Scattering theory without large-distance asymptotics

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ABSTRACT: In conventional scattering theory, to obtain an explicit result, one imposes a precondition that the distance between target and observer is infinite. With the help of this precondition, one can asymptotically replace the Hankel function and the Bessel function with the sine functions so that one can achieve an explicit result. Nevertheless, after such a treatment, the information of the distance between target and observer is inevitably lost. In this paper, we show that such a precondition is not necessary: without losing any information of distance, one can still obtain an explicit result of a scattering rigorously. In other words, we give an rigorous explicit scattering result which contains the information of distance between target and observer. We show that at a finite distance, a modification factor — the Bessel polynomial — appears in the scattering amplitude, and, consequently, the cross section depends on the distance, the outgoing wave-front surface is no longer a sphere, and, besides the phase shift, there is an additional phase (the argument of the Bessel polynomial) appears in the scattering wave function.

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1 Introduction

In conventional scattering theory, which is now a standard quantum mechanics textbook content, to seek an explicit result, one imposes a precondition that the distance between target and observer is infinite. As a result, the conventional scattering theory loses all the information of the distance and the result depends only on the angle of emergence. In this paper, we will show that without such a precondition, one can still achieve a rigorous scattering theory which, of course, contains the information of distance that is lost in conventional scattering theory.

The dynamical information of a scattering problem with a spherical potential $V(r)$ are embedded in the radial wave equation,

$$\frac{1}{r^2} \frac{d}{dr} \left( r^2 \frac{dR_l}{dr} \right) + \left[ k^2 - \frac{l(l+1)}{r^2} - V(r) \right] R_l = 0. \quad (1.1)$$

The scattering boundary condition in conventional scattering theory is taken to be

$$\psi(r, \theta) = e^{ikr \cos \theta} + f(\theta) \frac{e^{ikr}}{r}, \quad r \to \infty. \quad (1.2)$$

In conventional scattering theory, in order to achieve an explicit result, two kinds of asymptotic approximations are employed.

1) Replace the solution of the free radial equation, i.e., Eq. (1.1) with $V(r) = 0$, with its asymptotics:

$$R_l(r) \sim C_l h_l^{(2)}(kr) + D_l h_l^{(1)}(kr), \quad r \to \infty \quad (1.3)$$

$$r \to \infty \quad A_l \sim \frac{\sin (kr - l\pi/2 + \delta_l)}{kr}, \quad (1.4)$$
where \( h_l^{(1)}(z) \) and \( h_l^{(2)}(z) \) are the first and second kind spherical Hankel functions, \( e^{2i\delta_l} = D_l/C_l \) defines the scattering phase shift \( \delta_l \), and \( A_l = 2\sqrt{C_lD_l} \).

2) Replace the plane wave expansion in the boundary condition with its asymptotics:

\[
e^{ikr\cos \theta} = \sum_{l=0}^{\infty} (2l + 1) i^l j_l(kr) P_l(\cos \theta) \]

\[
r \to \infty \sum_{l=0}^{\infty} (2l + 1) i^l \sin \left( kr - \frac{l\pi}{2} \right) P_l(\cos \theta),
\]

where \( j_l(z) \) is the spherical Bessel function.

Technologically speaking, the above two treatments in conventional theory are to replace the spherical Hankel function, \( h_l^{(1)}(kr) \) and \( h_l^{(2)}(kr) \), and the spherical Bessel function, \( j_l(kr) \), with their asymptotics, and, thus, inevitably lead to the loss of information of the distance \( r \).

In this paper, we will show that the above two replacements is not necessary; without these two replacements, we can still obtain a rigorous scattering theory which contains the information of the distance between target and observer.

A systematic rigorous result of a scattering with the distance between target and observer is given in Sec. 2. The conclusion and outlook are given in Sec. 3.

2 Rigorous result of scattering without large-distance asymptotics

In this section, a rigorous treatment without large-distance asymptotics for short-range potentials is established. The scattering wave function, scattering amplitude, phase shift, cross section, and a description of the outgoing wave are rigorously obtained.

2.1 Phase shift

In conventional scattering theory, as mentioned above, one replaces the solution of the free radial equation, \( R_l(r) \), given by Eq. (1.3) with its asymptotics, Eq. (1.4), using the asymptotics of the spherical Hankel functions \( h_l^{(1)}(kr) \sim \frac{1}{kr} e^{i(kr-l\pi/2)} \) and \( h_l^{(2)}(kr) \sim -\frac{1}{kr} e^{-i(kr-l\pi/2)} \). Obviously, such a replacement will lose information.

In the following, with \( R_l(r) \) given by Eq. (1.3), rather than its asymptotics, Eq. (1.4), we solve the scattering rigorously.

The first step is to rewrite \( R_l(r) \) given by Eq. (1.3) as

\[
R_l(r) = C_l h_l^{(2)}(kr) + D_l h_l^{(1)}(kr) = M_l \left( \frac{i}{kr} \right) \frac{A_l}{x} \sin \left[ kr - \frac{l\pi}{2} + \delta_l + \Delta_l \left( \frac{i}{kr} \right) \right],
\]

where \( e^{2i\delta_l} = D_l/C_l \) and \( M_l(x) = |y_l(x)| \) and \( \Delta_l(x) = \arg y_l(x) \) are the modulus and argument of the Bessel polynomial \( y_l(x) \), respectively.

In order to achieve Eq. (2.1), we prove the relation

\[
C_l h_l^{(2)}(x) + D_l h_l^{(1)}(x) = M_l \left( \frac{i}{x} \right) \frac{A_l}{x} \sin \left[ x - \frac{l\pi}{2} + \delta_l + \Delta_l \left( \frac{i}{x} \right) \right].
\]
Proof. The first and second kind spherical Hankel functions, $h_l^{(1)}(x)$ and $h_l^{(2)}(x)$, can be expanded as [1]

\begin{align}
h_l^{(1)}(x) &= e^{ix} \sum_{k=0}^{l} \frac{i^{k-l-1}(l+k)!}{2^k k!(l-k)!x^{k+1}}, \tag{2.3} \\
h_l^{(2)}(x) &= e^{-ix} \sum_{k=0}^{l} \frac{(-i)^{k-l-1}(l+k)!}{2^k k!(l-k)!x^{k+1}}. \tag{2.4}
\end{align}

By the Bessel polynomial [1],

\begin{equation}
y_l(x) = \sum_{k=0}^{l} \frac{(l+k)!}{k!(l-k)!}\left(\frac{x}{2}\right)^k, \tag{2.5}
\end{equation}

we can rewrite $h_l^{(1)}(x)$ and $h_l^{(2)}(x)$ as

\begin{align}
h_l^{(1)}(x) &= e^{i(x-l\pi/2)} \frac{1}{ix} y_l\left(\frac{i}{x}\right), \\
h_l^{(2)}(x) &= -e^{-i(x-l\pi/2)} \frac{1}{ix} y_l\left(-\frac{i}{x}\right). \tag{2.6}
\end{align}

Using Eq. (2.6), we have

\begin{equation}
C_l h_l^{(2)}(x) + D_l h_l^{(1)}(x) = C_l \left[-\frac{e^{-i(x-l\pi/2)}}{ix} y_l\left(-\frac{i}{x}\right) + e^{2i\delta_l} \frac{e^{i(x-l\pi/2)}}{ix} \frac{y_l\left(i/x\right)}{-i} \right]. \tag{2.7}
\end{equation}

Writing the Bessel polynomial as $y_l = M_l e^{i\Delta_l}$, we prove the relation (2.2).

The wave function, then, by $\psi(r, \theta) = \sum_{l=0}^{\infty} R_l(r) P_l(\cos \theta)$, can be obtained immediately from Eq. (2.1),

\begin{equation}
\psi(r, \theta) = \sum_{l=0}^{\infty} M_l \left(\frac{i}{kr}\right) \frac{A_l}{kr} \sin \left[kr - \frac{l\pi}{2} + \delta_l + \Delta_l\left(\frac{i}{kr}\right)\right] P_l(\cos \theta). \tag{2.8}
\end{equation}

When the distance $r$ is finite, the coefficient becomes $M_l A_l$ and the phase becomes $\delta_l + \Delta_l$, where $M_l$ and $\Delta_l$ both depend on $r$. While, in conventional scattering theory, $r \to \infty$, the coefficient is $A_l$ and the phase is $\delta_l$, and they are both independent of $r$.

It should be emphasized that $\delta_l$ here is the same as that in conventional scattering theory. This is because $\delta_l$ is determined only by the coefficient $C_l$ and $D_l$ and $y_l\left(\frac{i}{kr}\right) \sim \infty$. Thus when $r \to \infty$, $C_l$, $D_l$, and, accordingly, $\delta_l$ remains unchanged.

The modification factors, $\Delta_l$ and $M_l$, are independent of potentials. When $r \to \infty$, $M_l (r \to \infty) = 1$ and $\Delta_l (r \to \infty) = 0$.

2.2 Asymptotic boundary condition

The outgoing wave is no longer a spherical wave when the observer stands at a finite distance from the target, other than that in large-distance asymptotics. The outgoing wave now becomes a surface of revolution around the incident direction, determined by
the potential and the observation distance. Because the outgoing waves are different at
different distances, there is no uniform expression of the asymptotic boundary condition
like Eq. (1.2). Here, we express the boundary condition as

\[ \psi (r, \theta) = e^{ikr \cos \theta} + f(r, \theta) \frac{e^{ikr}}{r}, \tag{2.9} \]

where \( f(r, \theta) \) depends not only on \( \theta \) but also on \( r \).

When the distance \( r \) is finite, however, the differential scattering cross section is no
longer the square modulus of \( f(r, \theta) \). Only when \( r \to \infty \), \( f(\infty, \theta) = f(\theta) \) and the differ-
ential cross section reduces to \( |f(\theta)|^2 \).

To calculate \( f(r, \theta) \), as that in conventional scattering theory, we expand the incoming
plane wave \( e^{ikr \cos \theta} \) by the eigenfunction of the angular momentum. Now, we prove that
the expansion of \( e^{ikr \cos \theta} \), Eq. (1.5), can be exactly rewritten as

\[ e^{ikr \cos \theta} = \sum_{l=0}^{\infty} (2l+1) i^l j_l(kr) P_l(\cos \theta) \]

\[ = \sum_{l=0}^{\infty} (2l+1) i^l M_l \left( i \frac{kr}{r} \right) \frac{1}{kr} \sin \left[ kr - \frac{l\pi}{2} + \Delta_l \left( i \frac{kr}{r} \right) \right] P_l(\cos \theta). \tag{2.10} \]

\textit{Proof.} A plane wave can be expanded as \[ e^{ikr \cos \theta} = \sum_{l=0}^{\infty} (2l+1) i^l j_l(kr) P_l(\cos \theta). \tag{2.11} \]

By the relations \( h_l^{(1)}(x) = j_l(x) + in_l(x) \) and \( h_l^{(2)}(x) = j_l(x) - in_l(x) \), the spherical
Bessel function \( j_l(x) \) can be rewritten as \( j_l(x) = \frac{i}{2} \left[ h_l^{(1)}(x) + h_l^{(2)}(x) \right] \), where \( n_l(x) \) is the
spherical Neumann function [1]. By Eq. (2.6), we have

\[ j_l(kr) = M_l \left( i \frac{kr}{r} \right) \frac{1}{kr} \sin \left[ kr - \frac{l\pi}{2} + \Delta_l \left( i \frac{kr}{r} \right) \right]. \tag{2.12} \]

Substituting this result into Eq. (2.11) proves Eq. (2.10).

The plane wave expansion (2.10) is exact, rather than the asymptotic one, Eq. (1.6),
used in conventional scattering theory. In conventional scattering theory, the spherical
Bessel function \( j_l(kr) \) given by Eq. (2.12) is replaced by its asymptotics: \( j_l(kr) \sim \frac{1}{kr} \sin (kr - l\pi/2) \), i.e., \( M_l \) and \( \Delta_l \) are asymptotically taken to be \( M_l \left( i \frac{kr}{r} \right) \sim 1 \) and \( \Delta_l \left( i \frac{kr}{r} \right) \sim 0 \); as a result, the information embedded in \( M_l \) and \( \Delta_l \) is lost.

The boundary condition, Eq. (2.9), then, by Eq. (2.10), can be expressed as

\[ \psi (r, \theta) = \sum_{l=0}^{\infty} (2l+1) i^l M_l \left( i \frac{kr}{r} \right) \frac{1}{kr} \sin \left[ kr - \frac{l\pi}{2} + \Delta_l \left( i \frac{kr}{r} \right) \right] P_l(\cos \theta) + f(r, \theta) \frac{e^{ikr}}{r}. \tag{2.13} \]
2.3 Scattering wave function

The scattering wave function can be calculated by imposing the boundary condition (2.13) on the asymptotic wave function (2.8).

Observing the outgoing part of the wave function (2.13), \( f(r, \theta) e^{ikr}/r \), we can see that the leading contribution of \( f(r, \theta) \) must only be a zero power of \( r \), or else the outgoing wave is not a spherical wave when \( r \to \infty \). Thus, we can expand \( f(r, \theta) \) by the Bessel polynomial, which is complete and orthogonal [3], as

\[
f(r, \theta) = \sum_{l=0}^{\infty} g_l(\theta) y_l \left( \frac{i}{kr} \right).
\]

The reason why only \( y_l \left( \frac{i}{kr} \right) \) appears in the expansion (2.14) is that only the flux corresponding to \( y_l \left( \frac{i}{kr} \right) e^{ikr}/r \) is an outgoing spherical wave; or, in other words, the requirement that the scattering wave must be an outgoing wave rules out the terms including \( y^*_l \left( \frac{i}{kr} \right) = y_l \left( -\frac{i}{kr} \right) \).

Equating Eqs. (2.8) and (2.13), using the expansion (2.14), and noting that \( M_l e^{i\Delta_l} = y_l \), we arrive at

\[
\frac{1}{2ik} \left[ (2l+1) - A_l e^{i(-\pi/2+\Delta_l)} \right] P_l(\cos \theta) + g_l(\theta) = 0,
\]

\[
(2l+1) e^{i\pi} - A_l e^{-i(-\pi/2+\Delta_l)} = 0.
\]

Solving these two equations gives

\[
A_l = (2l+1) e^{i\pi} e^{i(-\pi/2+\Delta_l)},
\]

\[
g_l(\theta) = -\frac{1}{2ik} (2l+1) \left( 1 - e^{i2\Delta_l} \right) P_l(\cos \theta).
\]

Then, we arrive at

\[
f(r, \theta) = \sum_{l=0}^{\infty} \frac{1}{2ik} (2l+1) \left( e^{i2\Delta_l} - 1 \right) P_l(\cos \theta) y_l \left( \frac{i}{kr} \right).
\]

When taking the limit \( r \to \infty \), the modification factor — the Bessel polynomial \( y_l \left( \frac{i}{kr} \right) \) — tends to 1, and \( f(r, \theta) \) recovers the scattering amplitude in conventional scattering theory: \( f(\infty, \theta) = f(\infty, \theta) = \frac{1}{2ik} \sum_{l=0}^{\infty} (2l+1) \left( e^{i2\Delta_l} - 1 \right) P_l(\cos \theta) \).

The leading is a \( p \)-wave modification, because the \( s \)-wave modification is \( y_0(x) = 1 \).

2.4 Outgoing wave-front surface

In conventional scattering theory, the observer is at \( r \to \infty \) and the outgoing wave is a spherical wave. When the observer is at a finite distance \( r \), the outgoing wave-front surface, however, is a surface of revolution around the incident direction, since for a spherical potential the outgoing wave must be cylindrically symmetric.

The outgoing wave-front surface is determined by the outgoing flux \( j^\infty \) which serves as its surface normal vector. The outgoing flux is \( j^\infty = j - j^\text{in} \), where \( j = \frac{\hbar}{m} \text{Im} (\psi^* \nabla \psi) \)
and \( j^{in} = \frac{h}{m} \text{Im}\left( \psi^{in} \ast \nabla \psi^{in} \right) \). Here we write the wave function (2.9) as \( \psi = \psi^{in} + \psi^{sc} \) with \( \psi^{in} = e^{ikr \cos \theta} \) and \( \psi^{sc} = f(r, \theta) e^{ikr}/r \).

The outgoing wave-front surface is a surface of revolution. Its generatrix, \( r = r(\theta) \), with \( j^{sc} \) as the normal vector, is determined by

\[
\frac{1}{r(\theta)} \frac{dr(\theta)}{d\theta} = -j^{sc}_\theta j^{sc}_r = -\tan \gamma^{sc},
\]

where \( \gamma^{sc} \) is the intersection angle between \( j^{sc} \) and the radial vector.

The equation of the generatrix, Eq. (2.19), is a differential equation. The integration constant can be chosen as \( r(0) = R \), where \( R \) is the intersection between the outgoing wave-front surface on which the observer stands and the target along the z-axis. Then the solution of Eq. (2.19) can be formally written as \( r = r(\theta, R) \).

Moreover, the Gaussian curvature of the outgoing wave-front surface reads

\[
K(\theta) = \frac{1}{r^2} \cos^2 \gamma^{sc} \left( 1 + \frac{d\gamma^{sc}}{d\theta} \right) (1 - \tan \gamma^{sc} \cot \theta).
\]

When \( r \to \infty, \gamma^{sc} \to 0 \), and then \( K = 1/r^2 \) reduces to a curvature of a sphere.

### 2.5 Differential scattering cross section

The differential scattering section is \( d\sigma = j^{sc} \cdot dS/j^{in} \). The scattering flux \( j^{sc} \), other than that in conventional scattering theory, is not along the radial direction. Thus,

\[
d\sigma = \frac{j^{sc} \cdot dS}{j^{in}} = \frac{j^{sc}}{j^{in} \cos \gamma^{sc}} \frac{r^2 d\Omega}{j^{in} r^2 d\Omega} = (1 + \tan^2 \gamma^{sc}) \frac{j^{sc}}{j^{in}} r^2 d\Omega,
\]

where \( j^{sc} = \sqrt{j^{sc}_r^2 + j^{sc}_\theta^2} \) and \( \tan \gamma^{sc} = j^{sc}_\theta/j^{sc}_r \). A straightforward calculation gives

\[
\frac{d\sigma}{d\Omega} = \left| f(r, \theta) \right|^2 + \eta(r, \theta) \left( 1 + \tan^2 \gamma^{sc} \right),
\]

where

\[
\eta(r, \theta) = \frac{1}{k} \text{Im}\left\{ f^* \frac{\partial f}{\partial r} + e^{ikr(1-\cos \theta)} \left\{ [ikr(1 + \cos \theta) - 1] f + r \frac{\partial f}{\partial r} \right\} \right\}.
\]

### 2.6 Total scattering cross section

For simplicity, we only consider the leading contribution of the total scattering cross section, \( \sigma_t(R) = 2\pi \int_{0}^{\pi} |f(R, \theta)|^2 \sin \theta d\theta \), in which the outgoing wave-front surface is approximately a sphere of radius \( R \).

The total cross section then reads

\[
\sigma_t(R) = \frac{4\pi}{k^2} \sum_{l=0}^{\infty} (2l + 1) \sin^2 \delta_l \left| y_l \left( \frac{i}{kR} \right) \right|^2.
\]

In comparison with conventional scattering theory, a modification factor \( \left| y_l \left( \frac{i}{kR} \right) \right|^2 \) appears.
3 Conclusions and outlook

We show that one can obtain a rigorous scattering theory without the precondition $r \to \infty$. A rigorous scattering theory contains the information of the distance between target and observer is presented. The conventional scattering theory can be recovered by setting $r \to \infty$.

In comparison with conventional scattering theory, there is an additional factor — the $l$-th Bessel polynomial — appears in the $l$-th partial-wave contribution. The leading modification is $p$-wave.

Quantum scattering theory plays an important role in many physical area and is intensively studied. Nevertheless, all studies are based on conventional scattering theory. Based on our result, we can further consider many scattering-related problems. For example, at low temperatures, the thermal wavelength has the same order of magnitude as the interparticle spacing, so the scattering in a BEC transition [4, 5] and in a transport of spin-polarized fermions [6, 7] may need to take the effect of the distance into account. The scattering spectrum method is important in quantum field theory [8–11]; a scattering spectrum method without asymptotics can also be discussed. Moreover, the relation between scattering spectrum method and heat kernel method, which is given by Ref. [12] based on Refs. [13, 14], can also be improved by the exact result of the scattering theory without infinite-distance asymptotics. Moreover, a related inverse scattering problems can also be systematically studied, and the result can be applied to, e.g., the interference pattern of Bose-Einstein condensates [15] and the Aharonov–Bohm effect [16].

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