spherical incident wave* from (2.10) becomes asymptotically *the plane incident wave* from (1.13) as the source goes off to infinity:

$$\frac{|q_D|}{|x-q_D|}e^{i|k|(|x-q_D|-|q_D|)} \to e^{ikx}, \qquad D\to\infty. \tag{2.13}$$

In this limit, the picture of Fig. 3 becomes the one of Fig. 2. We derive convergence (2.11) from asymptotics (2.10) by the Sobolev embedding theorem and the Ikebe uniqueness theorem for the Lippmann–Schwinger equation [12] (Theorem 3.1 of [3, Ch. 4]). Finally, we prove the second formula of (1.14) for the flux (1.20) in Theorem 8.2. We deduce it from the decay of the oscillatory integrals (8.9), which is due to the interference of the incident and scattered waves.

3. Limiting amplitude principle

We deduce the limiting amplitude principle (2.8) from the dispersion decay in weighted energy norms [14,15].

Lemma 3.1. *Assume that conditions* H0–H4 *hold and* $k\in\mathbb{R}^3$. *Then:*

i) *The limiting amplitude principle* (2.8) *holds in the norm of* $\mathcal{H}^2_{-\sigma}$ *with any* $\sigma>5/2$.
ii) C^l_q *converge to some limits* C^l *as* $|q|\to\infty$, *and the limiting amplitude is given by* (2.9).

Proof. We should prove that

$$\psi(x,t)=B_q(x)e^{-iE_kt}+\sum_1^N C^l_q\psi_l(x)e^{-iE^lt}+r(x,t), \tag{3.1}$$

where

$$C^l_q\to C^l, \qquad |q|\to\infty; \qquad \|r(\cdot,t)\|_{\mathcal{H}^2_{-\sigma}}\to 0, \qquad t\to\infty. \tag{3.2}$$

The solution to the Cauchy problem (2.1) is unique and is given by the Duhamel representation

$$\psi(t) = U(t)\psi^0 - i\int_0^t e^{-iE_k s}U(t-s)\rho_q\,ds. \tag{3.3}$$

Here, $U(t)$ is the dynamical group of equation (2.1) with $\rho_q = 0$, and the first term in the right-hand side admits the expansion

$$U(t)\psi^0 = \sum_1^N C^l\psi_l e^{-iE^l t} + r_0(t), \tag{3.4}$$

where C^l are independent of q, and

$$\|r_0(t)\|_{\mathcal{H}^2_{-\sigma}} \le C\langle t\rangle^{-3/2}. \tag{3.5}$$

This decay follows similarly to the dispersion decay in the norm $\mathcal{H}^0_{-\sigma}$, as established in (10.9) of [14], with suitable refinement of the resolvent high energy decay (see Theorem 17.1 of [15]). Here, the assumptions H0 and H3–H4 are essential.

On the other hand, the second term on the right-hand side of (3.3) can be written as

$$I(t) = -i\int_0^t e^{-iE_k s}U(t-s)\rho_q\,ds = -ie^{-iE_k t}\int_0^t e^{iE_k\tau}U(\tau)\rho_q\,d\tau. \tag{3.6}$$

Here, $\rho_q \in \mathcal{H}^2_{\sigma_1}$ with some $\sigma_1 > 5/2$ by H1. Hence, similarly to (3.4) and (3.5),

$$U(\tau)\rho_q = \sum_1^N D^l_q\psi_l e^{-iE^l\tau} + r_q(\tau), \tag{3.7}$$

where

$$\|r_q(\tau)\|_{\mathcal{H}^2_{-\sigma}} \le C_q\langle\tau\rangle^{-3/2}. \tag{3.8}$$

Finally, the eigenfunctions $\psi_l(x) \in \mathcal{H}^2_s$ with any $s \in \mathbb{R}$ by Agmon's theorem [1, Theorem 3.3] (see also Theorem 20.7 of [15]). Hence, (2.4) implies that

$$D^l_q = \langle\rho_q, \psi_l\rangle = |q|\int \rho(x-q)\psi_l(x)dx = \mathcal{O}(|q|^{-3-\varepsilon_1}), \qquad |q| \to \infty. \tag{3.9}$$

Therefore, $C^l_q = C^l + D^l_q \to C^l$ as $|q| \to \infty$, and

$$I(t) \sim B_q(x)e^{-iE_k t} + \mathcal{O}(|q|^{-3-\varepsilon_1}), \qquad t \to \infty. \tag{3.10}$$

Here, the asymptotics hold in $\mathcal{H}^2_{-\sigma}$, and the limiting amplitude is given by

$$B_q = -i\int_0^\infty e^{iE_k\tau}U(\tau)\rho_q\,d\tau = -i\int_0^\infty e^{i(E_k+i0)\tau}U(\tau)\rho_q\,d\tau, \tag{3.11}$$

which can be written as (2.9). This proves (3.1). $\square$

4. Spherical waves

In this section we obtain long-range asymptotics (2.10). Denote $R = R(E_k + i0)$ and $R_0 = R_0(E_k + i0)$, where $R_0(E) = (H_0 - E)^{-1}$ is the resolvent of the free Schrödinger operator $H_0 = -\frac{1}{2}\Delta$. Rewriting formula (2.9) for the limiting amplitude as the following 'spherical version' of the Lippmann–Schwinger equation, this gives

$$B_q(x) = R_0\rho_q(x) - R_0 V B_q(x), \tag{4.1}$$

since $R = R_0 - R_0 V R$. The free Schrödinger resolvent $R_0(E)$ is the integral operator with kernel

$$R_0(E, x, y) = \frac{e^{i\sqrt{2E}|x-y|}}{2\pi|x-y|}, \qquad E \in \mathbb{C} \setminus (0, \infty).$$

Therefore, R_0 is the integral operator with kernel

$$R_0(E_k + i0, x, y) = \frac{e^{i|k||x-y|}}{2\pi|x-y|}, \tag{4.2}$$

because $\sqrt{2(E_k + i0)} = |k|$.

For the first term on the right-hand side of (4.1), asymptotics (2.10) follow by a suitable modification of Lemma 3.2 from [3, Ch. 4]. Let

$$S = \{\theta \in \mathbb{R}^3 : |\theta| = 1\} \tag{4.3}$$

be the unit sphere.

Lemma 4.1. *Under condition* H1 *with* $\alpha = 0$*,*

$$R_0\rho_q(x) = b\Big(\frac{x-q}{|x-q|}\Big)\frac{|q|}{1+|x-q|}e^{i|k||x-q|} + K(x-q), \qquad x \in \mathbb{R}^3. \tag{4.4}$$

Here, the amplitude $b \in C^1(S)$*, and*

$$b(\theta) = \frac{1}{2\pi}\hat{\rho}(|k|\theta), \qquad |\theta| = 1, \tag{4.5}$$

where $\hat{\rho}(k)$ *denotes the Fourier transform* (1.9). *The remainder admits the bound*

$$|K(x-q)| \le C|q|(1+|x-q|)^{-1-\varepsilon_1}, \qquad x \in \mathbb{R}^3. \tag{4.6}$$

Proof. This lemma follows by the arguments from the proof of Lemma 3.2 from [3, Ch. 4], with $|x|$ substituted almost everywhere by $|x| + 1$. Moreover, H1 with $\alpha = 0$ implies that $\hat{\rho} \in C_b^1(\mathbb{R}^3)$. Hence, $b \in C^1(S)$ by (4.5). □

As a corollary, we obtain the bound

$$|R_0\rho_q(x)| \le \frac{C|q|}{1+|x-q|}, \qquad x \in \mathbb{R}^3. \tag{4.7}$$

Remark 4.2. Our asymptotics (4.4) and the estimate (4.6) differ from similar ones (3.50) and (3.51) of [3, Ch. 4], which hold only for $|x| \geq \delta > 0$.

For the second term on the right-hand side of (4.1) we need two additional technical lemmas.

Lemma 4.3. *Under conditions* H1 *and* H3 *the following bound holds for* $k \neq 0$:

$$\sup_{q\in\mathbb{R}^3} \|VB_q\|_{\mathcal{L}^2_\sigma} < \infty \quad \textit{for any} \quad \sigma < 5/2 + \varepsilon_2. \tag{4.8}$$

Proof. The Lippmann–Schwinger equation (4.1) implies

$$(1 + VR_0)VB_q = VR_0\rho_q. \tag{4.9}$$

On the other hand, $(1 + VR_0)^{-1} = 1 - VR$. Hence,

$$VB_q = (1 - VR)VR_0\rho_q = VR_0\rho_q - VRVR_0\rho_q. \tag{4.10}$$

Let us estimate each term on the right-hand side separately.

i) Condition (2.6) with $\alpha = 0$ and bound (4.7) imply

$$|VR_0\rho_q(x)| \leq \frac{C|q|}{(1 + |x - q|)(1 + |x|)^{5+\varepsilon_2}}, \quad x \in \mathbb{R}^3. \tag{4.11}$$

Therefore,

$$|VR_0\rho_q(x)| \leq \frac{C}{(1 + |x|)^{4+\varepsilon_2}}, \quad x \in \mathbb{R}^3. \tag{4.12}$$

Hence,

$$VR_0\rho_q \in \mathcal{L}^2_\sigma, \qquad \sigma < 5/2 + \varepsilon_2. \tag{4.13}$$

Thus, the bound (4.8) holds for the first term on the right-hand side of (4.10).

ii) It remains to estimate the last term of (4.10). By (4.13) we have $RVR_0\rho_q \in \mathcal{L}^2_{-s}$ for any $s > 1/2$, since the resolvent $R = R(E_k + i0) : \mathcal{L}^2_s \to \mathcal{L}^2_{-s}$ is continuous by [14, Theorem 9.2] because $E_k > 0$ for $k \neq 0$. Therefore, $VRVR_0\rho_q \in \mathcal{L}^2_\sigma$ for $\sigma < 4.5 + \varepsilon_2$ by (2.6) with $\alpha = 0$. □

Lemma 4.4. *Under conditions* H1 *and* H3 *the following uniform decay holds*:

$$\sup_{q\in\mathbb{R}^3} |R_0VB_q(x)| \leq C(1 + |x|)^{-2}, \quad x \in \mathbb{R}^3. \tag{4.14}$$

Proof. By (4.2),

$$|R_0VB_q(x)| \leq C\int \frac{|VB_q(y)|}{|x - y|}dy = C\int_0^\infty \Big[\int\int \frac{|VB_q(r,\varphi,\theta)|d\varphi \sin\theta d\theta}{\sqrt{|x|^2 + r^2 - 2|x|r\cos\theta}}\Big]r^2dr. \tag{4.15}$$

Applying the Cauchy–Schwarz inequality to the inner integral,

$$|R_0VB_q(x)| \le C\int\limits_0^\infty \Big[\int |VB_q(r,\varphi,\theta)|^2 d\varphi \sin\theta d\theta\Big]^{\frac12}\Big[\int \frac{d\varphi\sin\theta d\theta}{|x|^2+r^2-2|x|r\cos\theta}\Big]^{\frac12} r^2dr$$
$$= C\int\limits_0^\infty \Big[\int |VB_q(r,\varphi,\theta)|^2 d\varphi \sin\theta d\theta\Big]^{\frac12}\Big[\frac{1}{|x|r}\log\frac{|x|+r}{||x|-r|}\Big]^{\frac12} r^2dr. \tag{4.16}$$

Applying the same inequality to the last integral, this gives

$$|R_0VB_q(x)| \le C\Big[\int (1+r)^{2\sigma}|VB_q(r,\varphi,\theta)|^2 d\varphi\sin\theta d\theta r^2 dr\Big]^{\frac12} \times \Big[\int\limits_0^\infty \log\frac{|x|+r}{||x|-r|}\ \frac{r^2dr}{|x|r(1+r)^{2\sigma}}\Big]^{\frac12}$$
$$\le C(\sigma)\Big[\int\limits_0^\infty \log\frac{|x|+r}{||x|-r|}\ \frac{rdr}{|x|(1+r)^{2\sigma}}\Big]^{\frac12} = C(\sigma)\Big[\int\limits_0^\infty \log\frac{1+s}{|1-s|}\ \frac{|x|sds}{(1+s|x|)^{2\sigma}}\Big]^{\frac12} \tag{4.17}$$

for $\sigma < 5/2+\varepsilon_2$ by the uniform bound (4.8). Let us split the region of integration $(0,\infty) = (0,1/2)\cup(1/2,3/2)\cup(3/2,\infty)$ and observe that

$$\left.\begin{array}{ll} \log\frac{1+s}{|1-s|} = \mathcal{O}(s), & s\in(0,1/2)\\ \log\frac{1+s}{|1-s|} \in L^1(1/2,3/2) & \\ \log\frac{1+s}{|1-s|} = \mathcal{O}(s^{-1}), & s\in(3/2,\infty)\end{array}\right| \tag{4.18}$$

Then the integral (4.17) can be estimated as

$$C_1(\sigma)\Big[\int\limits_0^{1/2}\frac{|x|s^2ds}{(1+s|x|)^{2\sigma}} + (1+|x|)^{1-2\sigma} + \int\limits_{3/2}^\infty \frac{|x|ds}{(1+s|x|)^{2\sigma}}\Big]$$
$$= C_1(\sigma)\Big[|x|^{-2}\int\limits_0^{|x|/2}\frac{r^2dr}{(1+r)^{2\sigma}} + (1+|x|)^{1-2\sigma} + \int\limits_{3|x|/2}^\infty \frac{dr}{(1+r)^{2\sigma}}\Big]$$
$$\le C_2(\sigma)(1+|x|)^{1-2\sigma} \tag{4.19}$$

for $2\sigma > 1$. This gives (4.14), since we can take any $\sigma < 5/2+\varepsilon_2$ by (4.8). □

Now we are ready to prove (2.10).

Proposition 4.5. *Asymptotics* (2.10) *hold under conditions* H1–H3.

Proof. The Lippmann–Schwinger equation (4.1) yields

$$VB_q(x) = VR_0\rho_q(x) - VR_0VB_q(x).$$

Hence, (2.6) with $\alpha = 0$ and (4.12), (4.14) imply that

$$|VB_q(x)| \le \frac{C}{(1+|x|)^{4+\varepsilon_2}}. \tag{4.20}$$

Therefore, similarly to (4.4), we obtain the asymptotics

$$R_0 V B_q(x) = c_q\Big(\frac{x}{|x|}\Big)\frac{e^{i|k||x|}}{1+|x|} + L_q(x), \tag{4.21}$$

where

$$|L_q(x)| \le C(1+|x|)^{-1-\varepsilon_2}. \tag{4.22}$$

Now (4.1) and (4.4), (4.21) imply

$$B_q(x) \sim b\Big(\frac{x-q}{|x-q|}\Big)\frac{|q|}{|x-q|}e^{i|k||x-q|} + c_q\Big(\frac{x}{|x|}\Big)\frac{e^{i|k||x|}}{|x|} \tag{4.23}$$

as $|x-q|\to\infty$ and $|x|\to\infty$. Denote $B_D(x) := B_{q_D}(x)$, where $q_D = -nD$ with $n = k/|k|$ and $D > 0$. Then

$$B_D(x) \sim b(n)\Big[\frac{|q_D|}{|x-q_D|}e^{i|k||x-q_D|} + d_D(k,\theta)\frac{e^{i|k||x|}}{|x|}\Big] \tag{4.24}$$

as $|x-q_D|\to\infty$ and $|x|\to\infty$, where $\theta := x/|x|$, because

$$b(n) = \hat\rho(|k|n) \ne 0 \tag{4.25}$$

by (4.5) and the Wiener condition H2. This is the only point in our analysis, where the Wiener condition is called for. Finally, (4.24) can be written as (2.10) with $b_D(n) := b(n)e^{i|k|D}$ and $a_D(k,\theta) = d_D(k,\theta)e^{-i|k|D}$. □

The following corollary is of crucial importance in the next section.

Corollary 4.6. *Bound (4.7), asymptotics (4.21)–(4.22), and formula (4.1) imply*

$$|B_q(x)| \le \frac{C|q|}{1+|x-q|} + \frac{C}{(1+|x|)}, \qquad x, q \in \mathbb{R}^3. \tag{4.26}$$

5. Plane wave limit

In this section we prove convergence (2.11) from the uniqueness of solution to the Lippmann–Schwinger equation

$$A(x) = e^{ikx} - R_0 V A(x), \tag{5.1}$$

which is equivalent to (1.12) (see Lemma 7.1 below). First, we rewrite (4.1) with $q = q_D$ as

$$A_D(x) = R_0\rho_{q_D}(x)/b_D(n) - R_0 V A_D(x), \tag{5.2}$$

where $A_D(x) := B_D(x)/b_D(n)$. By (4.4) and (2.13) the first term on the right-hand side of (5.2) converges to the first term on the right-hand side of (5.1),

$$R_0\rho_{q_D}(x)/b_D(n) \to e^{ikx}, \qquad D\to\infty, \tag{5.3}$$

in $C(\mathbb{R}^3)$. Now (2.11) means the convergence of the corresponding solutions:

Proposition 5.1. *Let conditions* H1–H3 *hold and let $k \neq 0$. Then the convergence*

$$A_D \to A, \qquad D \to \infty \tag{5.4}$$

holds in $\mathcal{H}^s_{-\sigma}$ with any $s < 2$ and $\sigma > 5/2$, where the function $A(x)$ is defined by (1.12).

Proof. We deduce the convergence from the compactness of the family $\{A_D(x) : D > 0\}$ and Ikebe's uniqueness theorem [12] (Theorem 3.1 of [3, Ch. 4]).

Step i). By (5.2),

$$\|A_D\|_{\mathcal{H}^2_{-\sigma}} \leq C\|R_0\rho_{q_D}\|_{\mathcal{H}^2_{-\sigma}} + \|R_0 V B_D\|_{\mathcal{H}^2_{-\sigma}}.$$

The first term on the right-hand side is uniformly bounded for $D > 0$, since estimate of type (4.12) holds with $\langle x\rangle^{-\sigma}$ and σ instead of $V(x)$ and $5+\varepsilon_2$, respectively. The second term is uniformly bounded, since VB_q is uniformly bounded in $\mathcal{L}^2_\sigma$ with $\sigma < 5/2 + \varepsilon_2$ by (4.8), while the operator $R_0 : \mathcal{L}^2_s \to \mathcal{H}^2_{-s}$ is continuous for any $s > 1/2$ by Theorem 18.3 i) of [15], because $k \neq 0$. Hence,

$$\sup_{D>0} \|A_D\|_{\mathcal{H}^2_{-\sigma}} < \infty, \qquad \sigma > 5/2. \tag{5.5}$$

Step ii). Now the Sobolev embedding theorem [16] implies that the family $\{A_D(x) : D > 0\}$ is a precompact set in the Hilbert space $\mathcal{H}^s_{-\sigma}$ with any $s < 2$ and $\sigma > 5/2$. Hence, for any sequence $D_j \to \infty$, there is a subsequence $D_{j'} \to \infty$ such that

$$A_{D_{j'}}(x) \to A_*(x), \qquad j' \to \infty, \tag{5.6}$$

where the convergence holds in $\mathcal{H}^s_{-\sigma}$ with any $s < 2$ and $\sigma > 5/2$. Therefore,

$$VA_{D_{j'}}(x) \to VA_*(x), \qquad j' \to \infty, \tag{5.7}$$

where the convergence holds in $\mathcal{H}^s_\sigma$ with $s < 2$ and some $\sigma > 5/2$ by H3.

Step iii). At last, equation (5.2) and convergences (5.6), (5.7), and (5.3) imply equation (5.1) for $A_*(x)$:

$$A_*(x) = e^{ikx} - R_0 V A_*(x), \tag{5.8}$$

since the operator $R_0 := R_0(E_k + i0) : \mathcal{L}^2_\sigma \to \mathcal{L}^2_{-\sigma}$ is continuous for $\sigma > 1/2$ by Lemma 2.1 of [14].

The function $A_*(x)$ is bounded by (4.26) and is continuous by the Sobolev embedding theorem, since $A_*(x) \in \mathcal{H}^s_{-\sigma}$ with any $s < 2$ and $\sigma > 5/2$ by (5.6).

Finally, $A(x) = A_*(x)$ by Ikebe's uniqueness theorem [3,12], which holds for $k \neq 0$ under the condition (2.4) for bounded continuous solutions to the Lippmann–Schwinger equation (5.1). Hence, convergence (5.6) implies (5.4), since the limit function $A_*(x)$ does not depend on the subsequence j'. □

Remark 5.2. Let us emphasize that the right-hand side of (4.26) with $q = -nD$ is not uniformly bounded for $D > 0$: its value at $x = q$ tends to infinity as $D \to \infty$. Nevertheless, (4.26) implies that every limit function $A_*(x)$ is bounded.

6. Convergence of flux

We check the convergence (2.12) using (5.4).

Lemma 6.1. *Under conditions* H1–H3*,*

i) *the convergence* (2.12) *holds in* $\mathcal{L}^2_{\rm loc}(\mathbb{R}^3)$*.*
ii) *Moreover, the convergence holds 'in the sense of flux'; i.e.,*

$$\int\limits_S J_D(x)\nu(x)dS(x) \to \int\limits_S J_\infty(x)\nu(x)dS(x), \qquad D\to\infty, \quad t\in\mathbb{R}, \tag{6.1}$$

for any compact smooth two-dimensional submanifold $S\subset\mathbb{R}^3$ *with boundary, where* $\nu(x)$ *is the unit normal field to* S *and* $dS(x)$ *stands for the corresponding Lebesgue measure on* S*.*

Proof. Proposition 5.1 implies the convergence (5.4) in $C(\mathbb{R}^3)$, since $\mathcal{H}^s_{-\sigma}\subset C(\mathbb{R}^3)$ for $s>3/2$ by the Sobolev embedding theorem [16]. Further, the convergence of the derivatives

$$\nabla A_D(x)\to\nabla A(x), \qquad D\to\infty, \quad t\in\mathbb{R}, \tag{6.2}$$

holds in $\mathcal{H}^{s-1}_\sigma$ with any $s<2$. Hence, the convergence (2.12) holds in $\mathcal{L}^1_{\rm loc}(\mathbb{R}^3)$, and moreover,

$$\nabla A_D(x)\Big|_S \to \nabla A(x)\Big|_S, \qquad D\to\infty, \quad t\in\mathbb{R}, \tag{6.3}$$

in $\mathcal{L}^2(S)$ by the Sobolev trace theorem [16], for we can take $s>3/2$.

Similarly, (5.4) also implies the convergence in $\mathcal{L}^2(S)$

$$A_D(x)\Big|_S \to A(x)\Big|_S, \qquad D\to\infty, \quad t\in\mathbb{R}. \tag{6.4}$$

Therefore, the integrands in (6.1) converge in $\mathcal{L}^1(S)$. □

7. Long range asymptotics

We obtain asymptotics (1.13). The first lemma is well known [22].

Lemma 7.1. *Equation* (5.1) *admits a unique bounded continuous solution, which is given by* (1.12):

$$A(x) = e^{ikx} - RVe^{ikx}. \tag{7.1}$$

Proof. We should prove (7.1) assuming (5.1). First, we apply the general operator identity

$$P^{-1} = Q^{-1} + Q^{-1}(Q-P)P^{-1}$$

to $P = H_0 - E_k - i0$ and $Q = H - E_k - i0$. Then we obtain $R_0 = R + RVR_0$, and hence

$$R_0VA = RVA + RVR_0VA = RV(A + R_0VA) = RVe^{ikx}$$

by (5.1). Substituting into (5.1), we obtain (7.1). □

Next, we need an extension of Lemma 4.1 to functions from weighted Agmon–Sobolev spaces.

Lemma 7.2. *Let $r(x) \in \mathcal{H}^2_\sigma$ for some $\sigma > 7/2$. Then*

$$R_0 r(x) = \phi(\theta)\frac{e^{i|k||x|}}{|x|} + K(x), \qquad \theta := \frac{x}{|x|}, \qquad |x| > 1. \tag{7.2}$$

Here, the amplitude $\phi \in C^2(S)$, and

$$\phi(\theta) = \frac{1}{2\pi}\hat{r}(|k|\theta), \quad |\theta| = 1. \tag{7.3}$$

The remainder admits the bounds

$$|K(x)| \le C|x|^{-2}, \quad |\nabla K(x)| \le C|x|^{-2}, \quad |\nabla\nabla K(x)| \le C|x|^{-2}, \qquad |x| > 1. \tag{7.4}$$

Proof. First,

$$R_0 r(x) = \frac{e^{i|k||x|}}{2\pi|x|}\int e^{-i|k|\frac{x}{|x|}y} r(y)dy + \frac{1}{|x|}\int \frac{\langle y\rangle^2}{|x-y|}R(x,y)r(y)dy,$$

where the function $R(x,y)$ is bounded as in the proof of Lemma 3.2 from [3, Ch. 4]. Hence, formula (7.3) follows with $\phi \in C^2(S)$, since $\hat{r} \in \mathcal{H}^\sigma_2 \subset C^2_b(\mathbb{R}^3)$ for $\sigma > 7/2$ by the Sobolev embedding theorem.

To prove the first estimate of (7.4), it suffices to check that

$$J(x) := \int \frac{\langle y\rangle^2}{|x-y|}|r(y)|dy \le C|x|^{-1}, \qquad |x| > 1.$$

Using the Cauchy–Schwarz inequality, we obtain

$$|J(x)| \le \Big(\int \frac{1}{|x-y|^2\langle y\rangle^{2\sigma-4}}dy\Big)^{1/2}\|r\|_{\mathcal{L}^2_\sigma}.$$

Now it suffices to prove the bound

$$I(x) := \int \frac{1}{|x-y|^2\langle y\rangle^{2\sigma-4}}dy \le C|x|^{-2}, \qquad |x| > 1. \tag{7.5}$$

In the spherical coordinates, we obtain similarly to (4.17)–(4.19),

$$\begin{aligned}
I(x) &= 2\pi\int_0^\infty \frac{r^2 dr}{(1+r)^{2\sigma-4}}\int_0^\pi \frac{\sin\theta d\theta}{|x|^2 + r^2 - 2|x|r\cos\theta} \\
&= 2\pi|x|\int_0^\infty \frac{sds}{(1+s|x|)^{2\sigma-4}}\log\frac{|1+s|}{|1-s|} \\
&\le C\int_0^{1/2} \frac{|x|s^2 ds}{(1+s|x|)^{2\sigma-4}} + C|x|^{5-2\sigma} + C\int_{3/2}^\infty \frac{|x|ds}{(1+s|x|)^{2\sigma-4}} \\
&= C|x|^{-2}\int_0^{|x|/2} \frac{r^2 dr}{(1+r)^{2\sigma-4}} + C|x|^{5-2\sigma} + C\int_{3|x|/2}^\infty \frac{dr}{(1+r)^{2\sigma-4}} \\
&\le C_1(\sigma)|x|^{-2} + C_2|x|^{5-2\sigma} \le C|x|^{-2}, \qquad |x| > 1,
\end{aligned}$$

since $2\sigma > 7$. This proves the first bound in (7.4).

To prove the second bound in (7.4), we differentiate (7.2):

$$\nabla R_0 r(x) = \phi(\theta) i|k|\theta \frac{e^{i|k||x|}}{|x|} + \mathcal{O}(|x|^{-2}) + \nabla K(x), \qquad |x| \to \infty. \tag{7.6}$$

On the other hand, $\nabla R_0 r(x) = R_0 \nabla r(x)$, where $\nabla r \in \mathcal{H}^1_\sigma$. Hence, by the above arguments,

$$\nabla R_0 r(x) = \phi_1(\theta) \frac{e^{i|k||x|}}{|x|} + \mathcal{O}(|x|^{-2}), \qquad |x| \to \infty, \tag{7.7}$$

where

$$\phi_1(\theta) = \frac{1}{2\pi} \widehat{\nabla r}(|k|\theta) = \frac{1}{2\pi} i|k|\theta \hat{r}(|k|\theta) = i|k|\theta\phi(\theta).$$

So, the second bound in (7.4) follows by comparing (7.6) and (7.7).

The last bound of (7.4) follows similarly. □

Now asymptotics of type (1.13) follow from (7.1) and the next lemma, which is a refinement of Theorem 3.2 from [3, Ch. 4]. Let us denote $e_k(x) = e^{ikx}$.

Lemma 7.3. *Let condition* H3 *hold and let* $k \neq 0$. *Then*

$$-[RVe_k](x) = a(k,\theta) \frac{e^{i|k||x|}}{|x|} + K_1(x), \qquad \theta := \frac{x}{|x|}, \qquad |x| > 1. \tag{7.8}$$

The amplitude $a(k,\cdot) \in C^2(S)$ *is given by* (1.16), *and the remainder admits the bound*

$$|K_1(x)| + |\nabla K_1(x)| + |\nabla\nabla K_1(x)| \le C|x|^{-2}, \qquad |x| > 1. \tag{7.9}$$

Proof. First, $RV = R_0 T$, where $T := T(E_k + i0)$ (see (3.31) of [3, Ch. 4], and [22]). Hence,

$$-[RVe_k](x) = -[R_0 T e_k](x). \tag{7.10}$$

Therefore, (7.8)–(7.9) will follow from Lemma 7.2 if we verify that

$$Te_k \in \mathcal{H}^2_\sigma, \qquad \forall \sigma < 7/2 + \varepsilon_2/2. \tag{7.11}$$

Indeed,

$$Te_k = Ve_k - VRVe_k,$$

where $Ve_k \in \mathcal{H}^2_\sigma$ with any $\sigma < 7/2 + \varepsilon_2/2$ by H3. Hence, $RVe_k \in \mathcal{H}^2_s$ with any $s < -1/2$ by Corollary 19.3 of [15], since $k \neq 0$. Therefore, $VRVe_k \in \mathcal{H}^2_\sigma$ with any $\sigma < 9/2 + \varepsilon_2$ by H3.

Finally, applying Lemma 7.2 to the function $r(x) = Te^{ikx}$ and using (7.10), we obtain asymptotics (7.8)–(7.9) with the amplitude given by (1.16):

$$a(k,\theta) = -\frac{1}{2\pi}\hat{r}(|k|\theta) = -\frac{1}{2\pi}(Te_k, e_{|k|\theta}) = -4\pi^2 T(|k|\theta, k) \tag{7.12}$$

according to (1.8). □

Remark 7.4. Formula (1.16) for the amplitude in (7.8) is well known, see formula (97a) of [19]. On the other hand, the asymptotics (7.9) and the fact that $a(k,\cdot) \in C^2(S)$ are new, to our knowledge, and play the key role in the next section.

8. Differential cross section

Now we can justify formula (1.15). Lemma 3.1, Proposition 5.1, and the formula (7.1) imply the asymptotics of the limiting amplitudes,

$$\varphi_D(x,t)/b_D(n) \sim \mathcal{A}(x,t) = A(x)e^{-iE_k t} + \Sigma(x,t)$$
$$= [e^{ikx} + a^{\rm sc}(x)]e^{-iE_k t} + \Sigma(x,t), \quad D \to \infty. \tag{8.1}$$

Here, the amplitude $a^{\rm sc}(x) = -[RVe_k](x)$ decays at infinity together with its derivatives according to (7.8)–(7.9). Further, $\Sigma(x,t) = \sum C^l \psi_l(x) e^{-iE^l t}/b_D(n)$, and the asymptotics holds in $\mathcal{H}^s_{-\sigma}$ with any $s < 2$ and $\sigma > 5/2$. We will neglect the term $\Sigma(x,t)$ below since it does not contribute to the cross section, because

$$\int\limits_{|x|=R} [|\Sigma(x,t)|^2 + |\nabla\Sigma(x,t)|^2]dx \le C_N R^{-N}, \qquad \forall N > 0. \tag{8.2}$$

This follows by the Sobolev theorem on traces from the fact that $\psi_l(x) \in \mathcal{H}^2_s$ with any $s \in \mathbb{R}$ by Agmon's theorem [1, Theorem 3.3].

Let us denote by $j_\infty(x,t)$ the asymptotics of fluxes (1.4) corresponding to $\varphi_D(x,t)$ as $D \to \infty$. It can be "measured" in the double limit: first, $t \to \infty$, and then $D \to \infty$. The asymptotics (8.1) implies that $j_\infty(x,t)$ coincides with the flux corresponding to the wave field $\psi(x,t) := |b(n)|\mathcal{A}(x,t)$. Further, let us denote by $j^{\rm in}(x)$, $j^{\rm sc}(x)$ the incident and scattered fluxes defined by (1.20).

Finally, we should adjust the definition of $j^{\rm in}$ and $j^{\rm sc}_a$. First, the incident flux is defined in the following integral sense:

$$\int\limits_{|y-x|<1} |j_\infty(y,t) - j^{\rm in}|dy \to 0, \qquad |x| \to \infty, \qquad t \in \mathbb{R}. \tag{8.3}$$

Second, the angular density of the scattered flux is defined in the sense of distributions.

Definition 8.1. The limit (1.2) means that

$$R^2 \int\limits_S \phi(\theta) j^{\rm sc}(R\theta,t)\theta\, d\theta \to \int\limits_S \phi(\theta) j^{\rm sc}_a(\theta) d\theta, \qquad R \to \infty \tag{8.4}$$

for any test function $\phi \in C^\infty(S)$ with $\phi(\theta) = 0$ in a neighborhood of $\theta = \pm n$.

In other words, the limit (1.2) is understood in the sense of distributions on $S\setminus\{n,-n\}$. The test function ϕ physically corresponds to the "shape" (characteristic function) of a detector.

The main result of our paper is the following theorem.

Theorem 8.2. *Let all assumptions* H0–H4 *hold. Then for* $\theta \ne \pm n$

$$j^{\rm in} = |b(n)|^2 k, \qquad j^{\rm sc}_a(\theta) = |b(n)|^2 |a(k,\theta)|^2 |k|. \tag{8.5}$$

Proof. Using (8.1) and the definition (1.4), we obtain

$$\begin{aligned} j_\infty(x,t) &= |b(n)|^2\,\mathrm{Im}[\overline{\mathcal{A}(x,t)}\nabla\mathcal{A}(x,t)] \\ &= |b(n)|^2\,\mathrm{Im}[(\overline{e^{ikx}+a^{\mathrm{sc}}(x)})\nabla(e^{ikx}+a^{\mathrm{sc}}(x))]+j_\Sigma(x,t), \end{aligned} \tag{8.6}$$

where $j_\Sigma(x,t)$ denotes the terms containing $\Sigma(x,t)$ and its first derivatives in x. Here, the amplitude $a^{\mathrm{sc}}(x) = -RVe_k$ decays at infinity together with its derivatives according to (7.8)–(7.9). Hence, (8.2) implies that the flux (8.6) converges to $|b(n)|^2 k$ for large $|x|$ in the sense (8.3), which proves the first formula of (8.5).

It remains to prove the second formula of (8.5) neglecting $j_\Sigma(x,t)$. According to definition (8.4), we should check that for any test function $\phi \in C^\infty(S)$ with $\phi(\theta) = 0$ in a neighborhood of $\theta = \pm n$,

$$\begin{aligned} &R^2\int_S \phi(\theta)\,\mathrm{Im}[e^{-ikR\theta}\nabla a^{\mathrm{sc}}(R\theta)+\overline{a^{\mathrm{sc}}(R\theta)}ike^{ikR\theta}+\overline{a^{\mathrm{sc}}(R\theta)}\nabla a^{\mathrm{sc}}(R\theta)]\theta\,d\theta \\ &\to \int_S \phi(\theta)|a(k,\theta)|^2|k|d\theta, \qquad R\to\infty. \end{aligned} \tag{8.7}$$

Here,

$$\overline{a^{\mathrm{sc}}(R\theta)}\nabla a^{\mathrm{sc}}(R\theta)\theta = |a(k,\theta)|^2|k|R^{-2}+\mathcal{O}(R^{-3}) \tag{8.8}$$

by Lemma 7.3. Hence, it remains to prove that the oscillatory integrals in (8.7) vanish in the limit $R\to\infty$. This follows by the partial integration in view of Lemma 7.3, since the phase functions do not have stationary points outside $\theta = \pm n$. Indeed, let us consider, for example, the oscillatory integral

$$\begin{aligned} R^2\int_S \phi(\theta)e^{-ikR\theta}\nabla a^{\mathrm{sc}}(R\theta)\theta\,d\theta &= R^2\int_S \phi(\theta)e^{-ikR\theta}\nabla[a(k,\theta)\frac{e^{i|k|R}}{R}+K_1(R\theta)]\theta\,d\theta \\ &= R^2\int_S \phi(\theta)e^{-ikR\theta}[a(k,\theta)\frac{i|k|\theta e^{i|k|R}}{R}-a(k,\theta)\frac{e^{i|k|R}}{R^2}\theta \\ &\quad +\nabla a(k,\theta)\frac{e^{i|k|R}}{R}+\nabla K_1(R\theta)]\theta\,d\theta. \end{aligned} \tag{8.9}$$

Here, the phase functions $kR\theta$ and $kR\theta - |k|R$ admit exactly two stationary points $\theta = \pm n$ on the sphere S. Hence, the decay for each integral in the last line of (8.9) follows by the partial integration. The integrals with $a(k,\theta)$ vanish in the limit $R\to\infty$, since $a(k,\cdot)\in C^2(\mathbb{R}^3)$: the first integral vanishes by twofold partial integration, while the second and the third ones, by the single partial integration. The integral with ∇K_1 vanishes in the limit $R\to\infty$ by the single partial integration due to (7.9). □

Corollary 8.3. *According to (8.5), the differential cross section in the limit $D\to\infty$ is given by*

$$\sigma(\theta) := j^{\mathrm{sc}}_a(\theta)/|j^{\mathrm{in}}| = |a(k,\theta)|^2, \qquad \theta \neq \pm n$$

which justifies (1.15). Then (1.7) also holds by the known formula (1.16).

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