3D Schrödinger equation: scattering operator, scattering amplitude and ergodic property

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Abstract

Stationary scattering problem (when the distance \( r \) tends to infinity) and dynamical scattering problem (when the time \( t \) tends to infinity) are considered for the 3D Schrödinger equation. A simple interconnection between the scattering amplitude (stationary case) and scattering operator (dynamical case) is given in the paper. This result is a quantum mechanical analog of the ergodic formulas in the classical mechanics.

1 Introduction

In the present paper, we consider the Schrödinger operator \( \mathcal{L}u(r) = -\Delta u + V(r)u \), where \( \Delta \) denotes the 3-dimensional Laplacian, \( V(r) = \overline{V}(r) \) and \( r \in \mathbb{R}^3 \). The Schrödinger operator \( \mathcal{L} \) is one of the most important operators in mathematics and physics. Spectral and scattering problems for this operator were investigated by many authors (see, e.g. important works [1, 2, 4, 5, 6]).

In this paper we consider two types of scattering problems: stationary scattering problem (when the distance \( r \) tends to infinity) and dynamical scattering problem (when the time \( t \) tends to infinity).

The connection between the scattering amplitude (stationary scattering problem) and dynamical scattering operator is described by formula (3.11).
and presents the main result of the paper. Formula (3.11) is a quantum mechanical analog of the ergodic formulas in the classical mechanics. Works by Povzner [6], Ikebe [1] and Kato [2] were essential for our research.

For the radial case, where \( V(r) = V(|r|) \), the quantum mechanical analogs of the ergodic formulas in classical mechanics were obtained in our papers [9, 10]. Some ergodic results were obtained for the Dirac equation as well (see [11, 12]).

2 Preliminary results

In this section, we present the results that we will be needed later.

1. Let us consider the Schrödinger operator

\[
\mathcal{L} u(r) = -\Delta u + V(r) u, \quad \mathcal{L}_0 u(r) = -\Delta u,
\]

(2.1)

where \( r = (r_1, r_2, r_3) \in \mathbb{R}^3 \). Further we assume that

\[
V(r) = \overline{V(r)}.
\]

(2.2)

Let us write the Lippmann-Schwinger equation:

\[
\phi(r, k) = e^{i k \cdot r} - \frac{1}{4\pi} \int_{\mathbb{R}^3} \frac{e^{i|k||r-s|}}{|r-s|} V(s) \phi(s, k) ds,
\]

(2.3)

where \( |k| = \sqrt{\lambda}, \lambda > 0 \). We note that the solution \( \phi(r, k) \) of the Lippmann-Schwinger equation (2.3) satisfies the relation

\[
(\mathcal{L} - \lambda) \phi = \lambda \phi.
\]

(2.4)

The modified Lippmann-Schwinger equation has the form

\[
(I + K(\lambda)) \psi(r, k) = e^{i k \cdot r} |V(r)|^{1/2},
\]

(2.5)

where the operator \( K(\lambda) \) is defined by the relation

\[
K(\lambda) f(r) = \frac{1}{4\pi} \int_{\mathbb{R}^3} |V(r)|^{1/2} \frac{e^{i|k|r-s|}}{|r-s|} W(s) |V(s)|^{1/2} f(s) ds.
\]

(2.6)

2. We need the following definition:
Definition 2.1 The potential $V(r)$ belongs to Rollnik class if the operator

$$A(\lambda) = \int_{\mathbb{R}^3} \frac{|V(r)|^{1/2}e^{i|k||r-s|}V(s)|^{1/2}}{|r-s|}f(s)ds.$$  \hspace{1cm} (2.7)

belongs to the Hilbert-Schmidt class.

Remark 2.2 Further we assume that the potential $V(r)$ belongs to the Rollnik class. Hence the operator $K(\lambda)$ belongs to the Hilbert-Schmidt class.

Definition 2.3 The point $\lambda > 0$ is an exceptional value if the equation $[I + K(\lambda)]\psi = 0$ has nontrivial solution in the space $L^2(\mathbb{R}^3)$.

We denote by $\mathcal{E}_+$ the set of exceptional points and we denote by $E_+$ the set of such points $\lambda > 0$ that $\lambda \notin \mathcal{E}_+$.

Lemma 2.4 If $\lambda \in E_+$, then equation (2.3) has one and only one solution $\psi(r, k)$ in $L^2(\mathbb{R}^3)$.

Corollary 2.5 If $\lambda \in E_+$, then equation (2.1) has one and only one solution $\phi(r, k)$ which satisfies the condition $|V(r)|^{1/2}\phi(r, k) \in L^2(\mathbb{R}^3)$.

We formulate the following result (see [7], p.115).

Corollary 2.6 1) The operator $L$ has only discrete spectrum in the domain $\lambda < 0$.
2) The discrete spectrum of the operator $L$ has no limit points in the domain $\lambda < 0$.
3) The set $\mathcal{E}_+$ is bounded, closed and has Lebesgue measure equal to zero.

Let us consider the scattering operator $S(\lambda)$ in the energetic representation. It is proved (see [7], p.110) that $S(\lambda)$ is unitary. Let us introduce the operator function

$$T(\lambda) = (2i\pi)^{-1}[I - S(\lambda)].$$  \hspace{1cm} (2.8)

We need the following assertion ([2])

Proposition 2.7 For each $\lambda \in E_+$ the operator $T(\lambda)$ can be represented in the form

$$T(\lambda) = \mathcal{F}(\lambda)W(r)[I + K(\lambda)]^{-1}\mathcal{F}^*(\lambda)$$  \hspace{1cm} (2.9)
The operator $\mathcal{F}(\lambda)$ is defined by the formula
\[
\mathcal{F}(\lambda)f(r) = \mu \int_{\mathbb{R}^3} e^{-i|k|\omega \cdot r} |V(r)|^{1/2} f(r) dr, \quad |k|^2 = \lambda,
\] (2.10)
where $\mu = (1/4)(\lambda)^{1/4} \pi^{-3/2}$. The adjoint to $\mathcal{F}(\lambda)$ operator has the form
\[
\mathcal{F}^*(\lambda)h(\omega) = \mu \int_{S^2} e^{i|k|\omega \cdot r} |V(r)|^{1/2} h(\omega) d\Omega(\omega)
\] (2.11)
Here by $S^2$ we denote the surface $|\omega'| = 1$ in the space $\mathbb{R}^3$, $d\Omega$ is the standard measure on the surface $S^2$. Now we formulate the Povzner-Ikebe result (see [6] and [1]):

**Theorem 2.8** Let the function $V(r)$ belong to space $L^2(\mathbb{R}^3)$. If
\[
|V(r)| = O(|r|^{-3-\delta}), \quad \delta > 0, \quad |r| \to \infty,
\] (2.12)
then the solution $\phi(r,k)$ of Lippmann-Schwinger equation (2.3) has the form
\[
\phi(r,k) = e^{ik \cdot r} + \frac{e^{i\sqrt{\lambda} |r|}}{|r|} f(\omega,\omega',\lambda) + o(1/|r|), \quad |r| \to \infty,
\] (2.13)
where $\omega = r/|r|$, $\omega' = k/|k|$ and
\[
f(\omega,\omega',\lambda) = -\frac{1}{4\pi} \int_{\mathbb{R}^3} e^{-i\sqrt{\lambda}(s \cdot \omega)} V(s) \phi(s,k) ds.
\] (2.14)
The function $f(\omega,\omega',\lambda)$ is the scattering amplitude.

**Remark 2.9** If the conditions of Theorem 2.8 are fulfilled, then $V(r) \in L^{3/2}(\mathbb{R}^3)$. It follows from the theorem Kato [3] that $V(r)$ belongs to the Rollnik class.

**Remark 2.10** The following assertion is valid [1]:
If the conditions of Theorem 2.8 are fulfilled, then $E_+ = (0, \infty)$.  

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3 Scattering operator and scattering amplitude, ergodic property

1. The scattering operator $S(\lambda)$ is the solution of the dynamical scattering problem, when time $t \to \infty$ [1], [2]. The scattering amplitude $f(\omega, \omega', \lambda)$ is the solution of the stationary scattering problem, when distance $r \to \infty$. In this section we show that dynamical and stationary scattering problems are closely connected.

We begin with the statement.

**Theorem 3.1** Let $V(r)$ belong to the Rollnik class. Then for each $\lambda \in E_+$ the operator $T(\lambda)$ belong to the Hilbert-Schmidt class.

**Proof.** We use the relation

$$[\mathcal{F} \mathcal{F} f] = \frac{1}{4\pi^2} \int_{\mathbb{R}^3} |V(r)|^{1/2} \sin(|k(r-s)|) |V(s)|^{1/2} f(s) ds.$$  \hspace{1cm} (3.1)

The function $V(r)$ belongs to Rollnik class. Hence it follows from (3.1) that the operator $\mathcal{F}^* \mathcal{F}$ belongs to the Hilbert-Schmidt class. Now using (2.9) we obtain the assertion of the theorem.

Changing the order of integrals in (2.9) and using (2.5) we obtain

$$T(\lambda) h(\omega') = \mu^2 \int_{S^2} T(\omega, \omega', \lambda) h(\omega') d\Omega(\omega'),$$ \hspace{1cm} (3.2)

where

$$T(\omega, \omega', \lambda) = \int_{\mathbb{R}^3} e^{-i\sqrt{\lambda}(s \cdot \omega)} V(s) \phi(s, k') ds,$$ \hspace{1cm} (3.3)

and $\omega = k/|k|$, $\omega' = k'/|k'|$, $|k| = |k'| = \sqrt{\lambda}$. We note that $\omega$ and $\omega'$ are defined in the cases (2.13) and (3.3) differently. Comparing (2.14) and (3.3) we have

$$f(\omega, \omega', \lambda) = -\frac{1}{4\pi} T(\omega, \omega', \lambda), \quad \lambda > 0.$$ \hspace{1cm} (3.4)

2. We introduce the Hilbert space $\mathcal{H}$ of the functions $h(\omega)$. The norm in the space $\mathcal{H}$ is defined by the relation

$$\|h\|^2 = \int_{S^2} |h(\omega)|^2 d\Omega(\omega).$$ \hspace{1cm} (3.5)
We note that the operator $S(\lambda)$ is unitary in the space $\mathcal{H}$. Hence there exists a complete orthonormal system of eigenfunctions $G_j(\omega, \lambda)$ of the operator $S(\lambda)$. We denote the corresponding eigenvalues by $\nu_j(\lambda)$, where $|\nu_j(\lambda)| = 1$. The function $f(\omega, \omega', \lambda)$, where $\omega$ and $\lambda$ are fixed, belongs to the space $\mathcal{H}$. Hence the function $f(\omega, \omega', \lambda)$ can be represented in the form of series:

$$f(\omega, \omega', \lambda) = \sum_j a_j(\omega)G_j(\omega', \lambda), \quad \lambda > 0, \quad (3.6)$$

where

$$a_j(\omega, \lambda) = \int_{S^2} f(\omega, \omega', \lambda)G_j(\omega', \lambda)d\Omega(\omega') \quad (3.7)$$

It follows from (3.4) and (3.7) the relation

$$a_j(\omega, \lambda) = -\frac{1}{4\pi} \int_{S^2} T(\omega, \omega', \lambda)G_j(\omega', \lambda)d\Omega(\omega') \quad (3.8)$$

Taking into account (3.2) and (3.8) we have

$$a_j(\omega, \lambda) = -\frac{1}{4\pi \mu^2} T(\lambda)G_j(\omega, \lambda) \quad (3.9)$$

We recall that $T(\lambda) = [I - S(\lambda)]/(2i\pi)$ and $\mu = (1/4)(\lambda)^{1/4} - 3/2$. Hence the relation (3.9) can be written in the following form:

$$a_j(\omega, \lambda) = \frac{2\pi}{i\sqrt{\lambda}} [S(\lambda) - I]G_j(\omega, \lambda), \quad \lambda > 0. \quad (3.10)$$

Relations (3.6) and (3.10) imply the following assertion:

**Theorem 3.2** Let the conditions of Theorem 2.8 be fulfilled. Then we have

$$f(\omega, \omega', \lambda) = \frac{2\pi}{i\sqrt{\lambda}} \sum_j (\nu_j(\lambda) - 1)G_j(\omega, \lambda)\overline{G_j(\omega', \lambda)}, \quad \lambda > 0. \quad (3.11)$$

Let us define the total cross section

$$\sigma(\lambda) = \int_{S^2} \int_{S^2} |f(\omega, \omega', \lambda)|^2 d\Omega(\omega) d\Omega(\omega'). \quad (3.12)$$
Corollary 3.3 Let conditions of Theorem 2.8 be fulfilled. Then the total cross section has the form

\[ \sigma(\lambda) = \frac{4\pi^2}{\lambda} \sum_j |\nu_j(\lambda) - 1|^2. \] (3.13)

Remark 3.4 It follows from the conditions of Theorem 2.8, that the operator \( F^*F \) (see (3.1)) belongs to the Hilbert-Schmidt class (see [13], Ch.1). Then operator \( T(\lambda) \) belongs to the Hilbert-Schmidt class too. Hence the series (3.11) and (3.13) converge.

Remark 3.5 Formulas (3.11) and (3.13) give the connections between the stationary scattering results \( (f(\omega, \omega', \lambda)) \) and the dynamical scattering results \( (G_j(\omega, \lambda), \mu_j(\lambda)) \). So, formulas (3.11) and (3.13) are quantum mechanical analogues of the ergodic formulas in classical mechanics. For radial case, when \( V(r) = V(|r|) \), the quantum mechanical analogues of the ergodic formulas were obtained in our papers [9], [10].

3. Let us consider separately the classical case, when \( V(r) = V(|r|), \ \omega'(\theta', \phi') = \omega' (\pi/2, 0). \) (3.14)

In other words, we consider the case when the potential \( V(r) \) is spherically symmetric and the incoming wave has z-direction. If potential \( V(r) \) is spherically symmetric then the corresponding complete orthonormal system of eigenfunctions \( Y_{\ell,m}(\theta, \phi) \) of \( S(\lambda) \) have the form (see [4], section 28):

\[ Y_{\ell,m}(\theta, \phi) = P_{\ell,m}(\cos \theta)F_m(\phi), \] (3.15)

where

\[ P_{\ell,0}(\cos \theta) = \sqrt{\ell + 1/2}P_{\ell}(\cos \theta), \ \ell = 0, 1, 2, ..., \] (3.16)

\[ F_m(\phi) = \frac{1}{\sqrt{2\pi}}e^{im\phi}, \ -\ell \leq m \leq \ell. \] (3.17)

Here the functions \( P_{\ell}(\cos \theta) \) are Legendre polynomials. We do not write formulas for \( P_{\ell,m}(\cos \theta), (m \neq 0) \) since we do not use them further. In case (3.14) we have

\[ f(\omega, \omega', \lambda) = f(\theta, \phi, \lambda). \] (3.18)
The azimuthal rotational symmetry of plane wave and spherical potential ensures that
\[ f(\theta, \phi, \lambda) = f(\theta, \lambda). \quad (3.19) \]

Taking into account the relations
\[ P_{\ell,0}(1) = \sqrt{\ell + 1/2}, \quad F_0(\phi) = \frac{1}{\sqrt{2\pi}} \quad (3.20) \]
we write equality (3.11) for case (3.14):
\[ f(\theta, \lambda) = \frac{1}{2i\sqrt{\lambda}} \sum_{\ell=0}^{\infty} (2\ell + 1)[\nu_\ell(\lambda) - 1]P_\ell(\cos \theta). \quad (3.21) \]

Let us write the classical formula (see [4], section 122 and [5], Ch.II) for case (3.14)
\[ f(\theta, \lambda) = \frac{1}{2i\sqrt{\lambda}} \sum_{\ell=0}^{\infty} (2\ell + 1)[S_\ell(\lambda) - 1]P_\ell(\cos \theta), \quad (3.22) \]
where \( S_\ell(\lambda) \) is connected with phase shift \( \delta_\ell(\lambda) \) by the relation
\[ S_\ell(\lambda) = \exp(\delta_\ell(\lambda)). \quad (3.23) \]

Comparing relations (3.22) and (3.23) we obtain the assertion:

**Corollary 3.6** Let conditions of Theorem 2.8 and conditions (3.14) be fulfilled. Then
1. The equality
\[ \nu_\ell(\lambda) = S_\ell(\lambda), \quad \lambda > 0 \] is valid.
2. The classical equation (3.22) is the partial case of formula (3.11).

We proved ([9], [10]) relation (3.24) before by using ordinary differential equations theory. The total scattering cross-section \( \sigma(\lambda) \) is defined now by the relation
\[ \sigma(\lambda) = 2\pi \int_0^\pi |f(\theta, \lambda)|^2 \sin \theta d\theta, \quad \lambda > 0. \quad (3.25) \]
We note that
\[ \int_0^\pi |P_\ell(\cos \theta)|^2 \sin \theta d\theta = \ell/2 + 1 \quad (3.26) \]
It follows from (3.22), (3.23) and (3.25), (3.26) the well-known formula

\[ \sigma(\lambda) = \frac{4\pi}{\lambda} \sum_{\ell=0}^{\infty} (2\ell + 1) \sin^2 \delta_\ell(\lambda), \quad \lambda > 0. \]  

(3.27)

**Remark 3.7** The definitions (3.12) and (3.25) of scattering cross-section \( \sigma(\lambda) \) are different. The corresponding results (3.13) and (3.26) are different too.

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