On Dynamical Justification of Quantum Scattering Cross Section

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Abstract

We give a dynamical justification of a differential cross section for the Schrödinger equation in the context of long time transition to stationary regime. Our approach is based on spherical incident waves, produced by a harmonic source, and uniform long-range asymptotics for the corresponding spherical limiting amplitudes. The main result is the convergence of the spherical limiting amplitudes to a limit as the source is moving to infinity. The main technical ingredients are the Agmon-Jensen-Kato analytical theory of the Green function and the Ikebe uniqueness theorem for the Lippmann-Schwinger equation.

Keywords: Schrödinger equation, scattering, differential cross section, scattering operator, limiting amplitude principle, spherical waves, plane waves, Lippman-Schwinger equation.

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1 Introduction

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

$$\sigma(\theta) = \frac{j_{a}^{sc}(\theta)}{|j_{in}|}.$$  \hspace{1cm} (1.1)

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

$$j_{a}^{sc}(\theta) = \lim_{R \to \infty} R^2 j^{sc}(R\theta) \cdot \theta,$$  \hspace{1cm} (1.2)

where $j^{sc}(x)$ denotes the scattered stationary flux (see Fig. 1).

In both scattering processes, the differential cross section is well-established in the framework of the corresponding dynamical equations: the Maxwell equations in the case of the Rayleigh scattering and the Newton equations in the case of the Rutherford scattering. On the other hand, a satisfactory justification of the quantum scattering cross section is missing.

Our goal is to complete the theory of the quantum differential cross section in the framework of the Schrödinger equation,

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

The corresponding charge and flux densities are defined as

$$\rho(x, t) = |\psi(x, t)|^2, \quad j(x, t) = \text{Im} \left[\psi(x, t)\nabla \psi(x, t)\right].$$  \hspace{1cm} (1.4)

The densities satisfy the charge continuity equation (see [23])

$$\dot{\rho}(x, t) + \text{div} j(x, t) = 0, \quad (x, t) \in \mathbb{R}^4.$$  \hspace{1cm} (1.5)

We justify the formula for the differential cross section

$$\sigma(k, \theta) = 16\pi^4 |T(|k|\theta, k)|^2,$$  \hspace{1cm} (1.6)

which is universally recognized in physical and mathematical literature: see, for example, [13, 19, 21, 23, 27]. Here $k \in \mathbb{R}^3$ is the "wave vector" of the incident plane wave $e^{ikx}$ and the $T$-matrix is given by

$$T(k', k) := \frac{1}{(2\pi)^3} \left( T(E_k + i0)e^{ikx}, e^{ik'x} \right), \quad k', k \in \mathbb{R}^3.$$  \hspace{1cm} (1.7)
which is the integral kernel of the operator \( T(E_k + i0) := V - V R(E_k + i0)V \) in the Fourier transform and \( E_k = \frac{1}{2}k^2 \). It is well known that the \( T \)-matrix allows us to express the integral kernel \( S(k', k) \) of the scattering operator \( S \) in the Fourier transform, see \([3, 19, 21, 24]\):

\[
S(k', k) = \delta(k' - k) - i\pi \delta(E_{k'} - E_k)T(k', k), \quad k', k \in \mathbb{R}^3.
\] (1.8)

The problem of dynamical justification of the differential cross section is suggested by the discussion in \([21\text{ pp. 355–357}]\). Namely, the commonly used ”naive scattering theory” consists of the following statements \([21, 23, 24]\):

I. The incident wave is identified with the plane wave

\[
\psi_{in}(x, t) = e^{i(kx - E_k t)}, \quad k \in \mathbb{R}^3.
\] (1.9)

The wave 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 solution “intuitively” is identified as the long time asymptotics

\[
\psi(x, t) \sim A(x)e^{-iE_k t}, \quad t \to \infty,
\] (1.10)

where the amplitude \( A(x) \) is expressed by

\[
A(x) = e^{ikx} - R(E_k + i0)[V(x)e^{ikx}].
\] (1.11)

This amplitude admits the following “spherical” long range asymptotics \([3\text{ p. 279, formula (3.58)}]\)

\[
A(x) \sim e^{ikx} + a(k, \theta)\frac{e^{i[k|x|}(|x|}}{|x|}, \quad |x| \to \infty, \quad \theta := x/|x|;
\] (1.12)

see Fig. 2.
III. By (1.4), asymptotics (1.12) give

$$j^\text{in} = k , \quad j^\text{sc}_a(\theta) = |a(k, \theta)|^2 |k| ,$$

and hence the differential cross section reads

$$\sigma(k, \theta) = |a(k, \theta)|^2 .$$

It is well-known that $a(k, \theta)$ is proportional to the $T$-matrix [21, formula (97a)],

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

Hence, (1.14) reads as (1.6).

A heuristic derivation of relations (1.10), (1.11) can be found in [21, pp. 355–357]. However, a mathematically consistent treatment of the relations in a time dependent picture was not proved until now. Moreover, relation (1.6) is considered as a definition of the differential cross section: see [13, formulas (1.2), (A.1.6)], [21, formula (96)], and [28, Definition 7.9 on p. 254].

The main problem is mathematical justification of (1.10) and (1.11) is related to the lack of a mathematical model for incident wave $\psi^\text{in}(x, t)$ which would provide convergence (1.10) to a stationary regime, and at the same time satisfy the “adiabatic condition”

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

which corresponds to the spirit of scattering theory. The plane incident wave (1.9) in the “naive scattering theory” does not satisfy (1.16) since the wave occupies the entire space. The plane wave is a solution to the free Schrödinger equation

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

Adiabatic condition (1.16) in acoustic scattering is provided by the “semi-infinite” incident plane wave

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

for $t < 0$, where $\Theta$ is the Heaviside function. The incident wave is a solution to the acoustic equation

$$\ddot{\psi}(x, t) = \Delta \psi(x, t) , \quad x \in \mathbb{R}^3 \setminus B ,$$

for $t < -D$ if the scatterer $B$ is located in the region $|x| \leq D$. 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 could fix $R \gg |k|D$ and take the semi-infinite plane wave

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

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 the great importance also in the context of quantum field theory, where the incident and outgoing plane waves play the fundamental role [19, 22, 23, 27].
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 be an asymptotically free plane wave if the source is "monochromatic" and distant from the scatterer. This model corresponds obviously to spherical incident waves, which are standard devices in optical and acoustic scattering [4]. We justify relations (1.10), (1.11), and (1.13), (1.14) in the following steps:

A. First, we prove a limiting amplitude principle for the harmonic source, i.e., long time convergence to a stationary harmonic regime with a "spherical limit amplitude", which does not depend on initial state.

B. Second, we prove the convergence of the spherical limit amplitudes to a plane limit amplitude when the source goes to infinity: \( D \to \infty \).

Convergences A and B imply that relations (1.10), (1.11), and (1.13), (1.14) hold true in this double limit: first \( t \to \infty \) and then \( D \to \infty \).

Let us comment on our techniques. We use Agmon-Jensen-Kato theory of the resolvent (or the Green function) [1, 16] to prove the limiting amplitude principle, uniform bounds and long range asymptotics for the spherical limiting amplitudes. The proof of convergence B relies on an application of the Ikebe Uniqueness Theorem for the Lippmann-Schwinger equation. We refine the known estimates [3, Lemma 3.2 in Chapter 4] for the derivatives of the remainder in asymptotics (1.12).

Note that the flux in our approach is given by the second formula (1.4). It describes the wave flux in the one-particle Schrödinger equation (1.3). Respectively, a many-particle interpretation of cross section (1.5) is not straightforward. An alternative approach is based on a stationary random process for an infinite number of particles modeled as normalized wave packets [8, 10, 26]. It is instructive to note that both approaches give the same expression for the differential cross section. One could expect that a unified approach, combining both a stationary nonrandom flux with a many-particle interpretation, should be developed for the second quantized models [5].

Let us comment on the known arguments for formula (1.6). In the physical literature the formula is usually justified by squaring the Dirac delta function and the subsequent physical interpretation of arising divergence; see, e.g., [19, 22, 23, 27]. Another physical approach [24] is based on random incident wave packets \( \psi^{in}(x, 0) \) which are asymptotically proportional to the plane waves \( e^{ikx} \):

\[
|\hat{\psi}^{in}(k', 0)|^2 \to \delta(k' - k) .
\]  

(1.19)

The known mathematical justifications rely on Dollard’s fundamental result [7] on scattering into cones. For example, Dollard’s result is used in [26] for a clarifying treatment of formula (1.6). Namely, the normalized angular distribution of a finite charge, scattered for infinite time, converges to the normalized function (1.6) in limit (1.19).

There are also mathematical justifications of the approach [24]. Namely, Dollard’s result was refined in [6, 15] and [2, Section 3-3], where the flux across the surface theorem is proved. This result was later developed in [8, 9, 11, 25] and applied for a justification of formula (1.6) in context of the Bohmian particle mechanics and incident stationary random processes constructed of normalized wave packets (1.6) in limit (1.19). The survey can be found in [10].
Let us stress that previous results do not concern the long time transition to a stationary regime. Moreover, we do not exclude the discrete spectrum of the Schrödinger operator $H$ in contrast to [8].

Our paper is organized as follows. In Section 2 we state the main results. In Section 3 we establish the limiting amplitude principle. In Section 4 we obtain long range asymptotics and uniform bounds for the limit spherical amplitudes. In the next two sections we prove convergence B and the corresponding convergence for the flux. Finally, in Section 8 we check formulas (1.15) and (1.13), which justifies (1.14) and (1.6).

## 2 Main results

We consider the Schrödinger equation with the harmonic source:

$$
\begin{cases}
    i\dot{\psi}(x,t) = H\psi(x,t) - \rho_q(x)e^{-iE_k t}, & t > 0 \\
    \psi(x,0) = \psi_0(x)
\end{cases} \quad x \in \mathbb{R}^3. \tag{2.1}
$$

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

Let us define weighted Agmon-Sobolev spaces $H^s_\sigma = H^s_\sigma(\mathbb{R}^3)$ with $s, \sigma \in \mathbb{R}$.

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

$$
\|\psi\|_{H^s_\sigma} := \|\langle \nabla \rangle^s \psi(x)\|_{L^2_\sigma} < \infty. \tag{2.2}
$$

We will assume the following conditions.

**H0.** The initial state $\psi_0$ is a function from the space $H^0_{\sigma_0}$ with some $\sigma_0 > 5/2$.

**H1.** For some $\varepsilon' > 0$

$$
\sup_{x \in \mathbb{R}^3} \langle x \rangle^{4+\varepsilon'} |\rho(x)| < \infty. \tag{2.3}
$$

**H2.** The following Wiener condition holds:

$$
\hat{\rho}(|k|\theta) := \int e^{i|k|\theta x} \rho(x)dx \neq 0, \quad \theta \in \mathbb{R}^3, \quad |\theta| = 1. \tag{2.4}
$$

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

$$
\sup_{x \in \mathbb{R}^3} \langle x \rangle^{5+\varepsilon} |\partial^\alpha V(x)| < \infty, \quad |\alpha| \leq 2, \tag{2.5}
$$

with some $\varepsilon > 0$.

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 $R_0(\omega) := (-\frac{1}{2}\Delta - \omega)^{-1}$ is the free resolvent. The space $\mathcal{M}_\sigma = \mathcal{M}$ does not depend on $\sigma \in (1/2, (5 + \varepsilon)/2)$ by the arguments before Lemma 3.1 in [16].
H4. We assume:

\[ \textbf{Spectral Condition} : \quad \mathcal{M} = 0 . \]  

(2.6)

The condition holds \textit{generically}, see the discussion before Lemma 3.1 in [16].

Let us outline our plan.

\textbf{I.} First we will prove the \textit{limiting amplitude principle}:

\[ \psi(x, t) \sim \varphi_q(x, t) = B_q(x)e^{-iE_k t} + \sum_{l=1}^{N} C_l \psi_l(x) e^{-i\omega_l t} , \quad t \to \infty , \]  

(2.7)

where \( \psi_l(x) \) denote the eigenfunctions of \( H \) corresponding to the eigenvalues \( \omega_l < 0 \). The asymptotics hold in \( H^{2-\sigma} \) with \( \sigma > 5/2 \), and the \textit{limit amplitude} \( B_q(x) \) is given by

\[ B_q(x) = R(E_k + i0) \rho_q , \]  

(2.8)

where \( R(\omega) := (H - \omega)^{-1} \) is the resolvent of the Schrödinger operator \( H \).

The coefficients \( C_l \) depend on the initial state \( \psi(x, 0) \). On the other hand, it is crucially important that the coefficients \( C_l \) \textit{do not depend on} \( q \) in the limit \( |q| \to \infty \), while the eigenvectors \( \psi_l(x) \) rapidly decay at infinity by Agmon Theorem [1, Theorem 3.3]. Hence, the sum over the discrete spectrum on the RHS of (2.7) does not contribute to the scattering cross section.

\textbf{II.} Second, we denote \( B_D(x) := B_{qD}(x) \), where \( q_D = -nD \) with \( n = k/|k| \) and \( D > 0 \), and establish the following \textit{“spherical version”} of long range asymptotics (1.12):

\[ B_D(x) \sim b_D(n) \left[ \frac{|qD|}{|x - qD|} e^{i|k||x - qD| - |qD|}} + a_D(k, \theta) \frac{e^{i(k|\theta|)}}{|x|} \right] \]

as \( |x - qD| \to \infty , \quad |x| \to \infty \),

(2.9)

where \( \theta := x/|x| \) and \( b_D(n) := b(n) e^{i(k|\theta|D)} \) with \( b(n) \neq 0 \); see Fig. 3.

\textbf{III.} Further, we prove the long range convergence of the spherical limit amplitudes, which is our central result: for \( k \neq 0 \)

\[ A_D(x) := B_D(x)/b_D(n) \to A(x) , \quad D \to \infty , \]  

(2.10)

where \( A(x) \) is expressed by (1.11).

\textbf{IV.} At last, (2.10) implies the convergence of the corresponding \textit{limit solutions} \( \varphi_D(x, t) := \varphi_{qD}(x, t) \),

\[ \varphi_D(x, t)/b_D(n) \to A(x)e^{-iE_k t} , \quad D \to \infty , \quad (x, t) \in \mathbb{R}^4 , \]  

(2.11)

and of the corresponding flux (1.4):

\[ j_D(x) = \text{Im} [\varphi_D(x, t) \nabla \varphi_D(x, t)] \to j_\infty(x) = |b(n)|^2 \text{Im} [A(x) \nabla A(x)] \quad D \to \infty \]

(2.12)

\textbf{V.} Finally, we show that convergence (2.12) and formula (1.11) justify (1.1), (1.6) in the limit \( D \to \infty \).
We establish long range asymptotics (2.9) using a "spherical version" of the Lippmann-Schwinger equation and applying Lemma 3.2 from [3] together with the properties of the resolvent of the Schrödinger equation obtained in [16]. The asymptotics imply convergence (2.10) by a compactness argument and the Ikebe Theorem on the uniqueness of the solution to the Lippmann-Schwinger equation [3, 14] which holds under the condition \( k \neq 0 \). One of the key observations is that the spherical incident wave from (2.9) becomes the plane incident wave from (1.12) asymptotically when the source goes to infinity:

\[
\frac{|q_D|}{|x - q_D|} e^{i|k|(|x - q_D| - |q_D|)} \rightarrow e^{ikx}, \quad D \rightarrow \infty.
\]  

(2.13)

**Remark 2.2.** We suggest that our model of the incident wave suits the physics of quantum scattering. Namely, an incident electron beam is produced by a time periodic source like a heated cathode in an electron gun. The cathode is described by a density factor, and the source is not at infinity though its distance from the scatterer is sufficiently large.

### 3 Limiting amplitude principle

We deduce the limiting amplitude principle (2.7) from the dispersion decay in weighted energy norms established in [16].

**Lemma 3.1.** Let conditions H0–H4 hold and \( k \in \mathbb{R}^3 \). Then the limiting amplitude principle (2.7) holds in the norm of \( H^2_{-\sigma} \) with any \( \sigma > 5/2 \), where the coefficients \( C^t \) do not depend on \( q \) in the limit \( |q| \rightarrow \infty \), and the limit amplitude is given by (2.8).
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Proof. We should prove that

$$\psi(x,t) = B_q(x)e^{-iE_kt} + \sum_{l=1}^{N} C_l \psi_l(x)e^{-i\omega_l t} + r(x,t) \ ,$$  \hspace{1cm} (3.1)

where

$$\|r(\cdot,t)\|_{\mathcal{H}_2^\sigma} \to 0 \ , \quad t \to \infty \ .$$

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

$$\psi(t) = U(t)\psi_0 - i \int_0^t e^{-iE_k s}U(t-s)\rho_q \, ds \ .$$  \hspace{1cm} (3.2)

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

$$U(t)\psi_0 = \sum_{l=1}^{N} C_l^0 \psi_l e^{-i\omega_l t} + r_0(t) \ ,$$  \hspace{1cm} (3.3)

where $C_l^0$ do not depend on $q$ and

$$\|r_0(t)\|_{\mathcal{H}_2^\sigma} \leq C \langle t \rangle^{-3/2}$$  \hspace{1cm} (3.4)

by the dispersion decay \cite{16} (10.9)], which holds in our case due to $H_0$ and $H_3$–$H_4$. On the other hand, the second term in the RHS of (3.2) can be written as

$$I(t) := \int_0^t e^{-iE_k s}U(t-s)\rho_q \, ds = e^{-iE_k t} \int_0^t e^{iE_k \tau} U(\tau)\rho_q d\tau \ ,$$  \hspace{1cm} (3.5)

where $\rho_q \in \mathcal{H}_0^{\sigma'}$ with some $\sigma' > 5/2$ by H1. Hence, similarly to (3.3) and (3.4),

$$U(\tau)\rho_q = \sum_{l=1}^{N} C_l^q \psi_l e^{-i\omega_l \tau} + r_q(\tau) \ ,$$  \hspace{1cm} (3.6)

where

$$C_l^q = \langle \rho_q, \psi_l \rangle = \mathcal{O}(\langle q \rangle^{-M}) \ , \quad |q| \to \infty \ ,$$  \hspace{1cm} (3.7)

for any $M > 0$ since the eigenfunctions rapidly decay at infinity. Finally,

$$\|r_q(\tau)\|_{\mathcal{H}_2^\sigma} \leq C \langle \tau \rangle^{-3/2} .$$  \hspace{1cm} (3.8)

Therefore,

$$I(t) \sim B_q(x)e^{-iE_k t} + \mathcal{O}(\langle q \rangle^{-M}) \ , \quad t \to \infty \ ,$$  \hspace{1cm} (3.9)

where the asymptotics hold in $\mathcal{H}_2^\sigma$. In particular, contribution of $I(t)$ into the coefficients $C_l^q$ vanishes in the limit $|q| \to \infty$. Now (3.1) follows from (3.2)–(3.9) with the limit amplitude

$$B_q(x) = -i \int_0^\infty e^{iE_k \tau}U(\tau)\rho_q d\tau = -i \int_0^\infty e^{i(E_k+i\delta)\tau}U(\tau)\rho_q d\tau .$$  \hspace{1cm} (3.10)

Finally, this integral can be written as (2.8). \hfill \square
4 Spherical waves

Here we obtain long range asymptotics (2.9). Denote \( R = R(E_k + i0) \) and \( R_0 = R_0(E_k + i0) \), where \( R_0(\omega) = (H_0 - \omega)^{-1} \) is the resolvent of the free Schrödinger operator \( H_0 = -\frac{1}{2}\Delta \). Let us rewrite formula (2.8) for the limit amplitude as the following “spherical version” of the Lippmann-Schwinger equation:

\[
B_q(x) = R_0\rho_q(x) - R_0VB_q(x) \tag{4.1}
\]

since \( R = R_0 - R_0VR \). The free Schrödinger resolvent \( R_0(\omega) = (H_0 - \omega)^{-1} \) is an integral operator with the kernel

\[
R_0(\omega, x, y) = \frac{e^{i\sqrt{2\omega|x-y|}}}{2\pi|x-y|}, \quad \omega \in \mathbb{C} \setminus [0, \infty).
\]

Hence, \( R_0 \) is the integral operator with the kernel

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

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

For the first term on the right-hand side of (4.1) asymptotics (2.9) follows by Lemma 3.2 from [3, Chapter 4]:

**Lemma 4.1.** Under condition H1 the asymptotics

\[
R_0\rho_q(x) = b\left(\frac{x - q}{|x - q|}\right)\frac{|q|}{1 + |x - q|}e^{i|k||x - q|} + K(x - q), \quad x \in \mathbb{R}^3, \tag{4.3}
\]

hold, where

\[
b(\theta) = \sqrt{2\pi\hat{\rho}(|k|\theta)}, \quad |\theta| = 1, \tag{4.4}
\]

\[
|K(x - q)| \leq C|q|(1 + |x - q|)^{-1-\varepsilon'}. \tag{4.5}
\]

As a corollary, we obtain the bound

\[
|R_0\rho_q(x)| \leq \frac{C|q|}{1 + |x - q|}, \quad x \in \mathbb{R}^3. \tag{4.6}
\]

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

**Lemma 4.2.** Under conditions H1 and H3 the following bound holds:

\[
\sup_{q \in \mathbb{R}^3} \|VB_q(x)\|_{L^2_\sigma} < \infty \quad \text{for any} \quad \sigma < 2.5 + \varepsilon. \tag{4.7}
\]

**Proof.** The Lippmann-Schwinger equation (4.1) implies

\[
(1 + VR_0)VB_q = -VR_0\rho_q. \tag{4.8}
\]
On the other hand, \((1 + VR_0)^{-1} = 1 - VR\). Hence,

\[
VB_q = -(1 - VR)VR_0\rho_q = -VR_0\rho_q + VRV_0\rho_q.
\] (4.9)

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

i) Condition (2.5) with \(\alpha = 0\) and bound (4.6) imply

\[
|VR_0\rho_q(x)| \leq \frac{C|q|}{(1 + |x - q|)(1 + |x|)^{4+\varepsilon}}, \quad x \in \mathbb{R}^3.
\] (4.10)

Therefore,

\[
|VR_0\rho_q(x)| \leq \frac{C}{(1 + |x|)^{4+\varepsilon}}, \quad x \in \mathbb{R}^3.
\] (4.11)

Hence,

\[
VR_0\rho_q \in L_2^2, \quad \sigma < 2.5 + \varepsilon.
\] (4.12)

Thus the bound (4.7) holds for the first term on the right-hand side of (4.9).

ii) It remains to estimate the last term of (4.9). By (4.12) we have \(RV_0\rho_q \in L_2^2 - \sigma_1\) for any \(\sigma_1 > 1/2\) since the resolvent \(R = R(E_k + i0) : L_2^{\sigma_1} \to L_2^{-\sigma_1}\) is continuous by [16, Theorem 9.2] because \(E_k > 0\). Therefore, \(VRV_0\rho_q \in L_2^2\) for \(\sigma < 4.5 + \varepsilon\) by (2.5) with \(\alpha = 0\).

**Lemma 4.3.** Under conditions H1 and H3 the following uniform decay holds:

\[
\sup_{q \in \mathbb{R}^3} |R_0VB_q(x)| \leq C(1 + |x|)^{-2}, \quad x \in \mathbb{R}^3.
\] (4.13)

**Proof.** We adopt the arguments from the proof of Lemma 3.2 in [3, p. 275]. Namely,

\[
|R_0VB_q(x)| \leq C \int \frac{|VB_q(y)|}{|x - y|} dy
\]

\[
= C \int_0^{\infty} \left[ \int \frac{|VB_q(r, \varphi, \theta)| d\varphi \sin \theta d\theta}{\sqrt{|x|^2 + r^2 - 2|x|r \cos \theta}} \right] r^2 dr.
\] (4.14)

by (4.12). Applying the Cauchy-Schwarz inequality to the inner integral, we obtain

\[
|R_0VB_q(x)|
\leq C \int_0^{\infty} \left[ \int |VB_q(r, \varphi, \theta)|^2 d\varphi \sin \theta d\theta \right]^{\frac{1}{2}} \left[ \int \frac{d\varphi \sin \theta d\theta}{|x|^2 + r^2 - 2|x|r \cos \theta} \right]^{\frac{1}{2}} r^2 dr
\]

\[
= C \int_0^{\infty} \left[ \int |VB_q(r, \varphi, \theta)|^2 d\varphi \sin \theta d\theta \right]^{\frac{1}{2}} \left[ \frac{1}{|x|r} \log \frac{|x| + r}{|x| - r} \right]^{\frac{1}{2}} r^2 dr.
\] (4.15)
Applying the same inequality to the last integral, we obtain

\[
|R_0 VB_q(x)| \leq C \left[ \int \frac{(1 + r)^{2\sigma} |VB_q(r, \varphi, \theta)|^2 d\varphi \sin \theta dr r^2 dr}{|x|\left|\frac{r}{1 + r}\right|} \right]^{1/2} \times \left[ \int_0^\infty \log \frac{|x| + r}{|x| - r} \frac{r^2 dr}{|x| (1 + r)^{2\sigma}} \right]^{1/2} \\
\leq C(\sigma) \left[ \int_0^\infty \log \frac{|x| + r}{|x| - r} \frac{r dr}{|x| (1 + r)^{2\sigma}} \right]^{1/2} \\
= C(\sigma) \left[ \int_0^\infty \log \frac{1 + s}{1 - s} \frac{|x|ds}{(1 + s|x|)^{2\sigma}} \right]^{1/2} 
\]

by the uniform bound (4.7). Splitting the region of integration

\((0, \infty) = (0, 1/2) \cup (1/2, 3/2) \cup (3/2, \infty)\),

we estimate the last integral by

\[
C_1(\sigma) \left[ \int_0^{1/2} \frac{|x|s^2 ds}{(1 + s|x|)^{2\sigma}} + (1 + |x|)^{1-2\sigma} + \int_{3/2}^\infty \frac{|x|ds}{(1 + s|x|)^{2\sigma}} \right] \\
= C_1(\sigma) \left| x \right|^{-2} \left[ \int_0^{|x|/2} \frac{r^2 dr}{(1 + r)^{2\sigma}} + (1 + |x|)^{1-2\sigma} + \int_{3|x|/2}^\infty \frac{dr}{(1 + r)^{2\sigma}} \right] \\
\leq C_2(\sigma)(1 + |x|)^{1-2\sigma}
\]

if \(3 - 2\sigma < 0\). Hence, (4.13) follows since we can take any \(\sigma < 2.5 + \varepsilon\) by (4.7).

Now we are ready to prove (2.9).

**Proposition 4.4.** Asymptotics (2.9) hold under conditions H1–H3.

**Proof.** The Lippmann-Schwinger equation (4.1) yields

\[ VB_q(x) = -VR_0 \rho_q(x) - VR_0 VB_q(x) \, . \]

Hence, (2.5) with \(\alpha = 0\) and (4.11), (4.13) imply

\[
|VB_q(x)| \leq \frac{C}{(1 + |x|)^{4+\varepsilon}}. \quad (4.16)
\]

Therefore, similarly to (4.13), we obtain the asymptotics

\[
R_0 VB_q(x) = c_q \left( \frac{x}{|x|} \right) \frac{e^{ik|x|}}{1 + |x|} + L_q(x) \, , \quad (4.17)
\]
where

\[ |L_q(x)| \leq C(1 + |x|)^{-1-\varepsilon}. \]  

(4.18)

Now (4.1) and (4.3), (4.17) imply

\[ B_q(x) \sim b \left( \frac{x - q}{|x - q|} \right) \frac{|q|}{|x - q|} e^{i|k||x - q|} + c_q \left( \frac{x}{|x|} \right) e^{i|k||x|} \]  

(4.19)

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

\[ B_D(x) \sim b(n) \left[ \frac{|qD|}{|x - qD|} e^{i|k||x - qD|} + d_D(k, \theta) e^{i|k||x|} \right] \]  

(4.20)

as \(|x - qD| \to \infty\) and \(|x| \to \infty\), where \(\theta := x/|x|\) since \(b(n) \sim \hat{\rho}(|k|n) \neq 0\) by (4.4) and the Wiener condition \(H2\). This is the unique point in our proofs, where the Wiener condition is needed. Finally, (4.20) can be written as (2.20) with \(b_D(n) := b(n)e^{i|k|nD}\) and \(a_D(k, \theta) = d_D(k, \theta)e^{-i|k|D}\). □

**Corollary 4.5.** Bound (1.6), asymptotics (4.17), and formula (4.1) imply

\[ |B_q(x)| \leq \frac{C|q|}{1 + |x - q|} + \frac{C}{(1 + |x|)}, \quad x, q \in \mathbb{R}^3. \]  

(4.21)

## 5 Plane wave limit

Here we obtain convergence (2.10) from the uniqueness of solution to the Lippmann-Schwinger equation

\[ A(x) = e^{ikx} - R_0VA(x), \]  

(5.1)

which is equivalent to (1.11) (see Lemma 7.1 below). First, rewrite (4.1) with \(q = qD\) as

\[ A_D(x) = R_0\rho_{qD}(x)/b_D(n) - R_0VA_D(x), \]  

(5.2)

where \(A_D(x) := B_D(x)/b_D(n)\). Then the first term on the right-hand side of (5.2) converges to the first term on the right-hand side of (5.1):

\[ R_0\rho_{qD}(x)/b_D(n) \to e^{ikx}, \quad D \to \infty, \]  

(5.3)

in \(C(\mathbb{R}^3)\) due to (1.3) and (2.13).

It remains to prove the convergence of the corresponding solutions:

**Proposition 5.1.** Let conditions H1–H3 hold and \(k \neq 0\). Then

\[ A_D(x) \to A(x), \quad D \to \infty, \]  

(5.4)

in \(H^{s}_{-\sigma}\) with any \(s < 2\) and \(\sigma > 5/2\). The function \(A(x)\) is defined by (1.11).

**Proof.** We deduce the convergence from the compactness of the family \(\{A_D(x) : D > 0\}\) and the Ikebe Uniqueness Theorem [3, Theorem 3.1], which holds under the condition \(k \neq 0\).

**Step i** Formula (5.2) implies

\[ \|A_D\|_{H^2_{-\sigma}} \leq C\|R_0\rho_{qD}\|_{H^2_{-\sigma}} + \|R_0VB_D\|_{H^2_{-\sigma}}. \]
The first term on the right-hand side is uniformly bounded for $D > 0$ since estimates of type (4.10)–(4.11) hold with $\langle x \rangle^{-\sigma}$ instead of $V(x)$. The second term is uniformly bounded since $V B q$ is uniformly bounded in $L^2_\sigma$ with $\sigma < 5/2 + \varepsilon$ by (4.7) while the operator $R_0 : \mathcal{L}_\sigma^2 \to \mathcal{H}^2_{-\sigma}$ is continuous for $\sigma \in (1/2, 5/2 + \varepsilon)$. Indeed, $(-\frac{1}{2} \Delta - E_k)R_0 = I$, and hence the operator $(\frac{1}{2} \Delta + 1)R_0 = (I + E_k + 1)R_0 : \mathcal{L}_\sigma^2 \to \mathcal{L}^2_{-\sigma}$ is continuous by [16, Lemma 2.1]. Hence,

$$
sup_{D > 0} \|A_D\|_{\mathcal{H}^2_{-\sigma}} < \infty, \quad \sigma \in (5/2, 5/2 + \varepsilon). \tag{5.5}
$$

**Step ii)** Now the Sobolev Embedding Theorem [17] 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 $\sigma \in (5/2, 5/2 + \varepsilon)$. Hence, for any sequence $D_j \to \infty$ there is a subsequence $D_{j'} \to \infty$ such that

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

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

$$
V A_{D_{j'}}(x) \to VA_\ast(x), \quad j' \to \infty, \tag{5.7}
$$

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 the equation (5.1) for $A_\ast(x)$:

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

since the operator $R_0 := R_0(E_k + i0) : \mathcal{L}_\sigma^2 \to \mathcal{L}^2_{-\sigma}$ is continuous for $\sigma > 1/2$ by [16, Lemma 2.1].

The function $A_\ast(x)$ is bounded by (4.21), and continuous by the Sobolev Embedding Theorem since $A_\ast(x) \in \mathcal{H}^s_{-\sigma}$ with any $s < 2$ and $\sigma > 5/2$ by (5.6).

Finally, $A(x) = A_\ast(x)$ by the Ikebe Uniqueness Theorem [3, Theorem 3.1] for bounded continuous solutions to the Lippmann-Schwinger equation (5.1) under condition (2.3). Hence, convergence (5.6) implies (5.4) since the limit function $A_\ast(x)$ does not depend on the subsequence $j'$.

**Remark 5.2.** Let us emphasize that the right-hand side of (4.21) with $q = -nD$ is not uniformly bounded for $D > 0$: its value at $x = q$ tends to infinity as $D \to \infty$.

## 6 Convergence of flux

We check the convergence of the limit flux as the source goes to infinity. First we check (2.11) and (2.12) relying on (2.7) and (2.10).

**Lemma 6.1.** Under conditions H1 - H3 the long range convergence

$$
\varphi_D(x, t)/b_D(n) \to A(x)e^{-iE_k t}, \quad D \to \infty, \quad t \in \mathbb{R}, \tag{6.1}
$$

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


Proof. The convergence follows from Proposition 5.1 since
\[ \varphi_D(x, t)/b_D(n) = A_D(x)e^{-iE_k t} \] (6.2)
as \( t \to \infty \) by definition of \( \varphi_q(x, t) \) in (2.7) with \( q(D) = -nD \) (recall that we omit the sum over the discrete spectrum in (2.7)). Here \( |b_D(n)| \neq 0 \) by the Wiener condition (2.4).

Lemma 6.2. i) Convergence (2.12) holds:
\[ j_D(x) = \text{Im}[[\varphi_D(x, t)\nabla\varphi_D(x, t)]] \to j_\infty(x) = |b(n)|^2\text{Im}[A(x)\nabla A(x)] \] (6.3)
as \( D \to \infty \) in \( \mathcal{L}_{\text{loc}}^2(\mathbb{R}^3) \).

ii) Moreover, the convergence holds “in the sense of flux”, i.e.,
\[ \int_S j_D(x) \cdot \nu(x) dS(x) \to \int_S j_\infty(x) \cdot \nu(x) dS(x) , \quad D \to \infty , \quad t \in \mathbb{R} , \] (6.4)
for any compact smooth two-dimensional submanifold \( S \subset \mathbb{R}^3 \) with a boundary, where \( \nu(x) \) is the unit normal field to \( S \), and \( dS(x) \) stands for the corresponding Lebesgue measure on \( S \).

Proof. Convergence (6.1) also holds in \( C(\mathbb{R}^3) \) since \( \mathcal{H}_{\sigma}^s \subset C(\mathbb{R}^3) \) with \( s > 3/2 \) by the Sobolev Embedding Theorem [17]. Further, the convergence of the derivatives
\[ \nabla\varphi_D(x, t)/b_D(n) \to \nabla A(x)e^{-iE_k t} , \quad D \to \infty , \quad t \in \mathbb{R} , \] (6.5)
holds in \( \mathcal{H}_{\sigma}^{s-1} \) with any \( s < 2 \). Hence, convergence (6.3) holds in \( \mathcal{L}_{\text{loc}}^2(\mathbb{R}^3) \), and moreover,
\[ \nabla\varphi_D(x, t)/b_D(n) \big|_S \to \nabla A(x)e^{-iE_k t} \big|_S , \quad D \to \infty , \quad t \in \mathbb{R} , \] (6.6)
in \( \mathcal{L}^2(S) \) by Sobolev Trace Theorem [17] since we can take \( s - 1 > 1/2 \).

Therefore, the integrands in (6.4) converge in \( \mathcal{L}^2(S) \) by (6.3).

7 Long range asymptotics

We obtain asymptotics (1.12). The first lemma is well-known [24].

Lemma 7.1. Equation (5.1) admits a unique bounded continuous solution which is given by (1.11):
\[ A(x) = e^{ikx} - RV e^{ikx} \] (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 \( R_0 = R + RV R_0 \), and hence
\[ R_0 V A = RVA + RV R_0 VA = RV (A + R_0 VA) = RV e^{ikx} \]
by (5.1). Substituting into (5.1), we obtain (7.1).
Next we need a generalization of Lemma 4.1 to functions of weighted Agmon-Sobolev spaces.

**Lemma 7.2.** Let \( r(x) \in \mathcal{H}_2^2 \), where \( \sigma < 7/2 + \delta \) with a \( \delta > 0 \). Then

\[
R_0 r(x) = \phi(\theta) \frac{e^{i|k|x}}{|x|} + K(x) , \quad x \in \mathbb{R}^3 , \quad \theta := \frac{x}{|x|} ,
\]

(7.2)

where

\[
\phi(\theta) = \sqrt{2\pi} \hat{r}(|k|\theta) , \quad |\theta| = 1 ,
\]

and

\[
|K(x)| + |\nabla K(x)| \leq C|x|^{-2} .
\]

(7.4)

**Proof.** We adopt further the arguments from the proof of Lemma 3.2 in [3, p. 275]. First,

\[
R_0 r(x) = e^{i|k|x} \left( \frac{1}{2\pi |x|} \int e^{-i|k|y} r(y) dy + \frac{1}{|x|} \int \frac{\langle y \rangle^2}{|x - y|} B(x,y) r(y) dy \right) ,
\]

where the function \( B(x,y) \) is bounded. Hence, it remains to check that

\[
J(x) := \int \frac{\langle y \rangle^2}{|x - y|} |r(y)| dy \leq C|x|^{-1} .
\]

Using the Cauchy-Schwarz inequality, we obtain

\[
|J(x)| \leq \left( \int \frac{1}{|x - y|^2} \langle y \rangle^{2\sigma-4} dy \right)^{1/2} \| r \|_{L_2^\sigma} .
\]

Now it suffices to prove the bound

\[
I(x) := \int \frac{1}{|x - y|^2} \langle y \rangle^{2\sigma-4} dy \leq C|x|^{-2} .
\]

(7.5)

In the spherical coordinates, similarly to (4.16), we obtain

\[
I(x) = 2\pi \int_0^\infty \frac{r^2 dr}{(1 + r)^{2\sigma-4}} \int_0^\pi \frac{\sin \theta d\theta}{|x|^2 + r^2 + 2|x|r \cos \theta}
\]

\[
= 2\pi |x| \int_0^\infty \frac{\rho d\rho}{(1 + \rho|x|)^{2\sigma-4}} \log \frac{|1 + \rho|}{|1 - \rho|}
\]

\[
\leq C \int_0^{1/2} \frac{|x|^2 \rho^2 d\rho}{(1 + \rho|x|)^{2\sigma-4}} + C|x|^{5-2\sigma} + C \int_1^{\infty} \frac{|x| d\rho}{(1 + \rho|x|)^{2\sigma-4}}
\]

\[
= C|x|^{-2} \int_0^{1/2} \frac{r^2 dr}{(1 + r)^{2\sigma-4}} + C|x|^{5-2\sigma} + C \int_1^{\infty} \frac{dr}{(1 + r)^{2\sigma-4}}
\]

\[
\leq C_1(\sigma)|x|^{-2} + C_2|x|^{5-2\sigma}
\]
if $2\sigma > 7$. Hence, (7.5) holds since we can take any $\sigma < 7/2 + \delta$. Then the first bound in (7.4) follows. To prove the second bound, we differentiate (7.2):

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

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

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

where

$$\phi_1(\theta) = \sqrt{2\pi} \hat{\nabla} r(|k|\theta) = \sqrt{2\pi i|k|\theta} e^{i|k||x|}/|x| + \mathcal{O}(|x|^{-2}),$$

Hence, the second bound in (7.4) follows by comparison of (7.6) and (7.7).

Now asymptotics of type (1.12) follow from (7.1) and the next lemma, which is a modification of Theorem 3.2 from [3, Chapter 4].

**Lemma 7.3.** Let condition H3 hold. Then

$$-RV e^{ikx}(x) = a(k, \theta)e^{i|k||x|}/|x| + K_1(x), \quad |x| \to \infty,$$  \hfill (7.8)

where $\theta := x/|x|$, the amplitude $a(k, \theta)$ is given by (1.15), and

$$|K_1(x)| \leq C|x|^{-2}, \quad |
abla K_1(x)| \leq C|x|^{-2}.$$  \hfill (7.9)

**Proof.** First, $RV = R_0 T$, where $T := T(\omega + i0)$ (see [3, (3.31) of Chapter 4] and [24]); hence

$$-[RV e^{ikx}](x) = -[R_0 T e^{ikx}](x).$$  \hfill (7.10)

We cannot apply Lemma 4.1 directly to obtain asymptotics (7.8) for $R_0 T e^{ikx}$ since we did not prove a bound of type (2.3) for $T e^{ikx}$. Let us prove a weighted estimate for $T e^{ikx}$ and then apply Lemma 7.2.

Namely, $T e^{ikx} \in \mathcal{H}_\sigma^2$ with any $\sigma < 7/2 + \varepsilon/2$. Indeed,

$$T e^{ikx} = V e^{ikx} - RV e^{ikx},$$

where $V e^{ikx} \in \mathcal{H}_\sigma^2$ with $\sigma < 7/2 + \varepsilon/2$ by H3. Furthermore, $RV e^{ikx} \in \mathcal{H}_\sigma^2$ with $\sigma < 9/2 + \varepsilon$ since $RV e^{ikx} \in \mathcal{H}_\sigma^2$ with $\sigma < -1/2$. The latter follows from $RV e^{ikx} \in \mathcal{L}_\sigma^2$ with $\sigma < -1/2$ by the identity

$$(1 - \frac{1}{2}\Delta)R(\omega) = 1 + (1 - V + \omega)R(\omega).$$

Finally, applying Lemma 7.2 to the function $r(x) = T e^{ikx}$ and using (7.10), we obtain asymptotics (7.8) with

$$a(k, \theta) = -\sqrt{2\pi} \hat{\nabla}(|k|\theta) = -2\pi(2\pi)^2(T e_k, e_{|k|\theta}) = -4\pi^2 T(|k|\theta, k)$$  \hfill (7.11)

according to (1.7). Hence, formula (1.15) is proved. \hfill $\square$
8 Cross section

Now we can justify formula (1.14). Convergence (6.1) can be written as the long range asymptotics
\[ \varphi_D(x, t) \sim b_D(n) A(x)e^{-iE_k t} = b_D(n)e^{ikx}e^{-iE_k t} - b_D(n)RVe^{ikx}e^{-iE_k t}, \quad D \gg 1, \]
according to (7.1). Hence, asymptotics (7.8) and (7.9) imply that the incident and scattered waves should be identified asymptotically as
\[ \psi_{in}(x, t) = b_D(n)e^{ikx}e^{-iE_k t}, \quad \psi_{sc}(x, t) = -b_D(n)RVe^{ikx}e^{-iE_k t}, \quad D \gg 1. \]

Then the corresponding limit stationary flux is given by
\[ j_{in}(x) = |b(n)|^2 k, \quad j_{sc}(x) = |b(n)|^2 \text{Im} [a^{sc}(x)\nabla a^{sc}(x)], \]
where \( a^{sc}(x) := -RVe^{ikx} \). At last, (7.8) and (7.9) imply that the scattered flux admits the long range asymptotics
\[ j_{sc}(x) = |b(n)|^2 \frac{|a(k, x/|x|)|^2}{|x|^2} |k|\theta + O(|x|^{-3}), \quad |x| \to \infty, \quad (8.1) \]
with corresponding angular density (1.2) at infinity
\[ j_{a}^{sc}(\theta) = |b(n)|^2 |a(k, x/|x|)|^2 |k|. \quad (8.2) \]

Finally, according to definition (1.1), the differential cross section is given by
\[ \sigma(\theta) := j_{a}^{sc}(\theta)/|j_{in}| = |a(k, x/|x|)|^2, \]
which justifies (1.14). Then (1.6) also holds according to known formula (1.15).

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