Chapter 10: QUANTUM SCATTERING

Scattering is an extremely important tool to investigate particle structures and the interaction between the target particle and the scattering particle. For example, Rutherford scattering finds that atoms have small and massive nuclei, surrounded by tiny and light electrons. High-energy photons can be scattered by a neutron, revealing its inner structure formed by quarks. Quantum scattering is a very extensive subject, and we will study the basic ideas. We have briefly discussed photon scattering, now our focus is on matter particles, such as electrons and neutrons, within the formal and exact framework, though approximations will be taken as well in practice.

10.1 Cross Sections

**Goal:** finding the differential cross section $d\sigma / d\Omega$ of an incident particle beam with definite momentum scattered by an object described by a (localized) potential.

**Simplification:** A steady particle beam with definite momentum can be described by a planewave, and we can only consider one particle. The results for a current density of a particle beam can be obtained readily.

Let’s begin with **one dimension** (1D).

$$\psi_k \rightarrow \begin{cases} \begin{align*} &A e^{ikx} + Be^{-ikx} \quad (x \to -\infty) \\ &Ce^{ikx} + De^{-ikx} \quad (x \to +\infty) \end{align*} \end{cases} \quad (10.1)$$

1. $D = 0$.
3. The transition rate $T = |C|^2 / |A|^2$.

Both $R$ and $T$ are a function of $k$, therefore

4. Theoretically, if we know $V(x)$, we can calculate $R(k)$ and $T(k)$.
5. Experimentally, we can measure $R(k)$ and $T(k)$ to gain knowledge of $V(x)$.

Now let’s look at the 3D, which shares many features with the 1D case. However, it is much more complicated due to angle dependence. The differential scattering cross section is
\[
\frac{d\sigma}{d\Omega} = \frac{\text{number of particles scattered in } d\Omega/\text{sec}}{\text{number of incident particles/sec/area } \times d\Omega}.
\]

(10.2)

The following is the derivation of \(d\sigma / d\Omega\) based on definition of Eq. (10.2). Neglecting the trivial normalization factor, the total wave function is

\[
\psi_k = e^{ikr} + \psi_{sc}(r, \theta, \phi),
\]

(10.3)

where the incident wave is \(e^{ikr}\) and the scattered wave is \(\psi_{sc}(r, \theta, \phi)\). When \(r \to \infty\), assume \(rV(r) \to 0\) to guarantee a non-divergent solution of \(\psi_{sc}\):

\[
(\nabla^2 + k^2)\psi_{sc} = 0, \quad \text{for } r \to \infty.
\]

(10.4)

The general solution for the free-particle equation in spherical coordinates:

\[
\psi_{sc}(r, \theta, \phi)_{r \to \infty} = \sum_l \sum_m (A_l j_l(kr) + B_l n_l(kr))Y_l^m(\theta, \phi),
\]

(10.5)

where \(Y_l^m\) is the spherical harmonics, \(j_l\) and \(n_l\) the spherical Bessel and spherical Neumann functions, respectively. The asymptotic behaviors of \(j_l\) and \(n_l\):

\[
j_l(kr) \to \infty \quad \sin(kr - \pi l / 2) / kr,
\]

(10.6)

\[
n_l(kr) \to \infty \quad -\cos(kr - \pi l / 2) / kr.
\]

(10.7)

To get a purely outgoing wave for \(\psi_{sc} = e^{ikr} / r\), \(A_l\) and \(B_l\) must satisfy \(A_l / B_l = -i\), then

\[
\psi_{sc}(r, \theta, \phi)_{r \to \infty} = e^{ikr} \sum_l \sum_m (-i)^l (-B_l)Y_l^m(\theta, \phi) = e^{ikr} \frac{f(\theta, \phi)}{r}
\]

(10.8)

\[
\psi_k \to \infty \quad e^{ikr} + f(\theta, \phi) \frac{e^{ikr}}{r}
\]

(10.9)

where the scattering amplitude

\[
f(\theta, \phi) = \frac{1}{k} \sum_l \sum_m (-i)^l (-B_l)Y_l^m(\theta, \phi).
\]

(10.10)

The probability flux (current density) for a particle with mass \(m\) and wave function \(\psi\):

\[
\mathbf{j}(\mathbf{r}, t) = \frac{\hbar}{2im} \left( \psi^* \nabla \psi - \psi \nabla \psi^* \right),
\]

(10.11)

which satisfies the continuity equation

\[
\frac{\partial \rho}{\partial t} + \nabla \cdot \mathbf{j} = 0.
\]

(10.12)
Here $\rho(r, t) = |\psi(r, t)|^2$ is probability density, and Eq. (10.12) is derived from Schrödinger equation.

In polar coordinate systems,
\[
\nabla = \hat{r} \frac{\partial}{\partial r} + \hat{\theta} \frac{\partial}{\partial \theta} + \hat{\phi} \frac{1}{r \sin \theta} \frac{\partial}{\partial \phi}.
\]  
(10.13)

The magnitude of the incident flux:
\[
\mathbf{j}_{\text{inc}} = \frac{\hbar}{2im} \left( e^{-ikr \cos \theta} \nabla e^{ikr \cos \theta} - e^{ikr \cos \theta} \nabla e^{-ikr \cos \theta} \right) = \frac{\hbar k}{m}.
\]  
(10.14)

The scattered flux:
\[
\mathbf{j}_{\text{sc}} = \frac{\hbar}{2im} \left( \psi^*_\text{sc} \nabla \psi - \psi \nabla \psi^* \right).
\]  
(10.15)

At the limit of $r \to \infty$, the derivatives along $\hat{\theta}$ and $\hat{\phi}$ directions behave as $\sim \frac{1}{r^2}$ (Q: why?), while the derivative along $\hat{r}$ is
\[
\frac{\partial}{\partial r} \left[ f(\theta, \phi) e^{ikr} \right] = f(\theta, \phi) ik \frac{e^{ikr}}{r} + f(\theta, \phi) (-1) \frac{e^{ikr}}{r^2}.
\]  
(10.16)

Dropping the $\sim \frac{1}{r^2}$ terms at the limit of $r \to \infty$, we obtain
\[
\mathbf{j}_{\text{sc}} = \frac{\hbar k}{m} \frac{|f(\theta, \phi)|^2}{r^2} \hat{r}.
\]  
(10.17)

The probability (proportional to number of particles) flows into solid angle $d\Omega$ at the rate
\[
R(d\Omega) = \mathbf{j}_{\text{sc}} \cdot r^2 d\Omega,
\]  
(10.18)

The incident flux $\mathbf{j}_{\text{inc}}$ is proportional to the number of particles/sec/area, thus
\[
\frac{d\sigma}{d\Omega} = \frac{R(d\Omega)}{\mathbf{j}_{\text{inc}} d\Omega} \Rightarrow \frac{d\sigma}{d\Omega} = \frac{f(\theta, \phi)}{2k} |f(k, k')|^2.
\]  
(10.19)

Notes:

(1) $f(\theta, \phi)$ is also written as $f(k, k')$, with $k$ and $k'$ the incident and scattered wave vectors.

(2) We have considered elastic scattering, i.e., $k' = k$; in general, $\frac{d\sigma}{d\Omega} = \frac{k'}{k} |f(k, k')|^2$. 

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(3) We only study the elastic scattering in this class.

Methods to compute the scattering amplitude $f(\theta, \phi)$:
(1) Time-dependent perturbation theory
(2) Time-independent perturbation theory
(3) Exact theory

10.2 Formal Theory and the Born Series
Up to a normalization parameter, the wave function of a free particle is $\phi_k = e^{ikr}$, which satisfies
\[ (\nabla^2 + k^2)\phi_k = 0. \tag{10.20} \]

Under full potential $V(r)$ a particle’s wave function $\psi_k$ can be obtained by solving
\[ (\nabla^2 + k^2)\psi_k(r) = \frac{2m}{\hbar^2}V(r)\psi_k(r). \tag{10.21} \]

We write the total wave function in the form: $\psi_k = e^{ikr} + \psi_{sc}$, with eigenenergy $E_k = \frac{\hbar^2k^2}{2m}$, but momentum is not well defined. Here $k$ is the wave vector of the incident wave $\psi_{inc} = e^{ikr}$, while we have derived that the scattered wave $\psi_{sc} \rightarrow r \rightarrow \infty f(\theta, \phi) \frac{e^{ikr}}{r}$.

We need to solve the full potential Schrodinger equation [Eq. (10.21)] to obtain $f(\theta, \phi)$. We use Green’s function $G_0(k;r,r')$ to find the formally exact solution, which satisfies
\[ (\nabla^2 + k^2)G_0(k;r,r') = \frac{2m}{\hbar^2} \delta(r-r'). \tag{10.22} \]

The exact solution to Eq. (10.21) can be obtained by solving the Lippman-Schwinger equation:
\[ \psi_k(r) = e^{ikr} + \int G_0(k;r,r')V(r')\psi_k(r')dr'. \tag{10.23} \]
As usual, we can solve it iteratively starting from the zeroth order:
Zero-th order (for zero potential $V$): $\psi_k^{(0)} = e^{ikr}$.

First-order Born approximation:
\[ \psi_k^{(1)}(r) = e^{ikr} + \int G_0(k;r,r')V(r')e^{ikr'}dr'. \tag{10.24} \]
You might see the above expression in symbolic form in literature:

\[ \psi^{(1)} = \psi^{(0)} + G_0 V \psi^{(0)}. \]  

(10.25)

The **Born Series** for exact solution:

\[ \psi = \psi^{(0)} + G_0 V \psi^{(0)} + G_0 V G_0 V \psi^{(0)} + \cdots. \]

(10.26)

In this class, we focus on the first-order Born approximation, which requires an explicit form to Green’s function \( G_0(k; r - r') \), which can be obtained using contour integral:

\[ G_0(k; r, r') = G_0(k; r - r') = -\frac{e^{i|kr - r'|}}{|r - r'| \frac{2\pi \hbar}{m}}. \]

(10.27)

Then

\[ \psi_k(r) = e^{ikr} - \frac{m}{2\pi \hbar^2} \int \frac{e^{i|kr - r'|}}{|r - r'|} V(r') \psi_k(r') \, d^3r'. \]

(10.28)

and \( \psi_k(r) = e^{ikr} + \psi_{sc}(r) \).

Now we derive the formally exact \( f(\theta, \phi) \) for \( \psi_{sc} \rightarrow_{r \to \infty} f(\theta, \phi) \frac{e^{ikr}}{r} \). When \( r \to \infty \),

\[ |r - r'| \to r(1 - r \cdot r' / r^2), \]

then

\[ \frac{1}{|r - r'|} \to \frac{1}{r} \left( 1 + \frac{r \cdot r'}{r^2} \right), \]

\[ k |r - r'| \to kr \left( 1 - \frac{r \cdot r'}{r^2} \right) = kr - k' \cdot r', \]

(10.31)

where the scattered wave vector \( k' = \hbar \hat{r} \) for elastic scattering. Thus,

\[ \frac{e^{ikr}}{|r - r'|} \to \frac{e^{ikr}}{r} e^{-i \hat{r}'}, \]

(10.32)

\[ \psi_{sc}(r) \rightarrow_{r \to \infty} -\frac{m}{2\pi \hbar^2} \int e^{-i \hat{r}' \cdot r'} V(r') \psi_k(r') \, d^3r', \]

(10.33)

and finally we obtain the exact expression for scattering magnitude:

\[ f(\theta, \phi) = f(k, k') = -\frac{m}{2\pi \hbar^2} \int e^{-i \hat{r}' \cdot r'} V(r') \psi_k(r') \, d^3r'. \]

(10.34)
Note that
\[ \int e^{-kr'} V(r') \psi_k^*(r') d^3 r' = (2\pi)^3 \langle k' | V | \psi_k^* \rangle \] (10.35)

10.3 T-Matrix

Define the T-matrix as
\[ \mathcal{T}(k, k') \equiv \frac{1}{(2\pi)^3} \int e^{-kr'} V(r) \psi_k (r) d^3 r , \] (10.36)
so that
\[ \frac{d\sigma}{d\Omega} = \left[ \frac{4\pi^2 m}{\hbar^2} \right]^2 \left| \mathcal{T}(k, k') \right|^2 . \] (10.37)

The Born series \( \psi = \psi^{(0)} + G \psi^{(0)} + G^2 \psi^{(0)} + \cdots \) can be employed to obtain the T-matrix.

Under the (1st-order) Born approximation:
\[ \mathcal{T}^{(1)}(k, k') = \frac{1}{(2\pi)^3} \int e^{-k'r'} V(r) e^{ikr} d^3 r , \] (10.38)
which is essentially the Fourier transformation of potential:
\[ \tilde{V}(k - k') = \frac{1}{(2\pi)^3} \int e^{-kr'} V(r) e^{ikr} d^3 r . \] (10.39)

Let
\[ \tilde{T}(k, k') = \tilde{T}(k - k') = \int e^{-k'r'} T(r) e^{ikr} d^3 r , \] (10.40)
combining with the definition of T-matrix [Eq. (10.36)], we obtain
\[ T(r) \phi_k^*(r) = V(r) \psi_k (r) . \] (10.41)

Obviously, \( T^{(1)}(r) = V(r) \) and then \( \mathcal{T}^{(1)}(k, k') = \tilde{T}^{(1)}(k - k') = \tilde{V}(k - k') . \) The expansion (Born series) of \( T \) is similar to that of \( \psi \), as we expect.

Recast this problem more formally: \( H = H_0 + V \), and
\[ H_0 \phi_k = \varepsilon_k \phi_k \] (10.42)
with \( H_0 = p^2 / 2m, \varepsilon_k = \hbar^2 k^2 / 2m \), and \( \phi_k (r) = e^{ikr} \). The full-potential Schrödinger equation:
\[ H \psi_k = E_k \psi_k , \] (10.43)
and \( \psi_k = \phi_k + \phi_{sc} \). For elastic scattering, \( E_k = \varepsilon_k = \frac{\hbar^2 k^2}{2m} \). Eq. (10.43) \( \Rightarrow \)

\[(E_k - H_0)\psi_k = V\psi_k \Rightarrow (E_k - H_0)\psi_{sc} = V\psi_k, \quad (10.44)\]

because \( (E_k - H_0)\phi_k = 0 \). Operating \( (E_k - H_0)^{-1} \) on both sides of Eq. (10.44):

\[\psi_{sc} = (E_k - H_0)^{-1}V\psi_k, \quad (10.45)\]

we obtain the **Lippman-Schwinger equation**:

\[\psi_k = \phi_k + (E_k - H_0)^{-1}V\psi_k. \quad (10.46)\]

We introduce a **Green’s function** defined as

\[G_0 = G_{H_0}(E) = \lim_{\eta \to 0} (E - H_0 + i\eta)^{-1}. \quad (10.47)\]

Here \( H_0 \) is an operator, and positive \( \eta \) ensures that the scattered wave \( \psi_{sc} \) is outgoing. Thus

\[\psi_k(r) = \phi_k(r) + G_0 V(r)\psi_k(r). \quad (10.48)\]

Using Eq. (10.41), i.e., \( T(r)\phi_k(r) = V(r)\psi_k(r) \), we derive the **T-matrix equation** (Dyson’s Eq.):

\[T(r) = V(r) + V(r)G_0 T(r), \quad (10.49)\]

which can be solved iteratively:

\[T = V + VG_0 + VG_0 VG_0 + \cdots \quad (10.50)\]

Define

\[G = G_H(E) = \lim_{\eta \to 0} \frac{1}{E - H + i\eta} = \frac{1}{E - H_0 + i\eta}(1 - G_0 V) = \frac{G_0}{1 - G_0 V} \quad (10.51)\]

Then

\[T = V + VG_0, \quad (10.52)\]

We have derived the Born series for \( T \) and \( \psi \) using two slightly different approaches, but they essentially the same. One can verify that

\[G_0(k;r, r') = \langle r \rvert \frac{1}{E - H_0 + i\eta} \rvert r' \rangle = \langle r \rvert \frac{1}{\frac{\hbar^2 k^2}{2m} - H_0 + i\eta} \rvert r' \rangle = -\frac{m}{2\pi \hbar^2} e^{i(k-r)} \quad (10.53)\]

Alternatively,
\[ G_0(\mathbf{r}; \mathbf{r}') = \int \frac{\phi_k(\mathbf{r})\phi_k^*(\mathbf{r}')}{\varepsilon_k - \varepsilon_k' + i\eta} d^3k' = \frac{1}{\varepsilon_k - H_0 + i\eta} \int e^{i\mathbf{k} \cdot (\mathbf{r} - \mathbf{r}')} d^3k' \]

\[ = \frac{1}{\varepsilon_k - H_0 + i\eta} \delta(\mathbf{r} - \mathbf{r}'). \]

### 10.4 Applications and Validity of the First-order Born Approximation

With the dramatic progress in computational power, now we can calculate exact differential cross sections for any potential. But analytically, first-order Born approximation is still widely used to reveal the basic physics and estimate the magnitude. In the following, we discuss two examples using the first-order Born approximation.

To the first order, \( T^{(1)}(\mathbf{r}) = V(\mathbf{r}) \) and then

\[ \tilde{T}^{(1)}(\mathbf{k}, \mathbf{k}') = T^{(1)}(\mathbf{k} - \mathbf{k}') = \tilde{V}(\mathbf{k} - \mathbf{k}') \]

\[ = \frac{1}{(2\pi)^3} \int e^{i(k-k')\mathbf{r}} V(\mathbf{r}) d^3\mathbf{r}. \]  \hspace{1cm} (10.55)

The scattering magnitude

\[ j^{(1)}(\mathbf{k}, \mathbf{k}') = -\frac{4\pi^2 m}{\hbar^2} \tilde{T}^{(1)}(\mathbf{k}, \mathbf{k}'), \]  \hspace{1cm} (10.56)

and the differential cross section

\[ \frac{d\sigma}{d\Omega} = \left| \frac{4\pi^2 m}{\hbar^2} \tilde{T}^{(1)}(\mathbf{k}, \mathbf{k}') \right|^2. \]  \hspace{1cm} (10.57)

As shown in Fig. 9.3, for elastic scattering, \( T^{(1)}(\mathbf{k}, \mathbf{k}') = T^{(1)}(\mathbf{k} - \mathbf{k}') = T^{(1)}(\mathbf{q}) \), and here

\[ q = |\mathbf{k} - \mathbf{k}'| = 2k \sin(\theta / 2). \]  \hspace{1cm} (10.58)

For the special case of spherical potential, \( V(\mathbf{r}) = V(r) \), \( T^{(1)}(\theta) \) depends only on polar angle \( \theta \):

\[ T^{(1)}(\theta) = \frac{1}{8\pi^3} \int_0^\infty \int_0^{2\pi} \int_0^\pi V(r)e^{iqr\cos(\theta)} r^2 \sin(\theta') d\theta' d\phi dr \]

\[ = \frac{1}{2\pi^2 q} \int_0^\infty r V(r) \sin(qr) dr \] \hspace{1cm} (10.59)

**Example 1:** finite square well, a simple model for nuclei.

![Fig. 10.3: Scattering with angle \( \theta \).](image)

![Fig. 10.4: differential cross section.](image)
\[ V(r) = \begin{cases} V_0 & (r \leq a) \\ 0 & (r > a) \end{cases} \quad (10.60) \]

We use Eq. (10.59) to find that
\[ T^{(1)}(\theta) = \frac{V_0 a^3}{2\pi^2 (qa)^3} \left[ \frac{\sin(qa)}{qa} - \cos(qa) \right], \quad (10.61) \]
\[ \frac{d\sigma}{d\Omega} = \frac{4m^2 V_0^2 a^2}{\hbar^4 q^4} \left[ \frac{\sin(qa)}{qa} - \cos(qa) \right]^2. \quad (10.62) \]

**Question:** in Fig. 9.4 there are many minima in differential cross section, why?

**Example 2:** Yukawa potential (Screened Coulomb potential), for massive scalar fields.

\[ V(r) = \frac{V_0 e^{-\mu r}}{\mu r}. \quad (10.63) \]

Using Eq. (10.59) it is straightforward to obtain
\[ T^{(1)}(\theta) = \frac{1}{16\pi^2} \frac{V_0}{\mu} \frac{1}{q^2 + \mu^2}, \quad (10.64) \]
with (10.61)
\[ q^2 = 4k^2 \sin^2(\theta / 2) = 2k^2(1 - \cos \theta). \quad (10.65) \]

In the following we discuss the physics involved:

(1) Let \( \mu \to 0 \) but keep \( V_0 / \mu \) a constant, Yukawa potential reduces to Coulomb potential.

If \( V_0 / \mu = ZZ' e^2 \),
\[ \frac{d\sigma}{d\Omega} = \left( \frac{2mZZ' e^2}{\hbar^2} \right)^2 \frac{1}{4k^4(1 - \cos \theta)^2} = \frac{1}{16} \left( \frac{ZZ' e^2}{E_K} \right)^2 \frac{1}{\sin^4(\theta / 2)}. \quad (10.66) \]

It recovers the classical Rutherford scattering! The first-Born result is valid in the high-energy limit, for which classical and quantum results typically agree.

(2) The total cross section:
\[ \sigma = \left( \frac{2m V_0}{\mu \hbar^2} \right)^2 \frac{4\pi}{\mu^2(\mu^2 + 4k^2)}. \quad (10.67) \]
For Coulomb potential, it becomes infinity, which means that all incident probability current will be scattered, no matter how large the incident cross section is. Therefore, the Coulomb interaction is an infinite-range interaction, while the Yukawa potential is a finite-range interaction.

**Validity:** we replace \( \psi_k = e^{ikr} + \psi_{sc} \) by just \( e^{ikr} \) so that we need to ensure that

\[
|\psi_{sc}| \ll |e^{ikr}| = 1. \tag{10.68}
\]

The scattered wave has the maximum amplitude at scattering center \( r = 0 \), then \( |\psi_{sc}(0)| \ll 1 \).

\[
\psi_{sc}(r) = -\frac{m}{2\pi\hbar^2} \int \frac{e^{ik|r-r'|}}{|r-r'|} V(r')e^{ikr'}dr', \tag{10.69}
\]

Then \( |\psi_{sc}(0)| \ll 1 \Rightarrow \)

\[
\left| \frac{m}{2\pi\hbar^2} \int \frac{e^{ikr}}{r} V(r)e^{-ikr}dr \right| \ll 1. \tag{10.70}
\]

For spherical potential \( V(r) = V(r) \), the validity condition is

\[
\left| \frac{2m}{\hbar^2 k} \int e^{ikr} \sin(kr)V(r)dr \right| \ll 1. \tag{10.71}
\]

In the following we consider \( r \) within a small scatter region of \( r_0 \).

(1) For low energy, \( kr \to 0 \), \( e^{ikr} \to 1 \), \( \sin(kr) \to kr \). \( |\psi_{sc}(0)| \ll 1 \Rightarrow \)

\[
\frac{2m}{\hbar^2} \left| \int V(r)dr \right| \ll 1. \tag{10.72}
\]

Using the simplest finite square well model: \( V(r) = \begin{cases} V_0 & (r \leq r_0) \\ 0 & (r > r_0) \end{cases} \),

we obtain the condition for the first-order Born Approximation:

\[
\frac{mV_0r_0^2}{\hbar^2} \ll 1 \iff V_0 \ll \frac{\hbar^2}{mr_0^2}. \tag{10.73}
\]

(2) For high energy, \( kr \gg 1 \). \( e^{ikr} \sin(kr) = \frac{1}{2i}(e^{2ikr} - 1) \); since \( kr \gg 1 \), the \( e^{2ikr} \) term oscillates fast in the scattering range, which averages to zero. Therefore, \( |\psi_{sc}(0)| \ll 1 \Rightarrow \)
\[
\frac{m}{\hbar^2} \left| \int V(r) \, dr \right| \ll 1 \quad (10.74)
\]
we obtain the condition for the first-order Born Approximation:

\[
\frac{mV_0r_0}{\hbar^2 k} \ll 1 \quad \Rightarrow \quad V_0 \ll \frac{\hbar^2 k}{mr_0}. \quad (10.75)
\]

**Conclusions:** (i) If the Born approximation is good at low energy, it is also good for high energy; (ii) The Born approximation is normally good for high-energy limit, but it might fail miserably at the low-energy limit.

### 10.5 Partial Wave and Phase Shift; Optical Theorem

**Motivations:**
1. At low energy the first-Born approximation breaks down except for very weak scattering potential;
2. For the scattered spherical-like wave (especially at low energy), it is of great interest to study the angular momentum dependency on scattering amplitude.

The incident planewave can be decomposed of angular-momentum states

\[
e^{ikz} = e^{ikr \cos \theta} = \sum_{l=0}^{\infty} (2l+1)^{1/2} j_l(kr) P_l(\cos \theta), \quad (10.76)
\]

where \( j_l \) is the spherical Bessel function, and \( P_l \) the Legendre polynomials,

\[
P_l(\cos \theta) = \left( \frac{4\pi}{2l+1} \right)^{1/2} Y_l^0(\theta). \quad (10.77)
\]

For spherical potential \( V(r) = V(r) \), \( f(\theta, \phi) = f(\theta) \), and it also depends on \( k \):

\[
f(\theta, k) = \sum_{l=0}^{\infty} (2l+1)a_l(k) P_l(\cos \theta), \quad (10.78)
\]

where \( a_l(k) \) is the \( l \)-th partial wave amplitude, which is the measure of the scattering strength for the state with the (orbital) angular momentum \( lh \). For the low-energy case, \( l_{\text{max}} \approx kr_0 \) (Q: why?), so you don’t need to compute many \( a_l(k) \).

Now the task is to find \( a_l(k) \) for a given potential \( V(r) \). Let’s begin with a free particle,

\[
j_l(kr) \rightarrow_{r \to \infty} \frac{\sin(kr - l\pi / 2)}{kr}, \quad (10.79)
\]

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

\[
= \frac{1}{2ik} \sum_{l=0}^{\infty} (2l+1) \left[ \frac{e^{ikr}}{r} - \frac{e^{-i(kr-l\pi)}}{r} \right] P_l(\cos \theta) .
\] (10.80)

Here there are one incoming and one outgoing wave for each value of \( l \), and their probability current densities cancel out, i.e., no net probability flux flows into or comes out of the origin.

When potential \( V(r) \) is turned on, the wave function is not \( e^{ikz} \), instead,

\[ \psi_k(r) = \sum_{l=0}^{\infty} (2l+1)i^l R_l(kr)P_l(\cos \theta) , \] (10.81)

where the radial wave function \( R_l(kr) \) should reduce to that of a free-particle at \( r \to \infty \) for each value of \( l \):

\[ R_l(kr) \rightarrow r \to \infty \frac{A_l \sin[kr - l\pi/2 + \delta_l(k)]}{kr} = \frac{A_l}{2ikr} \left[ e^{i\delta_l}e^{i(kr-l\pi/2)} - e^{-i\delta_l}e^{-i(kr-l\pi/2)} \right] , \] (10.82)

where \( \delta_l(k) \) is the phase shift.

To keep the incoming wave unchanged, we set \( A_l = e^{i\delta_l} \). Then

\[ \psi_k(r) \rightarrow r \to \infty \frac{1}{2ik} \sum_{l=0}^{\infty} (2l+1) \left[ \frac{e^{2i\delta_l}e^{ikr}}{r} - \frac{e^{-i(kr-l\pi)}}{r} \right] P_l(\cos \theta) \]

\[
= e^{ikz} + \sum_{l=0}^{\infty} (2l+1) \left[ \frac{e^{2i\delta_l} - 1}{2ik} \right] P_l(\cos \theta) \frac{e^{ikr}}{r} .
\] (10.83)

Comparing with the expression for \( f(\theta, k) \), i.e., Eq. (10.78), we obtain

\[ a_l(k) = e^{2i\delta_l(k)} - 1 \frac{1}{2ik} = \frac{1}{k} e^{i\delta_l} \sin(\delta_l) . \] (10.84)

The scattering amplitude

\[ f(\theta) = \frac{1}{k} \sum_{l=0}^{\infty} (2l+1)e^{i\delta_l} \sin(\delta_l)P_l(\cos \theta) . \] (10.85)

The total cross section

\[ \sigma = \int \frac{d\sigma}{d\Omega} d\Omega = \int |f(\theta)|^2 d\Omega = \frac{4\pi}{k^2} \sum_{l=0}^{\infty} (2l+1) \sin^2(\delta_l) , \]

using the orthogonality of Legendre polynomials \( P_l(x) \):
\[ \int_0^\pi P_i(\cos \theta)P_i(\cos \theta) \sin(\theta) d\theta = \frac{2}{2l+1}. \]  \hspace{1cm} (10.86)

On the other hand, \( P_i(\cos 0) = P_i(1) = 1 \), then

\[ \text{Im}[f(0)] = \frac{1}{k} \sum_{l=0}^\infty (2l+1) \sin^2(\delta_k) \]  \hspace{1cm} (10.87)

Thus we have proved the famous **optical theorem**:

\[ \sigma = \frac{4\pi}{k} \text{Im}[f(0)]. \]  \hspace{1cm} (10.88)

An alternative proof is based on **Lippman-Schwinger equation**:

\[ |\psi_k\rangle = |k\rangle + G_0 V |\psi_k\rangle. \]  \hspace{1cm} (10.89)

Operating \( \langle k | V \psi_k \rangle \) from the left side on Eq. (10.89):

\[ \langle k | V \psi_k \rangle = \langle \psi_k | - \langle \psi_k | V^\dagger G_0^\dagger V \langle \psi_k | = \langle \psi_k | V \psi_k \rangle - \langle \psi_k | V^\dagger G_0^\dagger V \psi_k \rangle. \]  \hspace{1cm} (10.90)

Here the Green function (operator) is

\[ G_0^\dagger = \lim_{\eta \to 0} (E - \hat{H}_0 - i\eta)^{-1} \]
\[ = \lim_{\eta \to 0} \int_{-\infty}^{+\infty} \frac{\delta(E - E')}{E' - \hat{H}_0 - i\eta} dE' = i\pi \delta(E - \hat{H}_0). \]  \hspace{1cm} (10.91)

Since \( G_0^\dagger \) has purely imaginary part, we look at the imaginary parts on both sides of Eq. (10.90):

\[ \text{Im}(\langle k | V \psi_k \rangle) = -\pi \langle \psi_k | V^\dagger \delta(E - \hat{H}_0)V \psi_k \rangle = -\pi \langle k | T^\dagger \delta(E - \hat{H}_0)T | k \rangle. \]  \hspace{1cm} (10.92)

We have used Eq. (10.41), i.e., \( T | \psi_k \rangle = V | k \rangle \). Using \( \frac{d\sigma}{d\Omega} = \left( \frac{4\pi^2 m}{\hbar^2} \right)^2 |T(k,k')|^2 \), we can derive

\[ \langle k | T^\dagger \delta(E - \hat{H}_0)T | k \rangle = \langle k | T^\dagger \delta(E - \hat{H}_0) \int |k'\rangle \langle k'|d^3k' |T| k \rangle \]
\[ = \int \langle k | T^\dagger \delta(E - E') | k' \rangle \langle k'|d^3k' \]
\[ = \int |T(k,k')|^2 \delta(E - E') d^3k' \]
\[ = \left( \frac{\hbar^2}{4\pi^2 m} \right)^2 \int \frac{d\sigma}{d\Omega} \delta \left( \frac{\hbar^2 k^2}{2m} - \frac{\hbar^2 k'^2}{2m} \right) k'^2 dk' d\Omega \]
\[ = \left( \frac{\hbar^2}{4\pi^2 m} \right)^2 \frac{k^2}{2\hbar^2 k / 2m} \int \frac{d\sigma}{d\Omega} d\Omega = \frac{k\hbar^2}{(2\pi)^4 m} \sigma. \]  \hspace{1cm} (10.93)
Thus we have proved the optical theorem:

\[ \text{Im} \left[ f(\theta = 0) \right] = \left\{ -\frac{4\pi^2 m}{\hbar^2} \right\} (-\pi) \frac{\hbar^2 k}{(2\pi)^4 m} \sigma = \frac{k}{4\pi} \sigma \]  

(10.94)

Another interesting result is

\[ e^{i\phi} \sin(\delta_i) = -\frac{2mk}{\hbar^2} \int_0^\infty j_i(kr)V(r)R_i(kr)r^2 \, dr, \]

(10.95)

and one can use this to determine phase shift \( \delta_i \).

### 10.6 Determination of Phase Shifts

Let’s begin with a brief review of radial wave functions for central potential

\[-\frac{\hbar^2}{2m} \frac{d^2}{dr^2} + V_{\text{eff}}(r)\chi_i = E\chi_i, \]

(10.96)

where \( \chi_i(r) = rR_i(r) \), and the effective potential \( V_{\text{eff}}(r) = V(r) + \frac{l(l+1)\hbar^2}{2mr^2} \). For free particles,

\[ R_i(r) = c_1 j_i(kr) + c_2 n_i(kr). \]

(10.97)

Asymptotically, when \( kr \to 0 \),

\[ j_i(kr) \to \begin{cases} 0 & (l \neq 0) \\ 1 & (l = 0) \end{cases}; \quad n_i(kr) \to \infty. \quad \text{Thus } R_i(kr) = c_1 j_i(kr). \]

(10.98)

We want to determine phase shifts \( \delta_i \) for a scattering potential \( V(r) \) that vanishes for \( r > r_0 \). Outside the scattering center, it is a free particle, but \( R_i(r) = c_1 j_i(kr) + c_2 n_i(kr) \), since the origin is excluded. The wave function after scattering:

\[ \psi_i^k(r) = \sum_{l=0}^{\infty} (2l+1)i^l R_i(kr)P_l(\cos \theta). \]

(10.99)

We use the asymptotic behaviors of \( \psi_i^k \), \( j_i \) and \( n_i \) to determine \( c_1 \) and \( c_2 \):

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

(10.100)
we obtain $c_1 = e^{i\delta_0} \cos(\delta_0)$ and $c_2 = -e^{i\delta_0} \sin(\delta_0)$, so that

$$R_l(r) = e^{i\delta_0} \left[ \cos(\delta_0) j_l(kr) - \sin(\delta_0) n_l(kr) \right], \quad \text{for } r > r_0.$$  

We can match the radial wave function $R_l(r)$ at $r = r_0$ to find the phase shift $\delta_0$.

Example 1: The **Hard Sphere**

$$V(r) = \begin{cases} \infty, & r \leq r_0 \\ 0, & r > r_0 \end{cases}.$$  

Boundary condition $R_l(r_0) = 0 \Rightarrow$

$$\tan(\delta_0) = \frac{j_l(kr_0)}{n_l(kr_0)} \Rightarrow \delta_0 = \tan^{-1} \left[ \frac{j_l(kr_0)}{n_l(kr_0)} \right] \quad (10.103)$$

(1) Low energy limit $kr_0 \ll 1$, the $s$-wave ($l = 0$) scattering dominates.

$$\delta_0 = \tan^{-1} \left[ \frac{\sin(kr_0)}{kr_0} \right] = \tan^{-1} \left[ -\tan(kr_0) \right] \quad (10.104)$$

$$\Rightarrow \delta_0 = -kr_0. \quad \text{(This is actually exact!)}$$

$$f_0(\theta) = \frac{1}{k} e^{i\delta_0} \sin(\delta_0) P_0(\cos \theta), \quad (10.105)$$

and $P_0(x) = 1 \Rightarrow$

$$\frac{d\sigma_0}{d\Omega} = \left| f_0(\theta) \right|^2 = \frac{1}{k^2} \sin^2(\delta_0) = \frac{1}{k^2} \frac{\tan^2(-kr_0)}{1 + \tan^2(-kr_0)}. \quad (10.106)$$

At the low-energy limit, $\frac{d\sigma_0}{d\Omega} \rightarrow_{k_0 \ll 1} r_0^2$, and we obtain a surprising result:

$$\sigma_0 = \frac{4\pi}{k^2} \sin^2(\delta_0) \rightarrow_{k_0 \ll 1} 4\pi r_0^2, \quad (10.107)$$

Fig. 10.5: Phase shifts for attractive and repulsive scattering potentials.
The total cross section is *four times* the classical results. For other \( l \)-values,

\[
\begin{aligned}
j_l(x) &\rightarrow_{x=0} x^l \frac{x}{(2l+1)!!}, \\
n_l(x) &\rightarrow_{x=0} \frac{(2l-1)!!}{x^{-(l+1)}}.
\end{aligned}
\] (10.108)

Then

\[
\tan(\delta_i) \rightarrow_{kr_0 \ll 1} - \frac{(kr_0)^{2l+1}}{(2l+1)!!(2l-1)!!} \Rightarrow \\
\delta_i \rightarrow_{kr_0 \ll 1} - (kr_0)^{2l+1}.
\] (10.109)

At low energies, the scattering into the high angular momentum states is negligible.

(2) High-energy limit \( kr_0 \gg 1 \),

\[
\begin{aligned}
j_l(kr_0) &\rightarrow_{kr_0 \rightarrow \infty} \frac{\sin(kr_0 - l\pi/2)}{kr_0}, \\
n_l(kr_0) &\rightarrow_{kr_0 \rightarrow \infty} \frac{\cos(kr_0 - l\pi/2)}{kr_0}.
\end{aligned}
\] (10.110)

Then

\[
\tan(\delta_i) = -\tan(kr_0 - l\pi/2) \Rightarrow \delta_i \rightarrow_{kr_0 \gg 1} -kr_0 + l\pi/2, \\
\sin^2(\delta_i) = \sin^2(-kr_0 + l\pi/2) \Rightarrow \sin^2(\delta_i) + \sin^2(\delta_{i+1}) = 1,
\] (10.111) (10.112)

and we obtain

\[
\sigma = \frac{4\pi}{k^2} \sum_{l=0}^{k_0} (2l+1)\sin^2(\delta_i) = \frac{4\pi}{k^2} (kr_0)^2 \frac{1}{2} = 2kr_0^2.
\] (10.113)

The total cross section at high-energy limit is *twice* the classical results.

**Example 2:** The *finite Square Well* \( V(r) = \begin{cases} V_0, & r \leq r_0 \\ 0, & r > r_0 \end{cases} \) and \( V_0 > 0 \) (repulsive) \( V_0 < 0 \) (attractive).

To simplify our discussions, let’s consider only the \( s \)-wave scattering.

For \( r > r_0 \),

\[
R_0(r) = e^{ik_0r} \left[ \cos(\delta_0)j_0(kr) - \sin(\delta_0)n_0(kr) \right] = \frac{e^{ik_0r} \sin(kr + \delta_0)}{kr}. \] (10.114)

For \( r < r_0 \),

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\[ \chi_0(r) = rR_0(r) = A_0 \sin(kr), \quad (10.115) \]

where \( E - V_0 = \frac{\hbar^2 \kappa^2}{2m} \). **Note:** when \( E < V_0 \), \( \kappa = ik' \) with \( k' \) real. Then \( \sin(kr) = \sinh(k'r) \).

Boundary conditions: \( \chi_0(r) \) and its derivative \( \chi_0'(r) \) are continuous at \( r = r_0 \), then

\[
\frac{e^{i\delta}}{k} \sin(kr_0 + \delta_0) = A_0 \sin(\kappa r_0) \quad (10.116)
\]
\[
\frac{e^{i\delta}}{k} \cos(kr_0 + \delta_0) = A_0 \kappa \cos(\kappa r_0)
\]

\[
\Rightarrow \quad \tan(kr_0 + \delta_0) = \frac{k}{\kappa} \tan(\kappa r_0) \quad \Rightarrow \quad \tan(\delta_0) = \frac{k - \kappa \cot(\kappa r_0) \tan(\kappa r_0)}{\kappa \cot(\kappa r_0) + k \tan(\kappa r_0)}.
\]

Thus for attractive potential, \( V_0 < 0, \kappa > k, \delta_0 > 0 \); for repulsive potential, \( V_0 > 0, \kappa < k \), \( \delta_0 < 0 \), as illustrated in Fig. 9.5.

### 10.7 Ramsauer-Townsend Effect

Let’s focus on the attractive case. For a given \( k \) (\( E \) is fixed), when \( |V_0| \) increases, \( \delta_0 \) also increases; one can adjust the values of \( |V_0| \) and \( r_0 \) so that \( \delta_0 = \pi / 2 \), resulting in the maximum cross section for the \( s \)-wave scattering: \( \sigma_0 = \frac{4\pi}{k^2} \). If \( |V_0| \) increases still, eventually one can make \( \delta_0 = \pi \), so that \( \sigma_0 = 0 \), i.e., the \( s \)-wave partial cross section vanishes. Therefore, in the low-energy limit ( \( kr_0 \ll 1 \)), strong attractive potential could lead to perfect transmission without scattering. This is known as the **Ramsauer-Townsend effect**, which was first observed for electron scattering by rare gas atoms such as Ar, Kr and Xe in 1923.

To understand the Ramsauer-Townsend effect, we need to use **Levinson’s theorem**:

\[ \delta_i(k = 0) = N_i \pi \quad (10.118) \]
where $N_l$ is the number of bound states in the potential with angular momentum $l$, $N_l$ is finite for a potential of short range. Previously we have omitted $N_l \pi$ in $\delta_l$ when we discuss if the phase shift is positive and negative.

The phase shift is usually determined by the expression like $\tan(\delta_l) = F(k)$. We have encountered the case that $F(k = 0) = 0$; since $\tan(N \pi) = 0$, how do we determine $N$? The unique answer is obtained by graphing the phase shift as a function of $k$. For any finite attractive scattering potential, we demand that this graph has two characteristics: (1) The phase shift vanishes at very large values of $k$, and (2) The phase shift is a continuous function of $k$.

For the attractive square well potential $V(r) = \begin{cases} V_0, & r \leq r_0 \\ 0, & r > r_0 \end{cases}$ with $V_0 < 0$. Set $k_0^2 = \frac{-2mV_0}{\hbar^2}$, then

$$\kappa^2 = k^2 + k_0^2.$$

(Note: $k^2 = \frac{2mE}{\hbar^2}$)

We have derived

$$\tan(\delta_0) = \frac{k - \kappa \cot(\kappa r_0) \tan(k r_0)}{\kappa \cot(\kappa r_0) + k \tan(k r_0)}$$

previously, see Eq. (10.117). As plotted in Fig. 9.7, in case (1), there is no bound state, $N_0 = 0$. But in case (2), there are one bound state and two bound states in case (3). In case (3), the phase shift passes through $\pi$; however, the Ramsauer-Townsend effect occurs only when $kr_0 < 1$. Higher value of $k_0 r_0$ (i.e. higher $|V_0|$) is required. For example, $kr_0 \sim 0.324$ for the experiment of electron scattering by rare gas atoms.

At the low-energy limit:

![Fig. 10.7: The s-wave phase shift $\delta_0(k)$ for an attractive square well for three values of $k_0 r_0$: (1) $\pi / 4$, (2) $3\pi / 4$, and (3) $7\pi / 4$, as plotted in solid, long-dash and dashed lines.](image)
\[
\frac{d\sigma}{d\Omega} = r_0^2 \left[ 1 - \frac{\tan(k_0 r)}{k_0 r} \right]^2,
\]
so that the differential cross section can be either smaller or larger (sometimes much larger) than \( r_0^2 \).

**10.8 Resonance Scattering**

In atomic, nuclear and particle physics, the scattering for a given partial wave often has a *pronounced peak*, which is called the *resonance scattering*. This is because the phase shift \( \delta_l \) passes through \( \frac{\pi}{2} \) or \( (n+1/2)\pi \), then \( \sigma_l = 4\pi / k^2 \), the maximum value of \( \sigma_l \) for a given \( k \).

The following is an example to show that resonance condition is equivalent to the bound-state condition. Therefore if the potential is attractive enough to form a bound state, then there is a strong possibility that there still also be resonance scattering.

Let’s consider the attractive square well potential

\[
V(r) = \begin{cases} 
V_0, & r \leq r_0 \\
0, & r > r_0 
\end{cases}
\]

with \( V_0 < 0 \).

This time we look at the bound states for \( l \neq 0 \). The radial wave function

\[
R_l(r) = \begin{cases} 
A j_l(\kappa r), & r \leq r_0 \\
B h_l^{(1)}(ikr), & r > r_0 
\end{cases}
\]

where \( \kappa = \sqrt{2m(E - V_0)} / \hbar \), \( k = \sqrt{-2mE} / \hbar \), and the first type spherical Hankel function

\[
h_l^{(1)}(x) = j_l(x) + in_l(x).
\]

Under the low-energy and the strong-attraction limits, i.e., \( kr_0 \ll l \) and \( \kappa_0 r_0 \gg l \) (where \( \kappa_0 = \sqrt{-2mV_0} / \hbar \)), respectively, the asymptotic behaviors are

\[
j_l(x) \rightarrow_{x \rightarrow \pm \infty} \frac{\sin(x - l\pi/2)}{x},
\]

\[
h_l^{(1)}(x) \rightarrow_{x \rightarrow 0} -i \frac{(2l-1)!!}{x^{l+1}}.
\]

Employing the boundary conditions at \( r = r_0 \), i.e., continuity of radial wavefunction and its first-order derivative, one finds that the condition for a bound state to occur is

\[
\kappa_0 r_0 \cot(\kappa_0 r_0 - \frac{l\pi}{2}) = -l.
\]
Since \( \cot(\kappa_0 r_0 - \frac{l\pi}{2}) \approx 0 \) (for the strong-attraction limit), we obtain

\[
\kappa_0 r_0 - l\pi / 2 = (n + 1 / 2)\pi .
\]  (10.124)

The scattering states have \( E > 0 \), and the general expression for the phase shift \( \delta_i \) is:

\[
\cot(\delta_i) = \frac{k n_i'(k r_0) j_i(\kappa_0 r_0) - \kappa_0 n_i(k r_0) j_i'(\kappa_0 r_0)}{k j_i'(k r_0) j_i(\kappa_0 r_0) - \kappa_0 j_i(k r_0) j_i'(\kappa_0 r_0)} .
\]  (10.125)

At a resonance, \( \delta_i = \pi / 2 \) and \( \cot(\delta_i) = 0 \) \( \Rightarrow \)

\[
k n_i'(k r_0) j_i(\kappa_0 r_0) - \kappa_0 n_i(k r_0) j_i'(\kappa_0 r_0) = 0 .
\]  (10.126)

Using the asymptotic properties of \( j_i \) and \( n_i \) under the limits of \( k r_0 \ll l \) and \( \kappa_0 r_0 \gg l \):

\[
j_i(x) \to x^{-l} \frac{\sin(x - l\pi / 2)}{x},
\]

\[
n_i(x) \to x^{-l} \frac{(2l-1)!!}{x^{l+1}},
\]  (10.127)

we obtain

\[-(l+2)\sin(\kappa_0 r_0 - l\pi / 2) + \kappa_0 r_0 \cos(\kappa_0 r_0 - l\pi / 2) = 0 ,
\]  (10.128)

then again due to \( \kappa_0 r_0 \gg l \),

\[
\cos(\kappa_0 r_0 - l\pi / 2) \approx 0 \ \Rightarrow \ \kappa_0 r_0 - l\pi / 2 = (n + 1 / 2)\pi ,
\]  (10.129)

which is exactly the same condition for a bound state.

From Eq. (10.84) one can show that the partial wave amplitude

\[
a_i(k) = \frac{1}{k \cot(\delta_i) - ik} .
\]  (10.130)

We consider the neighborhood of resonance, \( k = k_R \) (or \( E = E_R \)), and \( \delta_i(k = k_R) = \pi / 2 \), by expanding \( \delta_i(E) \) as follows

\[
\cot[\delta_i(E)] \approx \cot[\delta_i(E = E_R)] - \frac{2}{\Gamma}(E - E_R) = -\frac{2}{\Gamma}(E - E_R) .
\]  (10.131)

Here the width \( \Gamma \) is defined by

\[
\frac{d \cot[\delta_i(E)]}{dE} \bigg|_{E=E_R} = -\frac{2}{\Gamma} ,
\]  (10.132)

which leads to

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\[ a_{l}(k) = -\frac{\Gamma / 2}{k \left[ (E - E_{R}) + \frac{i\Gamma}{2} \right]}, \quad (10.133) \]

and
\[ \sigma_{l} = \frac{4\pi}{k^2} \frac{(2l+1)(\Gamma / 2)^2}{(E - E_{R})^2 + (\Gamma / 2)^2}. \quad (10.134) \]

The peak cannot be infinitely sharp because
\[ \sigma_{l}(k) \leq \frac{4(2l+1)\pi}{k^2}. \quad (10.135) \]

Fig. 10.8: \( \sigma_{3} \) versus \( k \) in a resonance scattering.