Scattering theory

Let us consider a typical collision experiment which is illustrated by the schematic drawing below

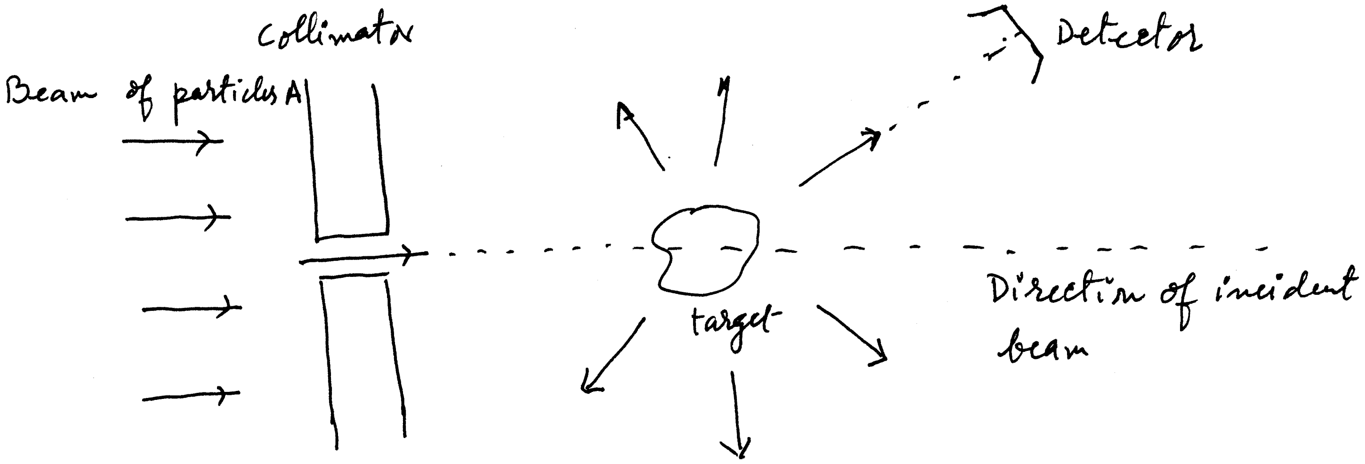


Fig. Schematic drawing of a collision process.

A beam of particles A, well collimated an nearly monoenergetic, is directed towards a target. The incident beam should be neither too intense — so that interactions between the incident particles may be neglected — nor too weak, because one wants to observe a ~~rea~~ reasonable number of 'events' during the experiment.

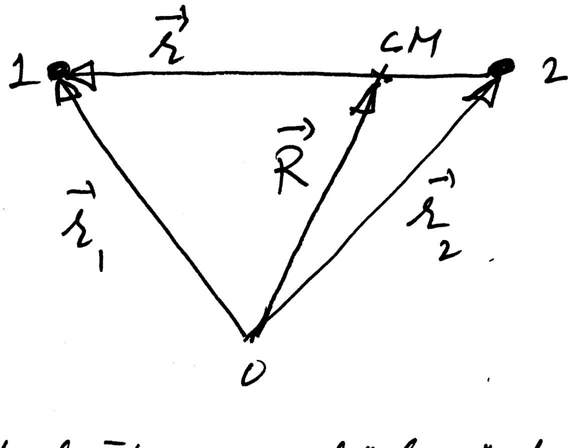
The target usually consists of a macroscopic sample containing a large number of scatterers B. The distance between these scatterers are in general quite large with respect to the de Broglie wavelength of the incident particles, in which case one can neglect coherence effects between the waves scattered by each of the scattering centers. In addition, if the target is sufficiently thin, multiple scattering by several scatterers may be neglected. One may then consider ~~then~~ that each scatterer acts as if it were alone and focus one's attention on the study of a typical collision between a particle A of the ~~beam~~ incident beam and a scatterer B of the target.

After the collision, some or all outgoing particles are detected by detectors at a macroscopic distance from the target.

In this course we will only study elastic scattering between particles, i.e., we will not consider the internal structure of the particles involved in the collision. Further, we will also neglect the spin of the particles. This simplifies the mathematical formalism.

Separation of the center of mass motion in a two-body problem.

Let us consider a non-relativistic system of two particles 1 and 2 with masses m_1 and m_2, coordinates $\vec{r}_1$ and $\vec{r}_2$ measured from some fixed origin O and momenta $\vec{p}_1, \vec{p}_2$.



We assume that these particles interact through a real potential $V(\vec{r}_1 - \vec{r}_2)$ which depends only on the relative coordinates $\vec{r}_1$ and $\vec{r}_2$. The classical Hamiltonian of the system is therefore given by

$$H = \frac{\vec{p}_1^{\,2}}{2m} + \frac{\vec{p}_2^{\,2}}{2m} + V(\vec{r}_1 - \vec{r}_2) \quad \cdots\cdots (1)$$

According to the principles of quantum mechanics, the dynamics of this two-body system is governed by the time-dependent Schrödinger equation

$$H\,\Psi(\vec{r}_1, \vec{r}_2, t) = i\hbar \frac{\partial}{\partial t} \Psi(\vec{r}_1, \vec{r}_2, t) \quad \cdots (2)$$

where $\Psi(\vec{r}_1, \vec{r}_2, t)$ is the wave function of the system and the Hamiltonian operator H, written in the coordinate representation $(\vec{r}_1, \vec{r}_2)$ is obtained by making the substitution $\vec{p}_1 \to -i\hbar \vec{\nabla}_{\vec{r}_1}$ and $\vec{p}_2 \to -i\hbar \vec{\nabla}_{\vec{r}_2}$ on the right hand side of Eq. (1). The Hamiltonian is therefore given by

$$H = -\frac{\hbar^2}{2m_1}\vec{\nabla}_1^{\,2} - \frac{\hbar^2}{2m_2}\vec{\nabla}_2^{\,2} + V(\vec{r}_1 - \vec{r}_2) \qquad (3)$$

where we have written $\vec{\nabla}_1 \equiv \vec{\nabla}_{\vec{r}_1}$ and $\vec{\nabla}_2 \equiv \vec{\nabla}_{\vec{r}_2}$.

The time-dependent Schrödinger equation (2) may be explicitly written as

$$\left(-\frac{\hbar^2}{2m_1}\nabla_1^2 - \frac{\hbar^2}{2m_2}\nabla_2^2 + V(\vec{r}_1 - \vec{r}_2)\right)\Psi(\vec{r}_1 \vec{r}_2, t)$$

$$= i\hbar\frac{\partial}{\partial t}\Psi(\vec{r}_1 \vec{r}_2 t) \quad \cdots (4)$$

This is a partial differential equation in seven variables, namely the six spatial variables and the time. Fortunately, however, several simplifications can be made.

First, since the Hamiltonian operator is time-independent, we may directly separate out the time dependence of the wave function. Indeed, we see that Eq. (4) admits particular solutions of the form

$$\Psi(\vec{r}_1, \vec{r}_2 t) = \psi(\vec{r}_1, \vec{r}_2)\exp\left\{-\frac{i}{\hbar}E_{total}\,t\right\}. \qquad (5)$$

These states are stationary states for which the total energy E_{total} of the system has a definite value. A general solution of Eq. (4) can be obtained as a sum of such particular solutions.

Substituting the expression (5) of Ψ into the Schrödinger equation (4), we find that the time-independent wave function $\psi(\vec{r}_1 \vec{r}_2)$ satisfies the equation

$$\left[-\frac{\hbar^2}{2m_1}\nabla_1^2 - \frac{\hbar^2}{2m_2}\nabla_2^2 + V(\vec{r}_1 - \vec{r}_2)\right]\psi(\vec{r}_1, \vec{r}_2) = E_{total}\,\psi(\vec{r}_1 \vec{r}_2). \quad (6)$$

This is the time-independent Schrödinger equation of our two-body problem.

We now proceed to simplify Eq. (6) by using the fact that the potential only depends on the difference of coordinates $\vec{r}_1 - \vec{r}_2$. We introduce the relative coordinate

$$\vec{r} = \vec{r}_1 - \vec{r}_2 \qquad \text{- - - - - - - (7)}$$

together with the vector

$$R = (m_1 \vec{r}_1 + m_2 \vec{r}_2)/(m_1 + m_2) \qquad \text{- - - - (8)}$$

which determines the position of the center of mass of the system as shown in the figure above.

Changing variables from the coordinates $(\vec{r}_1, \vec{r}_2)$ to the new coordinates $(\vec{r}, \vec{R})$, we see that Eq. (6) can be written in terms of the new coordinates as

$$\left(-\frac{\hbar^2}{2M}\nabla^2_{\vec{R}} - \frac{\hbar^2}{2m}\nabla^2_{\vec{r}} + V(\vec{r})\right)\psi(\vec{R},\vec{r})$$
$$= E_{total}\,\psi(\vec{R},\vec{r}), \qquad (9)$$

where

$$M = m_1 + m_2 \qquad (10)$$

is the total mass of the system and

$$m = m_1 m_2/(m_1+m_2) \qquad (11)$$

is the reduced mass of the particles 1 and 2. In order to avoid the introduction of a new symbol we have adopted here a rather loose notation, writing $\psi(\vec{r}_1,\vec{r}_2) = \psi(\vec{R},\vec{r})$.

Let us now analyze eq. (9) in more detail. Since the potential depends only on $\vec{r}$, a separation of the wave function $\psi(\vec{R},\vec{r})$ can be made into a product of functions of the relative coordinates and the center of mass coordinates. In fact, eq. (9) has a complete set of solutions of the form

$$\Psi(\vec{R},\vec{r}) = \Phi(\vec{R})\psi(\vec{r}) \quad \cdots\cdots\cdots \quad (12)$$

where $\Phi(\vec{R})$ and $\psi(\vec{r})$ satisfy respectively the equations

$$-\frac{\hbar^2}{2M}\nabla^2_{\vec{R}}\Phi(\vec{R}) = E_{CM}\Phi(\vec{R}) \quad \cdots\cdots \quad (13)$$

and

$$\left(-\frac{\hbar^2}{2m}\nabla^2_{\vec{r}} + V(\vec{r})\right)\psi(\vec{r}) = E\,\psi(\vec{r}) \quad \cdots\cdots \quad (14)$$

with

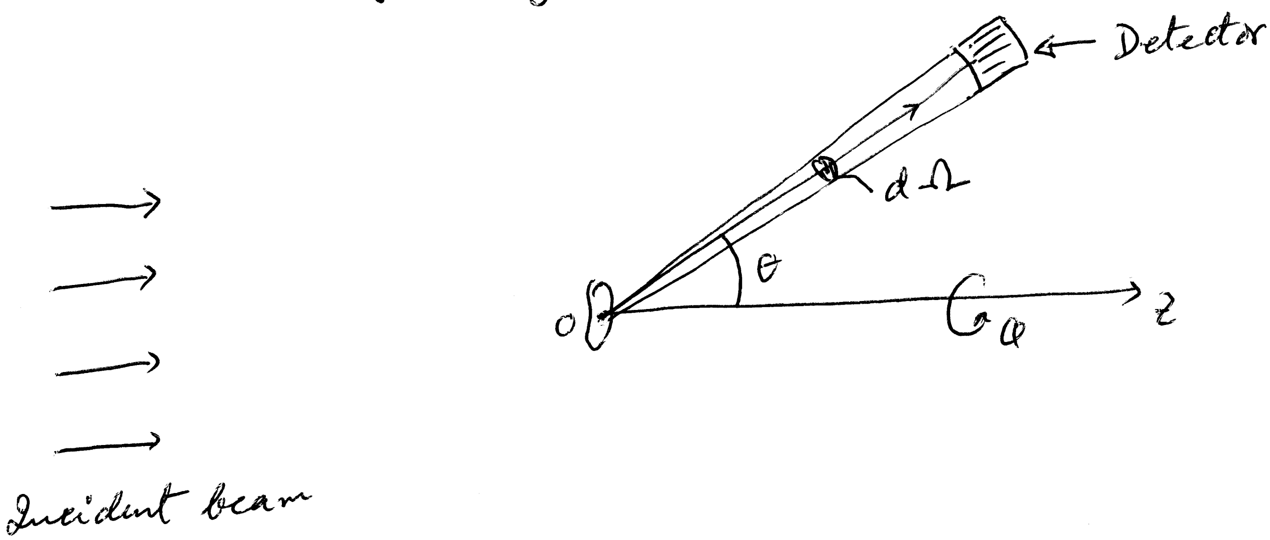
$$E_{total} = E_{CM} + E \,. \quad \cdots\cdots\cdots \quad (15)$$

We see that eq. (13) is a time-independent Schrödinger equation describing the center of mass as a free particle of mass M and energy E_{CM}. The other time-independent Schrödinger equation (eq. (14)), represents a particle of mass m in the potential $V(\vec{r})$.

We have therefore "decoupled" the original two-body problem into two one-body problems, that of a free particle (the center of mass) and that of a single, "relative" particle of reduced mass m in a potential $V(\vec{r})$. Furthermore, if we elect to work in the CM frame of the two colliding particles, as we will do in what follows, we need not be concerned about the motion of the center of mass, whose coordinates are thus eliminated. The problem of scattering of two particles interacting through a potential $V(\vec{r})$ which depends only on their relative coordinates $\vec{r}$ is therefore entire equivalent, in the center of mass frame, to the scattering of a particle of reduced mass m by the potential $V(\vec{r})$.

Definition of cross section.

consider a beam of incident particles each having the same energy ~~being~~ falling on a thin target.



Let J_{inc} be the flux of particles in the incident beam, i.e., number of particles transported by the beam per unit area perpendicular to the beam and per unit time.

A detector is placed far away from the zone of influence of the target particles. The detector's direction is (θ, ϕ) and it subtends a solid angle $d\Omega$ at O.

Let dn be the number of particles scattered into the solid angle $d\Omega$ per unit time and per unit target particle. We have

$$dn \propto d\Omega,\ J_{inc},\ N_{target}$$

where N_{target} is the number of target particles exposed to the beam. We write

$$dn = \sigma(\theta,\varphi)\, d\Omega\, J_{inc}\, N_{target}$$

or

$$\sigma(\theta,\phi)\, d\Omega = \frac{dn}{J_{inc}\, N_{target}}, \qquad \text{.....} \quad (16)$$

The proportionality constant $\sigma(\theta,\phi)$ has the dimensions of an area and is called the differential cross section for scattering by a single scatterer in the direction (θ,φ). For a central potential $(V(\vec{r}) \equiv V(|\vec{r}|))$, the differential cross section does not depend on φ.

The integrated cross section σ is found by integrating the differential cross section over all solid angles. Thus

$$\sigma = \int_{\Omega} \sigma(\theta,\phi)\, d\Omega = \int_{0}^{\pi} d\theta \sin\theta \int_{0}^{2\pi} d\phi\ \sigma(\theta,\phi) . \quad \cdots (17)$$

An alternative notation for differential cross section is $d\sigma/d\Omega$. Thus we write

$$\sigma(\theta,\phi)\, d\Omega = \frac{d\sigma}{d\Omega}\, d\Omega$$

Scattering amplitude

To obtain the scattering cross-section we have to solve the Schrödinger equation

$$\left[-\frac{\hbar^2}{2m}\nabla^2 + V(\vec{r})\right]\psi(\vec{r}) = E\,\psi(\vec{r}) \quad \cdots\cdots (18)$$

i.e.,

$$\left[\nabla^2 + k^2 - U(\vec{r})\right]\psi(\vec{r}) = 0$$

where

$$k^2 = \frac{2mE}{\hbar^2}$$

$$U(\vec{r}) = \frac{2m}{\hbar^2}V(\vec{r}) .$$

We now have to find the appropriate boundary condition that the wavefunction $\psi(\vec{r})$ must satisfy.

We assume that the potential is short-ranged so that at large distances $V(\vec{r}) \to 0$ and $\psi(\vec{r})$ satisfies the free particle wave equation

$$(\nabla^2 + k^2)\psi(\vec{r}) = 0 \quad \cdots\cdots (19).$$

Let us further assume that the incident particles are prepared in a state of definite momentum $\vec{p} = \hbar \vec{k}$ and that the beam is propagating along the z-axis. The initial state is then described by a plane wave

$$\psi_{inc} = e^{ikz} \quad \cdots\cdots (20)$$

After the collision, in addition to the plane wave there must be an outgoing spherical wave originating at the scattering center. This is illustrated in the figure below:

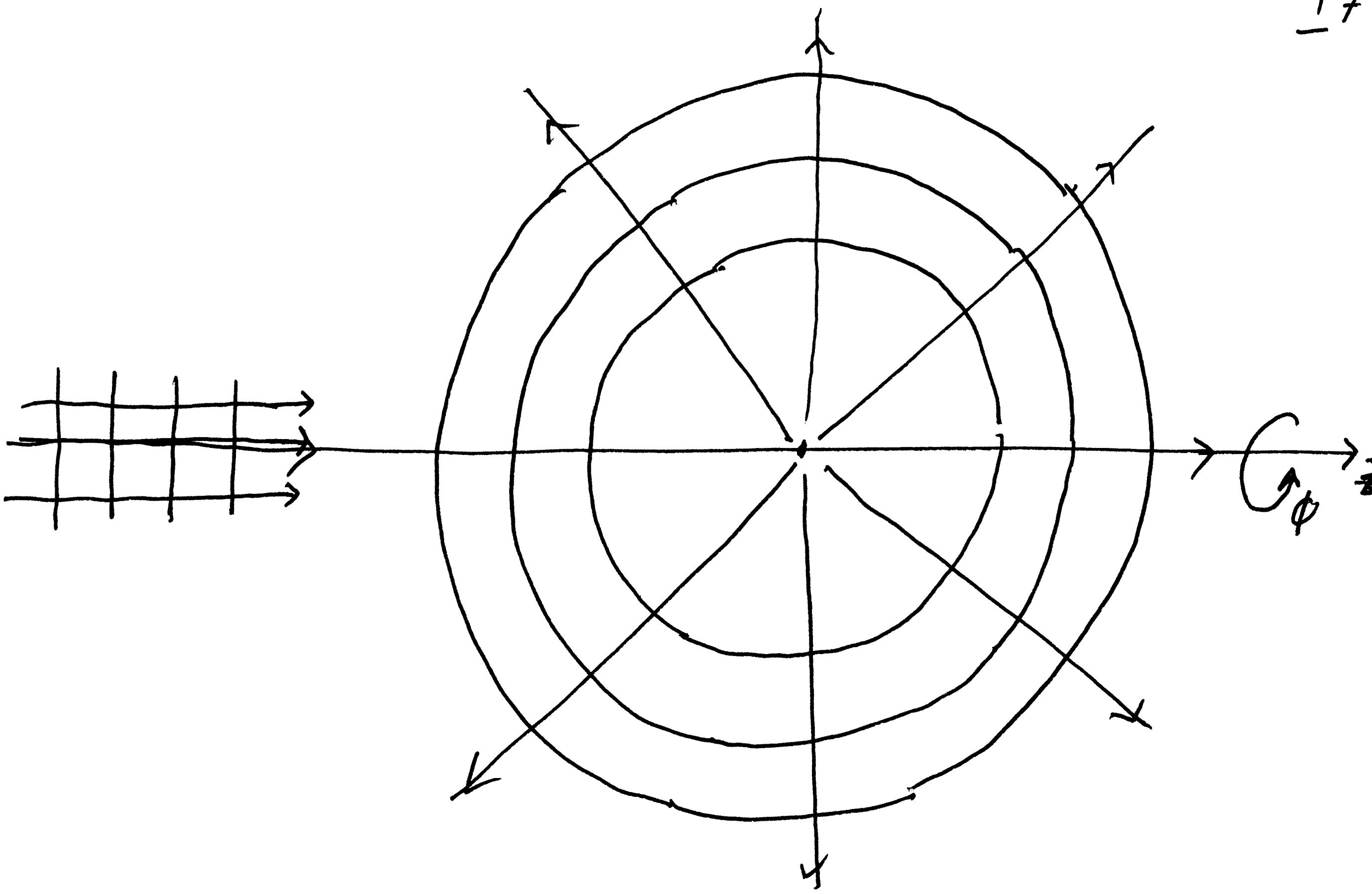


Fig: An incoming wave and an outgoing spherical wave originating from the scattering center.

The asymptotic form of the wavefunction must therefore be of the form

$$\psi(\vec{r}) \underset{r\to\infty}{\sim} e^{ikz} + f(\theta,\phi)\,\frac{e^{ikr}}{r}. \quad \cdots\cdots (21)$$

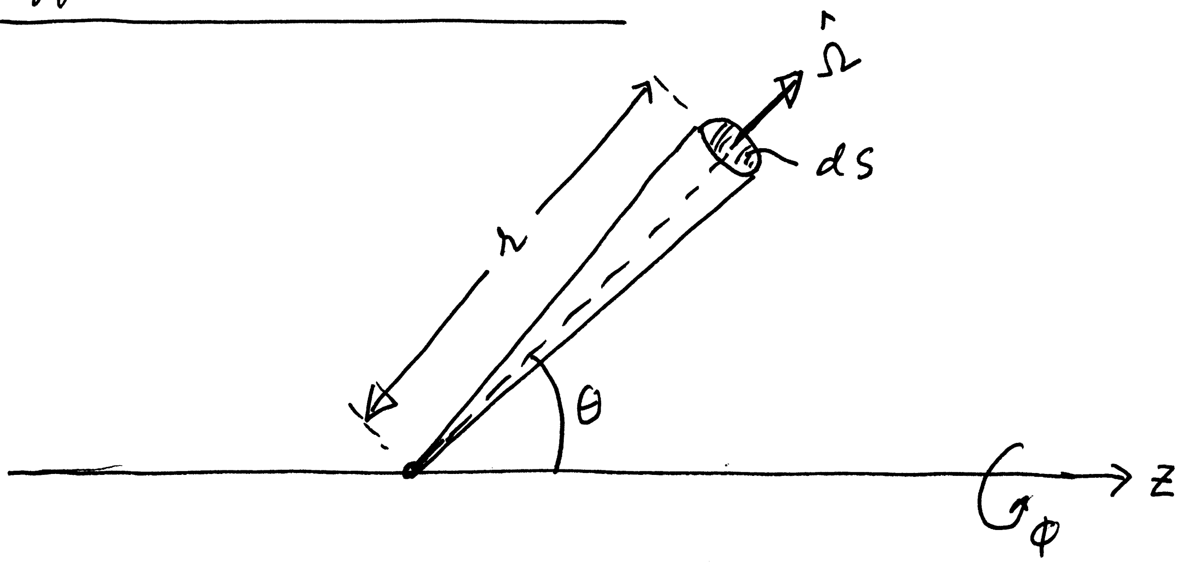
The second term in the above equation corresponds to the outgoing spherical wave.

It represents the probability of a particle moving outward from the scattering center. The amplitude of the outgoing wave, $f(\theta,\varphi)$, called the <u>scattering amplitude</u>, may in general depend on the polar angle θ and the azimuthal angle φ. However, for a spherically symmetric, i.e., a central potential, f depends only upon the polar angle θ.

The reason for the $\frac{1}{r}$ dependence of the scattered wave is as follows. Suppose that the scattering is isotropic, i.e., f is a constant. Then the intensity or the probability flux of the scattered wave must obey the inverse square law. Indeed, for the scattered spherically outgoing wave (second term on the right hand side of Eq. (21)), we have

$$\text{probability flux} \propto |\psi_{sc}|^2 \propto \frac{1}{r^2} .$$

Differential cross section.



Experimentally, the differential cross-section for scattering into a solid angle $d\Omega$ in the direction $\hat{\Omega} = (\theta, \phi)$ is defined as

$$\sigma(\theta,\phi)\, d\Omega \equiv \frac{d\sigma}{d\Omega}\, d\Omega$$

$$= \frac{\text{No. of particles scattered in the solid angle } d\Omega \text{ per unit time}}{\text{No. of particles incident on the scattering center per unit time and per unit area.}} \qquad (22).$$

~~(18)~~

In terms of probability flux, the definition of differential cross section reads

$$\sigma(\theta,\phi)\,d\Omega = \frac{\text{Scattered probability flux through the solid angle } d\Omega}{\text{Incident probability flux per unit area } (J_{inc})} \qquad (23)$$

The flux through the solid angle $d\Omega$ can be calculated from the probability current density $\vec{J}$ given by

$$\vec{J} = \frac{\hbar}{2mi}\left(\psi^* \vec{\nabla}\psi - \psi \vec{\nabla}\psi^*\right)$$

$$= \frac{\hbar}{m}\, \mathrm{Im}\left(\psi^* \vec{\nabla}\psi\right) \quad \cdots\cdots \quad (24)$$

Let us now calculate the scattered flux into the solid angle $d\Omega$.

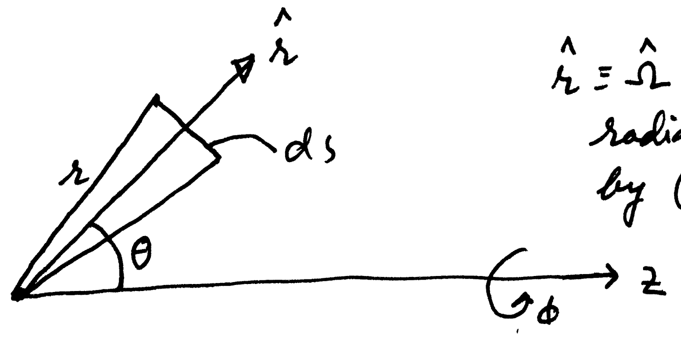
We take the scattered wave as in Eq. (21), i.e.,

$$\psi_{sc} = f(\theta,\phi)\,\frac{e^{ikr}}{r} \,. \qquad \text{------ (25)}$$

The gradient operator $\vec{\nabla}$ in spherical polar coordinates is

$$\vec{\nabla} = \hat{r}\,\frac{\partial}{\partial r} + \hat{\theta}\,\frac{1}{r}\,\frac{\partial}{\partial \theta} + \hat{\phi}\,\frac{1}{r\sin\theta}\,\frac{\partial}{\partial \phi} \,. \qquad \text{--- (26)}$$

Using ψ_{sc} and $\vec{\nabla}$ as given in the above two equations we can easily calculate $\vec{J}_{sc}$. Now we can calculate the probability flow rate $dP(\Omega)$ through a small area ds at right angles to the radial direction $\hat{r}$ given by (θ, ϕ). This is also the probability flow rate through the solid angle $d\Omega$ subtended by ds.



$\hat{r} \equiv \hat{\Omega}$ = unit vector in the radial direction specified by (θ, ϕ).

Now

$$dP(\Omega) = \vec{J}_{sc} \cdot \hat{r}\, ds$$

$$= J_{sc,r}\, ds$$

$$= J_{sc,r}\, r^2 d\Omega$$

$$= \frac{\hbar}{m} \operatorname{Im}\left[f^*(\theta,\phi) \frac{e^{-ikr}}{r} \frac{\partial}{\partial r}\left(f(\theta,\phi) \frac{e^{ikr}}{r} \right)\right] r^2 d\Omega$$

$$= \frac{\hbar}{m} |f|^2 \operatorname{Im}\left[\frac{e^{-ikr}}{r}\left(ik \frac{e^{ikr}}{r} - \frac{e^{ikr}}{r^2} \right)\right] r^2 d\Omega$$

$$= \frac{\hbar}{m} |f|^2 \operatorname{Im}\left[\frac{ik}{r^2} - \frac{1}{r^3} \right] r^2 d\Omega$$

$$= \frac{\hbar}{m} |f|^2 \cdot \frac{k}{r^2}\, r^2 d\Omega$$

$$= \frac{\hbar k}{m} |f|^2 d\Omega \quad \cdots\cdots\cdots (27)$$

The incident flux (i.e., the probability flow per unit time and per unit area) is

$$\phi_{inc} = |\vec{J}_{inc}| = \left| \frac{\hbar}{m} \operatorname{Im}\left(\psi_{inc}^* \vec{\nabla} \psi_{inc} \right) \right|$$

With

$$\psi_{inc} = e^{ikz}$$

we have

$$\phi_{inc} = \frac{\hbar}{m} \left| \operatorname{Im}\left(e^{ikz} \frac{d}{dz} e^{ikz} \right) \right|$$

or

$$\phi_{inc} = \frac{\hbar k}{m} \quad \cdots\cdots\cdots (28)$$

Therefore

$$\frac{d\sigma}{d\Omega}(\theta,\phi)\, d\Omega = \frac{dP(\Omega)}{\phi_{inc}}$$

$$= \frac{\frac{\hbar k}{m} |f|^2 d\Omega}{\frac{\hbar k}{m}}$$

$$= |f|^2 d\Omega$$

or

$$\boxed{\frac{d\sigma}{d\Omega}(\theta,\phi) = |f(\theta,\phi)|^2.} \quad \cdots\cdots\cdots (29)$$

This is the central result of ~~scattering~~ the theory of elastic scattering.

Partial wave analysis

The incident wave $\psi_{inc} = e^{ikz}$ is a plane wave propagating along the z-axis. The wave function ψ_{inc} is an eigenstate of the free Hamiltonian H_0 with eigenvalue $\hbar^2 k^2/2m$, i.e.,

$$-\frac{\hbar^2}{2m}\nabla^2 e^{ikz} = \frac{\hbar^2 k^2}{2m} e^{ikz} \quad \cdots\cdots (30)$$

We can rewrite this equation as

$$(\nabla^2 + k^2) e^{ikz} = 0 \quad \cdots\cdots (31)$$

where

$$k = \sqrt{\frac{2mE}{\hbar^2}} \, .$$

The plane wave is also an eigenstate of the momentum operator $\hat{\vec{p}} = -i\hbar\vec{\nabla}$ with eigenvalue $\hbar k \hat{z}$:

$$-i\hbar\vec{\nabla} e^{ikz} = -i\hbar\, \hat{z} \frac{\partial}{\partial z} e^{ikz} = \hat{z}\hbar k\, e^{ikz} \quad \cdots (32).$$

Thus e^{ikz} represents a free particle of energy $\hbar^2 k^2/2m$ and momentum $\hbar k$ propagating along the positive z-axis.

Even in the practical case of a well-collimated incident beam, the position of the particle with respect to the x and y-coordinates cannot be specified completely and the angular momentum of the particle relative to the scattering center can have any value. It is therefore convenient to replace the plane wave e^{ikz} by an equivalent series of spherical waves each of which represents a particle of definite orbital angular momentum.

Now, $\{H_0, L^2, L_z\}$ form a maximal set of mutually commutating operators and so it is possible to find simultaneous eigenstates of this set of operators. The plane wave e^{ikz}, which is a simultaneous eigenstate of $\hat{H}_0$ and $\hat{\vec{P}}$, can be expanded in terms of the simultaneous eigenstates of $\hat{H}_0$, $\hat{L}^2$ and $\hat{L}_z$. Such an expansion is called the partial wave expansion of e^{ikz}.

1. Partial wave expansion of e^{ikz}

First, we will work out the basis states for the expansion of e^{ikz}. The basis states are $\phi_{E\ell m}(\vec{r})$ which are simultaneous eigenstates of H_0, L^2 and L_z:

$$H_0 \phi_{E\ell m}(\vec{r}) = E\, \phi_{E\ell m}(\vec{r})$$

$$L^2 \phi_{E\ell m}(\vec{r}) = \ell(\ell+1)\hbar^2 \phi_{E\ell m}(\vec{r}) \qquad (33)$$

$$L_z \phi_{E\ell m}(\vec{r}) = m\hbar\, \phi_{E\ell m}(\vec{r}) .$$

The eigenstates of $\hat{L}^2$ and $\hat{L}_z$ are the spherical harmonics $Y_{\ell m}(\theta,\phi)$:

$$\hat{L}^2 Y_{\ell m}(\theta,\phi) = \ell(\ell+1)\hbar^2 Y_{\ell m}(\theta,\varphi)$$

$$\hat{L}_z Y_{\ell m}(\theta,\phi) = m\hbar\, Y_{\ell m}(\theta,\varphi) .$$

Therefore, $\phi_{E\ell m}(\vec{r})$ must be ~~f~~ of the form

$$\phi_{E\ell m}(\vec{r}) = R_\ell^{(0)}(r)\, Y_{\ell m}(\theta,\phi) \quad \cdots\cdots (34)$$

where $R_\ell^{(0)}(r)$ has to be determined from the requirement that $\phi_{E\ell m}(\vec{r})$ is an eigenfunction of H_0 with eigenvalue $E = \hbar^2 k^2/2m$ (first of Eqs (33)).

Therefore, we must have

$$\left(\nabla^2 + k^2\right)\phi_{E\ell m}(\vec{r}) = 0 \qquad \cdots\cdots (35).$$

Substituting Eq. (34) in Eq. (35) we get the appropriate differential equation satisfied by $R_\ell^{(0)}(r)$. First, ∇^2 in spherical polar coordinates can be written as

$$\nabla^2 = \frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right) - \frac{L^2}{\hbar^2 r^2} \qquad \cdots\cdots (36).$$

The first term on the right hand side of this equation can be expressed as

$$\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right) = \frac{1}{r}\frac{\partial^2}{\partial r^2} r .$$

Now, substitute Eqs. (34) and (36) in Eq. (35). We get

$$\left(\frac{1}{r}\frac{\partial^2}{\partial r^2} r - \frac{L^2}{\hbar^2 r^2} + k^2\right) R_\ell^{(0)}(r)\, Y_{\ell m}(\theta,\phi) = 0$$

or

$$\left(\frac{1}{r}\frac{d^2}{dr^2} r - \frac{\ell(\ell+1)}{r^2} + k^2\right) R_\ell^{(0)}(r) = 0$$

$$\left(\frac{d^2}{dr^2}+\frac{2}{r}\frac{d}{dr}+k^2-\frac{\ell(\ell+1)}{r^2}\right)R_\ell^{(0)}(r)=0 \quad \cdots\cdots (37)$$

The solutions of this differential equation are standard in mathematical physics. The two linearly independent solutions can be taken to be the spherical Bessel function $j_\ell(kr)$ and the spherical Neuman function $n_\ell(kr)$. These functions can be expressed in terms of the Bessel functions as

$$j_\ell(kr) = \left(\frac{\pi}{2kr}\right)^{1/2} J_{\ell+\frac{1}{2}}(kr)$$

$$n_\ell(kr) = (-1)^{\ell+1}\left(\frac{\pi}{2kr}\right)^{1/2} J_{-\ell-1/2}(kr).$$

The exact expressions for $j_\ell(kr)$ and $n_\ell(kr)$ for $\ell=0$ and 1 are

$$j_0(kr) = \frac{\sin kr}{kr}, \qquad n_0(kr) = -\frac{\cos kr}{kr}$$

$$j_1(kr) = \frac{\sin kr}{(kr)^2} - \frac{\cos kr}{kr}, \qquad n_1(kr) = -\frac{\cos kr}{(kr)^2} - \frac{\sin kr}{kr}.$$

For very small values of kr we have

$$j_\ell(kr) \underset{kr\to 0}{\sim} \frac{(kr)^\ell}{(2\ell+1)!!}$$

$$n_\ell(kr) \underset{kr\to 0}{\sim} -\frac{(2\ell-1)!!}{(kr)^{\ell+1}}$$

We see that $j_\ell(kr)$ are regular at the origin while $n_\ell(kr)$ tend to $-\infty$ at the origin.

Asymptotically for large values of kr, the functions $j_\ell(kr)$ and $n_\ell(kr)$ are oscillatory with decreasing amplitude:

$$j_\ell(kr) \underset{kr\to\infty}{\sim} \frac{\sin(kr - \ell\pi/2)}{kr}$$

$$n_\ell(kr) \underset{kr\to\infty}{\sim} -\frac{\cos(kr - \ell\pi/2)}{kr}.$$

Another useful pair of linearly independent solutions are the spherical Hankel function of the first kind $h_\ell^{(1)}(kr)$ and the spherical function of the second kind $h_\ell^{(2)}(kr)$ defined as

$$h_\ell^{(1)} = j_\ell + i n_\ell$$

$$h_\ell^{(2)} = j_\ell - i n_\ell \, .$$

Asymptotically we have

$$h_\ell^{(1)} \underset{kr \to \infty}{\sim} \frac{e^{i(kr - \ell\pi/2)}}{i\,kr}$$

$$h_\ell^{(2)} \underset{kr \to \infty}{\sim} - \frac{e^{-i(kr - \ell\pi/2)}}{i\,kr} \, .$$

Thus, asymptotically $h_\ell^{(1)}$ represents an outgoing spherical wave and $h_\ell^{(2)}$ represents an incoming spherical wave.

Since $R_\ell^{(0)}(r)$ must be regular everywhere including the origin, we take

$$R_\ell^{(0)}(r) = j_\ell(kr) \, . \quad \cdots\cdots (38)$$

Therefore

$$\phi_{E\ell m}(\vec{r}) = j_\ell(kr)\, Y_{\ell m}(\theta,\phi) \, . \quad \cdots\cdots (39) .$$

We can now write

$$e^{ikz} = \sum_{l=0}^{\infty}{}' \sum_{m=-l}^{l} c_{lm}\, j_l(kr)\, Y_{lm}(\theta,\varphi). \qquad (40)$$

Since $e^{ikz} = e^{ikr\cos\theta}$ is independent of ϕ, we must set $m=0$ on the right hand side of (30) because unless $m=0$ the spherical harmonic $Y_{lm}(\theta,\phi)$ has a φ-dependence of the form $e^{im\varphi}$. Now for $m=0$ we have $Y_{l0} = \sqrt{\frac{2l+1}{4\pi}}\, P_l(\cos\theta)$. Hence we can write Eq. (30) as

$$e^{ikz} = \sum_{l=0}^{\infty}{}' a_l\, j_l(kr)\, P_l(\cos\theta). \quad \text{- - - -} \quad (41)$$

To find a_l we have to make use of the orthogonality of the ~~the~~ Legendre polynomials

$$\int_0^{\pi} P_l(\cos\theta) P_{l'}(\cos\theta) \sin\theta \, d\theta = \frac{2}{2l+1}\,\delta_{ll'}.$$

Next, multiplying both sides of Eq. (31) by $P_{l'}(\cos\theta)\sin\theta$ and integrating over θ we obtain

$$\int_0^{\pi} e^{ikz} P_{l'}(\cos\theta)\sin\theta\, d\theta$$

$$= \sum_l a_l j_l(kr) \int_0^{\pi} P_l(\cos\theta) P_{l'}(\cos\theta)\sin\theta\, d\theta$$

$$= \sum_l a_l j_l(kr) \frac{2}{2l+1}\delta_{ll'}$$

$$= a_{l'} j_{l'}(kr)\frac{2}{2l'+1}$$

Thus (writing $l' = l$)

$$a_l \frac{2}{2l+1} j_l(kr) = \int_0^{\pi} e^{ikr\cos\theta} P_l(\cos\theta)\sin\theta\, d\theta$$

Making the change of variable

$$\mu = \cos\theta$$

we have

$$a_l \frac{2}{2l+1} j_l(kr) = \int_{-1}^{+1} P_l(\mu) e^{ikr\mu} d\mu$$

Integrating by parts we have

$$a_\ell \frac{2}{(2\ell+1)} j_\ell(kr) = \frac{1}{ikr}\left[P_\ell(\mu)e^{ikr\mu}\right]_{-1}^{+1} - \underbrace{\frac{1}{ikr}\int_{-1}^{+1} P_\ell'(\mu)e^{ikr\mu}\,d\mu}_{O\left(\frac{1}{r^2}\right)}.$$

For large r

$$a_\ell \frac{2}{(2\ell+1)} \frac{\sin(kr-\ell\pi/2)}{kr} = \frac{1}{ikr}\left[P_\ell(1)e^{ikr} - P_\ell(-1)e^{-ikr}\right]$$

Since

$$P_\ell(1) = 1, \quad P_\ell(-1) = (-1)^\ell$$

we have

$$\frac{2a_\ell \sin(kr-\ell\pi/2)}{(2\ell+1)\,kr} = \frac{e^{ikr} - (-1)^\ell e^{-ikr}}{ikr}$$

$$= \frac{e^{ikr} - e^{i\ell\pi}e^{-ikr}}{ikr} \qquad \Big| -1 = e^{i\pi}$$

$$= e^{i\ell\pi/2}\,\frac{e^{i(kr-\ell\pi/2)} - e^{-i(kr-\ell\pi/2)}}{ikr}$$

$$= 2e^{i\ell\pi/2}\,\frac{\sin(kr-\ell\pi/2)}{kr}$$

Hence

$$a_l = e^{il\pi/2}(2l+1)$$

i.e., $$a_l = i^l (2l+1). \qquad \text{- - - - - - . (42)}$$

Substituting Eq. (42) in Eq. (41) we finally obtain

$$\boxed{e^{ikz} = \sum_{l=0}^{\infty} i^l (2l+1) j_l(kr) P_l(\cos\theta)} \qquad \text{- - - (43)}$$

This is the partial wave expansion of the plane wave.

Partial wave expansion for the full wave function ψ and the scattering amplitude $f(\theta)$.

In the case of a particle being scattered from a fixed potential we have to solve the time-independent Schrödinger equation

$$\left(-\frac{\hbar^2}{2m}\nabla^2 + V\right)\psi(\vec{r}) = E\,\psi(\vec{r}) \quad \cdots\cdots (44)$$

i.e

$$\left(\nabla^2 + k^2 - U\right)\psi(\vec{r}) = E\,\psi(\vec{r})$$

subject to the boundary condition

$$\psi(\vec{r}) \underset{r\to\infty}{\sim} e^{ikz} + f(\theta)\frac{e^{ikr}}{r}, \qquad (45)$$

where we have defined

$$k^2 = \frac{2mE}{\hbar^2}$$

$$U = \frac{2mV}{\hbar^2}.$$

We assume that V is central, i.e., V depends only on the distance of the particle from the scattering centre, i.e.,

$$V = V(|\vec{r}|) = V(r).$$

In such a situation f does not depend on the azimuthal angle φ so that $f = f(\theta)$.

If the potential is <u>central</u>, L^2 and L_z both commute with H, i.e.,

$$[H, L^2] = [H, L_z] = 0.$$

$\{H\ L^2, L_z\}$ form a complete (or maximal) set of mutually commutating opertors and so simultaneous eigenstates of H, L^2 and L_z can be found. Let us denote the eigenstates as $\psi_{Elm}(\vec{r})$. Each of these eigenstates will satisfy the time-independent Schrödinger equation.

We can write $\psi_{E\ell m}(\vec{r})$ as

$$\psi_{E\ell m}(\vec{r}) = R_\ell(r)\, Y_{\ell m}(\theta,\varphi) \quad \ldots\ldots (46)$$

In this form $\psi_{E\ell m}(\vec{r})$ is an eigenfunction of L^2 and L_z with eigenvalues $\ell(\ell+1)\hbar^2$ and $m\hbar$, respectively, no matter what the function $R_\ell(r)$ is. However, $\psi_{E\ell m}(\vec{r})$ should be an eigenfunction of H with eigenvalue $E = \hbar^2 k^2/2m$. In order to ensure this, $R_\ell(r)$ cannot be chosen arbitrarily, it must satisfy the radial Schrödinger equation

$$\left[\frac{d^2}{dr^2} + \frac{2}{r}\frac{d}{dr} + \left(k^2 - \frac{\ell(\ell+1)}{r^2} - U(r)\right)\right] R_\ell(r) = 0 \quad \ldots (46)$$

Now, a general solution of the time independent Schrödinger equation can be written as a linear superposition of the various $\psi_{E\ell m}(\vec{r})$. We write

$$\psi(\vec{r}) = \sum_{\ell=0}^{\infty} \sum_{m=-\ell}^{\ell} C_{\ell m} R_\ell(r)\, Y_{\ell m}(\theta,\varphi) \quad \ldots (47)$$

Since the potential is central, there cannot be any φ-dependence in the wave function. So we must set $m=0$ on the right hand side of Eq. (47). ~~Since~~ Since $Y_{\ell 0} \propto \cos\theta$, Now, for large r, i.e., outside the range of the potential, the radial equation (46) becomes that of a free particle with solutions $j_\ell(kr)$ and $n_\ell(kr)$ or $h_\ell^{(1)}(kr)$ and $h_\ell^{(2)}(kr)$. Therefore

$$R_\ell(r) \underset{r\to\infty}{\sim} c_\ell\, j_\ell(kr) + d_\ell\, n_\ell(kr)$$

$$= c_\ell \frac{\sin(kr - \ell\pi/2)}{kr} - d_\ell \frac{\cos(kr - \ell\pi/2)}{kr}. \qquad (48)$$

We note that the coefficients c_ℓ and d_ℓ may be complex. We can write Eq. (48) in the alternative form

$$R_\ell(r) \underset{r\to\infty}{\sim} F_\ell \frac{\sin(kr - \ell\pi/2 + \delta_\ell)}{kr} \quad \ldots (49)$$

where F_ℓ and δ_ℓ are constants related to c_ℓ and d_ℓ. Both F_ℓ and δ_ℓ may be complex. Without loss of generality we can set the overall multiplicative constant F_ℓ to 1, i.e., $F_\ell = 1$, since we have already included a multiplicative constant b_ℓ in each partial wave in the expansion for $\psi(\vec{r})$, Eq. (47a)

Therefore we take the asymptotic form of $R_\ell(r)$ to be

$$R_\ell(r) \underset{r\to\infty}{\sim} \frac{\sin(kr - \ell\pi/2 + \delta_\ell)}{kr} \qquad (50)$$

Using Eq (50), the asymptotic form of $\psi(r)$ (Eq. (47a)) is

$$\psi(\vec{r}) \underset{r\to\infty}{\sim} \sum_\ell b_\ell \frac{\sin(kr - \ell\pi/2 + \delta_\ell)}{kr} P_\ell(\cos\theta) .$$

Writing $\sin(kr - \ell\pi/2 + \delta_\ell)$ in terms of exponentials we have

$$\psi(\vec{r}) \underset{r\to\infty}{\sim} \sum_\ell b_\ell \frac{e^{i(kr-\ell\pi/2+\delta_\ell)} - e^{-i(kr-\ell\pi/2+\delta_\ell)}}{2ikr} P_\ell(\cos\theta)$$

$$= -\sum_{\ell=0}^{\infty} b_\ell e^{-i\delta_\ell} \frac{e^{-i(kr-\ell\pi/2)} - e^{2i\delta_\ell} e^{i(kr-\ell\pi/2)}}{2ikr} P_\ell(\cos\theta)$$

$$\ldots (51)$$

We now rewrite Eq. (51) as

$$\lim_{r\to\infty} \psi(\vec{r}) =$$

$$-\sum_{l=0}^{\infty} b_l e^{-i\delta_l} \frac{e^{-i(kr-l\pi/2)} - e^{i(kr-l\pi/2)} - (e^{2i\delta_l}-1)\, e^{i(kr-l\pi/2)}}{2ikr} P_l(\cos\theta)$$

$$= -\sum_{l=0}^{\infty} b_l e^{-i\delta_l} \frac{e^{-i(kr-l\pi/2)} - e^{i(kr-l\pi/2)}}{2ikr} P_l(\cos\theta)$$

$$+ \sum_{l=0}^{\infty} b_l e^{-i\delta_l} \frac{1}{2ikr} (e^{2i\delta_l}-1)\, e^{i(kr-l\pi/2)} P_l(\cos\theta) \qquad (52)$$

Next, we have to determine the values of b_l by requiring that $\psi(\vec{r})$ satisfies the boundary condition (45) i.e.,

$$\psi(\vec{r}) \underset{r\to\infty}{\sim} e^{ikz} + f(\theta)\frac{e^{ikr}}{r} \quad \ldots\ldots\ldots (53)$$

The partial wave expansion of e^{ikz} is

$$e^{ikz} = \sum_{l=0}^{\infty} i^l (2l+1)\, j_l(kr)\, P_l(\cos\theta).$$

Asymptotically

$$e^{ikz} \underset{r\to\infty}{\sim} \sum_{l=0}^{\infty} i^l (2l+1) \frac{\sin(kr - l\pi/2)}{kr} P_l(\cos\theta)$$

i.e.,

$$e^{ikz} \underset{r\to\infty}{\sim} -\sum_{l=0}^{\infty} i^l (2l+1) \frac{e^{-i(kr-l\pi/2)} - e^{i(kr-l\pi/2)}}{2ikr} P_l(\cos\theta) \quad \cdots (54)$$

Now, comparing Eq. (52) with Eq. (53) and keeping in mind the asymptotic partial wave expansion of e^{ikz} (Eq. 54), we see that the first term of Eq. (52) on the right side is equal to e^{ikz} provided

$$b_l e^{-i\delta_l} = i^l (2l+1)$$

i.e.,

$$\boxed{b_l = i^l (2l+1) e^{i\delta_l}} \quad \cdots\cdots (55)$$

With this value of b_l the second term ~~of~~ on the right ~~sec~~ hand side of Eq. (52) is equated to the second term on the right hand side of Eq. (53), thus giving us the partial wave expansion of $f(\theta)$.

We find

$$\sum_{l=0}^{\infty} b_l e^{-i\delta_l} \frac{1}{k}\left(\frac{e^{2i\delta_l}-1}{2i}\right) e^{-il\pi/2} P_l(\cos\theta) \frac{e^{ikr}}{r}$$

$$= f(\theta)\frac{e^{ikr}}{r}$$

or,

$$f(\theta) = \sum_{l=0}^{\infty} b_l e^{-i\delta_l} \frac{1}{k}\left(\frac{e^{2i\delta_l}-1}{2i}\right) e^{-il\pi/2} P_l(\cos\theta)$$

Using Eq. (55)

$$f(\theta) = \sum_{l=0}^{\infty} i^l (2l+1) e^{-il\pi/2} \frac{1}{k}\left(\frac{e^{2i\delta_l}-1}{2i}\right) P_l(\cos\theta).$$

since

$$i^l e^{-il\pi/2} = e^{il\pi/2} e^{-il\pi/2} = 1$$

we finally have

$$f(\theta) = \sum_{l=0}^{\infty} (2l+1)\left(\frac{e^{2i\delta_l}-1}{2ik}\right) P_l(\cos\theta) \quad \cdots\cdots (56)$$

This expression is the partial wave expansion of the scattering amplitude $f(\theta)$.

Nature of δ_l

Using Eq. (55), the asymptotic form of the full wave function (Eq. 51) is

$$\psi(\vec{r}) \underset{r\to\infty}{\sim} -\sum_l i^l (2l+1) \frac{e^{-i(kr - l\pi/2)} - e^{2i\delta_l} e^{i(kr - l\pi/2)}}{2ikr} P_l(\cos\theta). \quad \text{... (57)}$$

Defining

$$S_l = e^{2i\delta_l} \quad \text{... (58)}$$

we can write

$$\psi(\vec{r}) \underset{r\to\infty}{\sim} -\sum_l i^l (2l+1) \frac{e^{-i(kr - l\pi/2)} - S_l e^{i(kr - l\pi/2)}}{2ikr} P_l(\cos\theta). \quad \text{... (59)}$$

We now compare this with the asymptotic expansion of the plane wave e^{ikz} (Eq. 54). The plane wave can be considered as a series of incoming spherical waves $\exp[-i(kr - l\pi/2)]/r$ each with orbital angular momentum l converging on the scattering center and an outgoing spherical wave $\exp[i(kr - l\pi/2)]/r$ with an amplitude equal in modulus to the incoming wave.

The potential modifies only the outgoing spherical wave. This is in accord with the principle of causality.

If $|S_l| = 1$, then the outgoing wave is only effected in phase, not in amplitude. This will be the case only when elastic scattering can occur. Then δ_l is a real number. In general, when non-elastic processes can occur, we have $|S_l| < 1$, i.e., both the phase and the amplitude of the outgoing wave may change. In either case, Eq (59) represents the asymptotic wave function for elastically scattered particles. In situations where non-elastic processes (like inelastic scattering, reactions) can occur, there will be fewer elastically scattered outgoing particles than ~~incoming particles~~ when only elastic scattering is possible because some particles are lost to non-elastic channels. This is why $|S_l| < 1$ when both elastic scattering and non-elastic processes can occur.

Now, if $|S_l| < 1$, the parameter δ_l is complex:

$$\delta_l = \mathrm{Re}\,\delta_l + i\,\mathrm{Im}\,\delta_l$$

so that

$$S_l = e^{2i\delta_l} = e^{-2\,\mathrm{Im}\,\delta_l}\, e^{2i\,\mathrm{Re}\,\delta_l}$$

The factor $e^{-2\,\mathrm{Im}\,\delta_l}$ is less than 1 provided $\mathrm{Im}\,\delta_l > 0$. Taking $\mathrm{Im}\,\delta_l > 0$ and denoting $e^{-2\,\mathrm{Im}\,\delta_l}$ by η_l we can write

$$S_l = \eta_l\, e^{2i\,\mathrm{Re}\,\delta_l} \qquad (\eta_l < 1)$$

Letting $\mathrm{Re}\,\delta_l = \delta_l'$ we can write

$$S_l = \eta_l\, e^{2i\delta_l'}$$

where both η_l and δ_l' are real numbers. Now simply omitting the prime in the above equation, we write

$$S_l = \eta_l\, e^{2i\delta_l} \qquad (\eta_l, \delta_l \text{ are real}, \ \eta_l < 1) \qquad (60)$$

Of course, δ_l in this equation is not the same δ_l appearing in Eq. (58). The δ_l in Eq (60) is the real part of the δ_l in Eq. (58).

In summary, $S_l(k)$ can be written as

$$S_l(k) = \eta_l(k)\, e^{2i\delta_l(k)} \qquad (61)$$

where both $\eta_l(k)$ and $\delta_l(k)$ are real parameters. The parameter $\delta_l(k)$ is called the phase shift and $\eta_l(k)$ is called the inelasticity parameter. In the case when elastic scattering is the only possibility, $\eta_l(k) = 1$ and if non-elastic channels are also open, we must have $|\eta_l(k)| < 1$. To find $S_l(k)$ we have to solve the Schrödinger equation (Eq. 44) with the boundary condition (45).

Note that, in our present discussion we are only considering potential scattering of a particle, i.e., scattering of a particle of mass m and energy E by a real potential. So there is no possibility of inelastic scattering or reaction in our case. As a consequence $|S_l| = |e^{2i\delta_l}| = 1$, for potential scattering.

Elastic cross section

The differential cross-section for elastic scattering into a solid angle in the direction (θ, φ) is given by

$$\frac{d\sigma}{d\Omega}(\theta,\varphi) = |f(\theta)|^2 \quad \cdots\cdots \quad (62)$$

where the scattering amplitude $f(\theta)$ is given in Eq. (56), i.e.,

$$f(\theta) = \frac{1}{k} \sum_l (2l+1)\left(\frac{e^{2i\delta_l}-1}{2i}\right) P_l(\cos\theta)$$

Defining the partial wave scattering amplitude $f_l(k)$ as

$$f_l(k) = \frac{e^{2i\delta_l}-1}{2i} = \frac{S_l - 1}{2i} \quad \cdots\cdots \quad (63)$$

we can write

$$f(\theta) = \frac{1}{k}\sum_l (2l+1) f_l(k) P_l(\cos\theta) \quad \cdots\cdots \quad (64)$$

The integrated elastic cross-section, σ_{el}, is found by integrating Eq. (62) over all solid angles.

$$\sigma_{el} = \int_\Omega \frac{d\sigma}{d\Omega}\, d\Omega \qquad \Big| \; d\Omega = \sin\theta\, d\theta\, d\phi$$

$$= \sum_{l,l'}{}' \frac{1}{k^2} (2l+1)(2l'+1)\, f_l^*(k) f_{l'}(k) \int_\Omega P_l(\cos\theta) P_{l'}(\cos\theta)\, d\Omega$$

$$= \frac{2\pi}{k^2} \sum_{l,l'}{}' (2l+1)(2l'+1)\, f_l^*(k) f_{l'}(k) \underbrace{\int_0^\pi P_l(\cos\theta) P_{l'}(\cos\theta) \sin\theta\, d\theta}_{\frac{2}{2l+1}\delta_{ll'}}$$

$$= \frac{2\pi}{k^2} \sum_{l,l'}{}' (2l+1)(2l'+1) \cdot \frac{2}{2l+1} \delta_{ll'}\, f_l^*(k) f_{l'}(k)$$

$$= \frac{4\pi}{k^2} \sum_{l}{}' (2l+1) \left| f_l(k) \right|^2$$

$$= \frac{4\pi}{k^2} \sum_{l} (2l+1) \frac{\left| 1 - S_l \right|^2}{4}$$

i.e.,

$$\sigma_{el} = \frac{\pi}{k^2} \sum_{l} (2l+1) \left| 1 - S_l \right|^2 \qquad \ldots\ldots\ldots \quad (65)$$

If only the elastic channel is open,

$$S_l = e^{2i\delta_l} \qquad \delta_l = \text{real}$$

$$\therefore \quad S_l - 1 = e^{2i\delta_l} - 1$$

$$= e^{i\delta_l}\left(e^{i\delta_l} - e^{-i\delta_l}\right)$$

$$= 2i\, e^{i\delta_l} \sin\delta_l$$

Hence

$$|1 - S_l|^2 = 4\sin^2\delta_l$$

Therefore

$$\sigma_{el} = \frac{4\pi}{k^2} \sum_l{}' (2l+1)\sin^2\delta_l \,. \quad \cdots\cdots \quad (66)$$

(only elastic channel open).

Since only elastic scattering is possible, σ_{el} is also the total cross-section. Next, write (66) as

$$\sigma_{el} = \sum_l \sigma_{el,l}$$

where

$$\sigma_{el,l} = \frac{4\pi}{k^2}(2l+1)\sin^2\delta_l(k)$$

is the contribution to the elastic cross-section by the

l^{th} partial wave. We note that the maximum contribution of each partial wave

$$\sigma_{el,l}^{max} = \frac{4\pi}{k^2}(2l+1)$$

and occurs when

$$\delta_l(k) = \left(n+\tfrac{1}{2}\right)\pi \;;\; n = 0, \pm 1, \pm 2, \ldots .$$

This maximum value of $\sigma_{el,l}^{max}$ is called the unitarity limit of $\sigma_{el,l}$.

When $\delta_l(k) = n\pi$, there is no contribution to the scattering from the partial wave l at the energy $E = \hbar^2 k^2/2m$.

Optical theorem

For potential scattering of a particle only elastic scattering is possible. Therefore,

$$\sigma_{tot} = \sigma_{el} = \frac{4\pi}{k^2} \sum_{l} (2l+1) \sin^2 \delta_l$$

The scattering amplitude is

$$f(\theta) = \frac{1}{k} \sum_{l} (2l+1)\, e^{i\delta_l} \sin \delta_l \, P_l(\cos\theta)$$

Noting that $P_l(1) = 1$ for all l, we can easily show that

$$\boxed{\sigma_{tot} = \frac{4\pi}{k} \operatorname{Im} f(0)} \qquad \text{- - - - - - -} \quad (67)$$

This relation is called the optical theorem. Optical theorem is valid in general, even in situations where non-elastic channels are open.

Advantage of partial wave expansion.

For calculating cross sections, the phase shift δ_l must be known for different partial waves. It may appear at first sight that calculation of the cross section using Eq. (66) would be difficult because an infinite number of partial waves of different l are involved. In practice, only a few l values are necessary depending on the energy.

We will now give a semiclassical argument to show why only a few l values need be considered. The figure below shows a particle approaching the scattering center with an impact parameter b. The range of the potential is r_0.

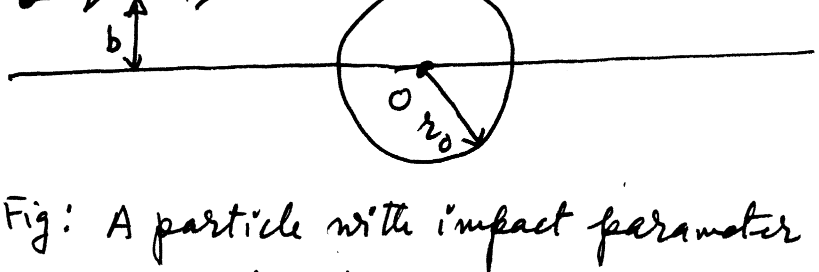


Fig: A particle with impact parameter b is scattered from a fixed potential of range r_0.

Scattering will take place only if $b < r_0$. For $b > r_0$, the incident particle will not "feel" the potential and hence they will not be scattered. Thus the largest impact parameter for which scattering will occur is $b_{max} = r_0$.

Now, an approaching particle with impact parameter b has an orbital angular momentum

$$L = mvb$$

about the scattering center O. The maximum orbital angular momentum that the incident particle may have and yet be scattered by the potential is that which corresponds to the maximum impact parameter b_{max}, i.e.,

$$L_{max} = mvb_{max} = mvr_0 . \qquad \ldots\ldots(68)$$

Particles with L smaller than L_{max} will be scattered by the potential while those particles with $L > L_{max}$ will not be scattered.

Now, in quantum mechanics, angular momentum does not vary in a continuous manner and can only assume discrete values given by

$$L = \sqrt{l(l+1)}\,\hbar \; ; \; l = 0, 1, 2, \ldots,$$

We approximate this value of L as

$$L \simeq l\hbar . \qquad \ldots \qquad (69)$$

Using Eq. (69) in Eq. (68) we have

$$l_{max}\hbar = m v r_0$$

or

$$l_{max} = \frac{p}{\hbar} r_0$$

i.e.,

$$l_{max} = k r_0 \qquad \ldots \qquad (70)$$

Here l_{max} is the maximum orbital angular momentum quantum number the particle can have and yet be scattered by the potential. If the particle's orbital angular momentum quantum number is less than or equal to l_{max}, the particle would be scattered. Thus, for scattering to occur we must have

$$l \leq l_{max}$$

i.e., $\quad l \leq kr_0 . \quad \ldots\ldots\ldots\ldots (71)$

If the incident energy is very small so that $kr_0 << 1$, then only the s-wave $l=0$ will contribute to scattering. The contribution of higher partial waves will be negligible. If the incident energy is increased so that kr_0 becomes larger, the $l=1$ wave (p-wave) begins to contribute also, while the dominant contribution is in the $l=0$ (s-wave). Thus, with increasing energy more and more partial waves have to be included in our calculations.

s-wave scattering

If we retain only the s-wave ($l=0$) in the partial wave expansion of the scattering amplitude, (Eq. 56), we have

$$f(\theta) = \frac{1}{2ik}\left(S_0(k) - 1\right) P_0(\cos\theta)$$

or

$$f(\theta) = \frac{1}{2ik}\left(S_0(k) - 1\right) \qquad \Big|\ P_0(\cos\theta) = 1$$

We see that $f(\theta)$ does not depend upon the angle θ. In other words, s-wave scattering of a particle from a fixed potential is isotropic. This means that for the two-body scattering problem, the s-wave scattering is isotropic in the <u>center-of-mass frame</u>, not in the lab frame.

An integral expression of δ_l in terms of the potential and the radial wavefunction.

The radial wavefunction $R_l(r)$ in the presence of the potential satisfies the differential equation

$$\frac{1}{r^2}\frac{d}{dr}\left(r^2\frac{dR_l}{dr}\right) + \left(k^2 - U(r) - \frac{l(l+1)}{r^2}\right)R_l(r) = 0 \quad \cdots\cdots (1)$$

where

$$k^2 = \frac{2mE}{\hbar^2}$$

$$U = \frac{2mV(r)}{\hbar^2}.$$

In the absence of the potential the radial wavefunction is denoted by $R_l^{(0)}$ and the differential equation for $R_l^{(0)}(r)$ is

$$\frac{1}{r^2}\frac{d}{dr}\left(r^2\frac{dR_l^{(0)}}{dr}\right) + \left(k^2 - \frac{l(l+1)}{r^2}\right)R_l^{(0)}(r) = 0, \quad \cdots\cdots (2)$$

The two linearly independent solutions of Eq. (2) are $j_l(kr)$ and $n_l(kr)$. Since $n_l(kr)$ is irregular at the origin (tends to ∞ as $r \to 0$), we take

$$R_l^{(0)}(r) = j_l(kr) \quad \cdots\cdots\cdots (3)$$

which is regular everywhere.

Now, from Eqs. (1) and (2) we obtain

$$\int_0^\infty \left[\frac{R_l^{(0)}}{r^2}\frac{d}{dr}\left(r^2\frac{dR_l}{dr}\right) - \frac{R_l}{r^2}\frac{d}{dr}\left(r^2\frac{dR_l^{(0)}}{dr}\right) - U(r)R_l^{(0)}R_l \right] r^2 dr = 0$$

or $$\int_0^\infty \left[R_l^{(0)}\frac{d}{dr}\left(r^2\frac{dR_l}{dr}\right) - R_l\frac{d}{dr}\left(r^2\frac{dR_l^{(0)}}{dr}\right)\right] dr = \int_0^\infty U(r)\, R_l^{(0)} R_l\, r^2 dr$$

or $$\int_0^\infty \frac{d}{dr}\left[R_l^{(0)} r^2 \frac{dR_l}{dr} - R_l r^2 \frac{dR_l^{(0)}}{dr}\right] dr = \int_0^\infty R_l^{(0)} U R_l\, r^2 dr$$

or $$\left[R_l^{(0)} r^2 \frac{dR_l}{dr} - R_l r^2 \frac{dR_l^{(0)}}{dr}\right]_0^\infty = \int_0^\infty R_l^{(0)} U R_l\, r^2 dr \quad \cdots\cdots (4)$$

Since $R_\ell^{(0)}$ and R_ℓ are both regular at the origin, the left hand side of the above equation in the lower limit is zero.

Let us now calculate the l.h.s. of Eq. (4) in the upper limit. Now, as $r \to \infty$, we have

$$R_\ell^{(0)}(r) = j_\ell(kr) \underset{r\to\infty}{\sim} \frac{\sin(kr - \ell\pi/2)}{kr} .$$

Next, we 'normalize' $R_\ell(r)$ such that

$$R_\ell(r) \underset{r\to\infty}{\sim} \frac{\sin(kr - \ell\pi/2 + \delta_\ell)}{kr} .$$

Therefore, the upper limit in the l.h.s. of Eq. (4) is

$$\frac{\sin(kr - \ell\pi/2)}{kr}\, r^2\, \frac{k\cos(kr - \ell\pi/2 + \delta_\ell)}{kr}$$
$$- \frac{\sin(kr - \ell\pi/2 + \delta_\ell)}{kr}\, r^2\, \frac{k\cos(kr - \ell\pi/2)}{kr}$$

$$= \frac{1}{k}\sin(-\delta_\ell)$$
$$= -\frac{1}{k}\sin\delta_\ell$$

where we have used the trigonometrical identity

$$\sin A \cos B - \cos A \sin B = \sin(A-B)$$

with $A = (kr - l\pi/2)$ and $B = (kr - l\pi/2 + \delta_l)$.

Therefore, Eq. (4) becomes

$$-\frac{1}{k}\sin\delta_l = \int_0^\infty dr\, r^2 j_l(kr)\, U(r)\, R_l(r)$$

or,

$$\boxed{\sin\delta_l = -k\int_0^\infty dr\, r^2 j_l(kr)\, U(r)\, R_l(r)\,.} \qquad (5)$$

When the potential is weak, $R_l(r) \simeq R_l^{(0)}(r) = j_l(kr)$,

so that

$$\sin\delta_l \simeq -k\int_0^\infty dr\, r^2 j_l^2(kr)\, U(r)\,. \quad \text{- - - - (6)}$$

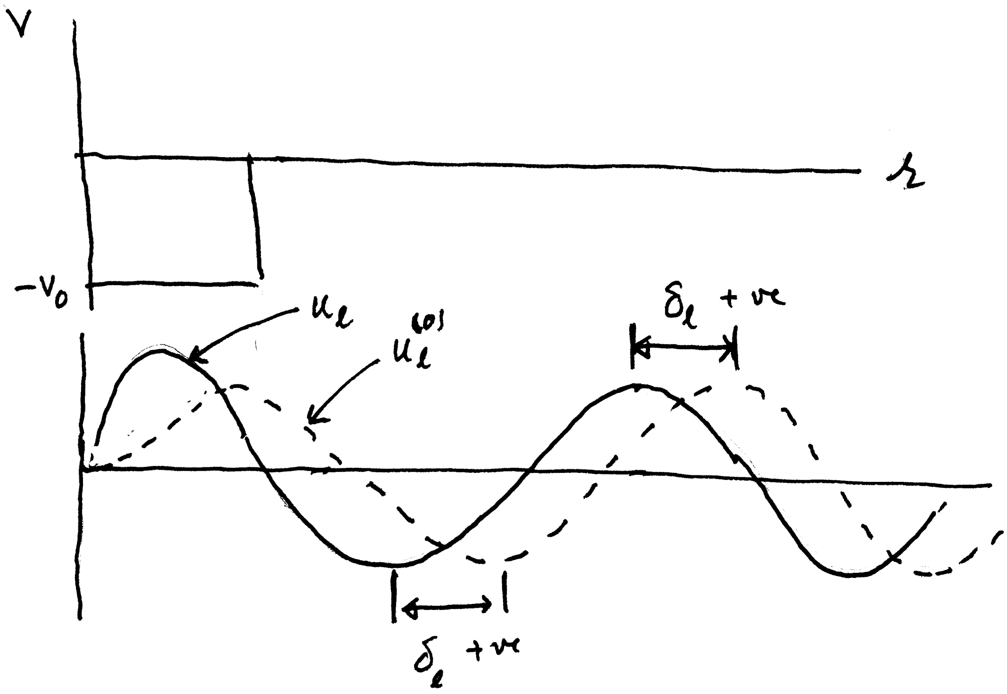
(Weak potential)

This is called the Born approximation for the phase shift. From (6) we see that for a weak attractive potential ($U(r) = -ve$), δ_l is positive, and, for a weak repulsive potential ($U(r) = +ve$), δ_l is negative.

In the figure below we have plotted free radial auxiliary wave function $u_\ell^{(0)} = kr\, j_\ell(kr)$ and $u_\ell(r) = kr\, R_\ell(r)$ for a weak attractive potential. Note that

$$u_\ell^{(0)}(r) \underset{r\to\infty}{\sim} \sin(kr - \ell\pi/2)$$

$$u_\ell(r) \underset{r\to\infty}{\sim} \sin(kr - \ell\pi/2 + \delta_\ell)$$



The attractive potential pulls in the free wavefunction producing a positive phase shift. In contrast, a weak positive (repulsive) potential pushes out the free wavefunction producing a negative phase shift.

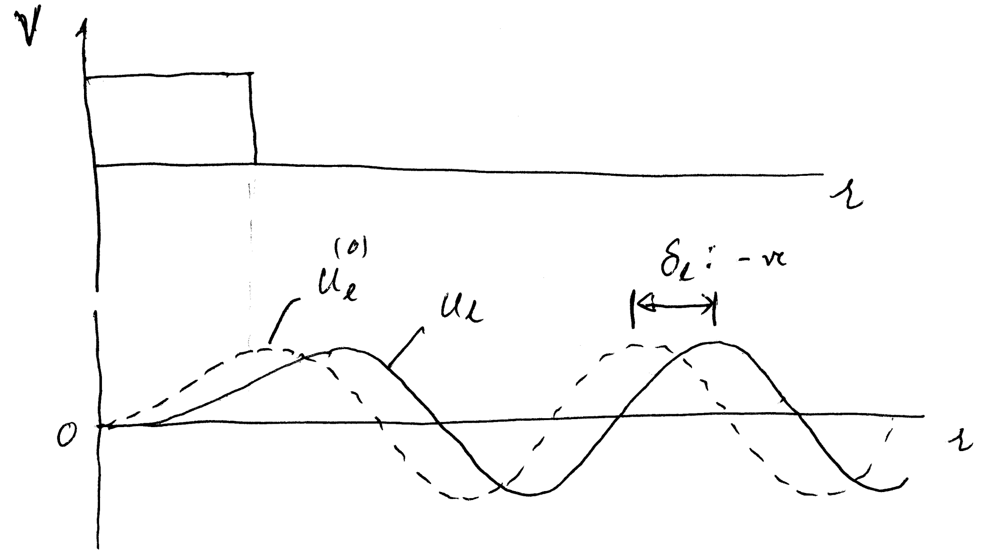


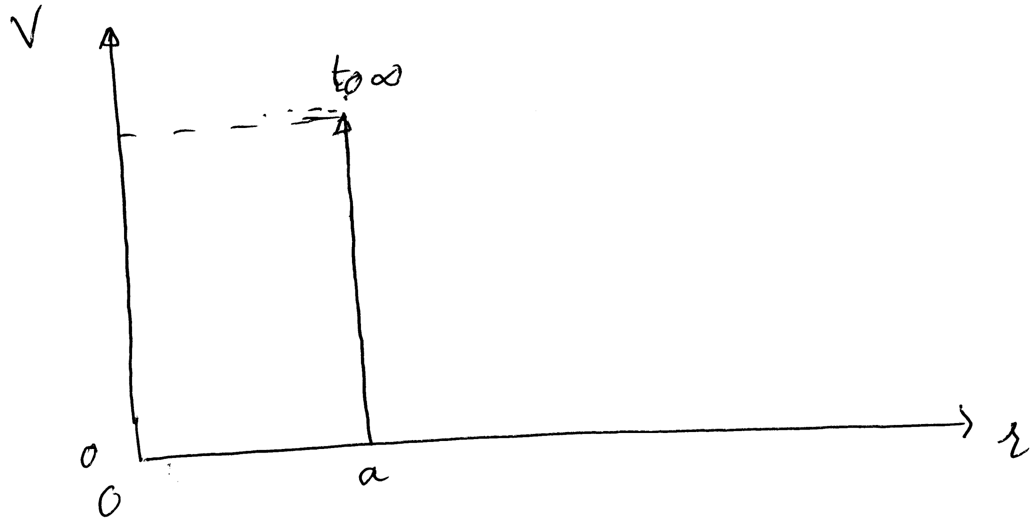
Fig: A repulsive potential pushes out the wave function producing a negative phase shift.

Some simple examples of phase shift calculations.

Ex Hard rigid sphere

Consider the "hard sphere" potential

$$V(r) = \begin{cases} +\infty & r < a \\ 0 & r > a. \end{cases}$$



For $r > a$, the radial Schrödinger equation is that of a ~~fre~~ free particle:

$$\frac{d^2 R_\ell}{dr^2} + \frac{2}{r}\frac{dR_\ell}{dr} + \left(k^2 - \frac{\ell(\ell+1)}{r^2}\right)R_\ell(r) = 0 \quad \cdots \quad (1)$$

$$(r > a).$$

and for $r \leq a$

$$R_\ell(r) = 0 \quad (r \leq a) \quad \cdots \quad (2)$$

The solutions of Eq. (1) are $j_\ell(kr)$ and $n_\ell(kr)$. Therefore, the wave function exterior to the potential ($r > a$) is of the form

$$R_\ell(r) = a_\ell j_\ell(kr) + b_\ell n_\ell(kr)$$

$$\underset{r\to\infty}{\sim} a_\ell \frac{\sin(kr - \ell\pi/2)}{kr} - b_\ell \frac{\cos(kr - \ell\pi/2)}{kr}$$

We 'normalize' $R_\ell(r)$ as

$$R_\ell(r) \underset{r\to\infty}{\sim} \frac{\sin(kr - \ell\pi/2 + \delta_\ell)}{kr}.$$

Therefore, we choose

$$a_\ell = \cos\delta_\ell$$

$$b_\ell = -\sin\delta_\ell.$$

Hence for $r > a$

$$R_\ell(r) = \cos\delta_\ell\, j_\ell(kr) - \sin\delta_\ell\, n_\ell(kr)$$

$$= \cos\delta_\ell \left(j_\ell(kr) - \tan\delta_\ell\, n_\ell(kr) \right)$$

Now, the exterior wavefunction must vanish at $r = a$,

i.e.,

$$R_l(r \to a^+) = 0$$

or $$j_l(ka) - \tan\delta_l \, n_l(ka)$$

i.e., $$\boxed{\tan\delta_l = \frac{j_l(ka)}{n_l(ka)}}, \qquad (3)$$

S-wave phase shift

For s-wave, $l = 0$. Therefore

$$\tan\delta_0 = \frac{j_0(ka)}{n_0(ka)} = \frac{\sin ka/ka}{-\cos ka/ka}$$

or $$\tan\delta_0 = -\tan ka$$

or $$\boxed{\delta_0 = -ka} \quad \ldots\ldots\ldots \quad (4)$$

The s-wave radial wavefunction is

$$R_0(r) = \cos\delta_0 \frac{\sin kr}{kr} + \sin\delta_0 \frac{\cos kr}{kr}$$

$$= \frac{\sin(kr + \delta_0)}{kr} = \frac{\sin(kr - ka)}{kr} = \frac{\sin k(r-a)}{kr}.$$

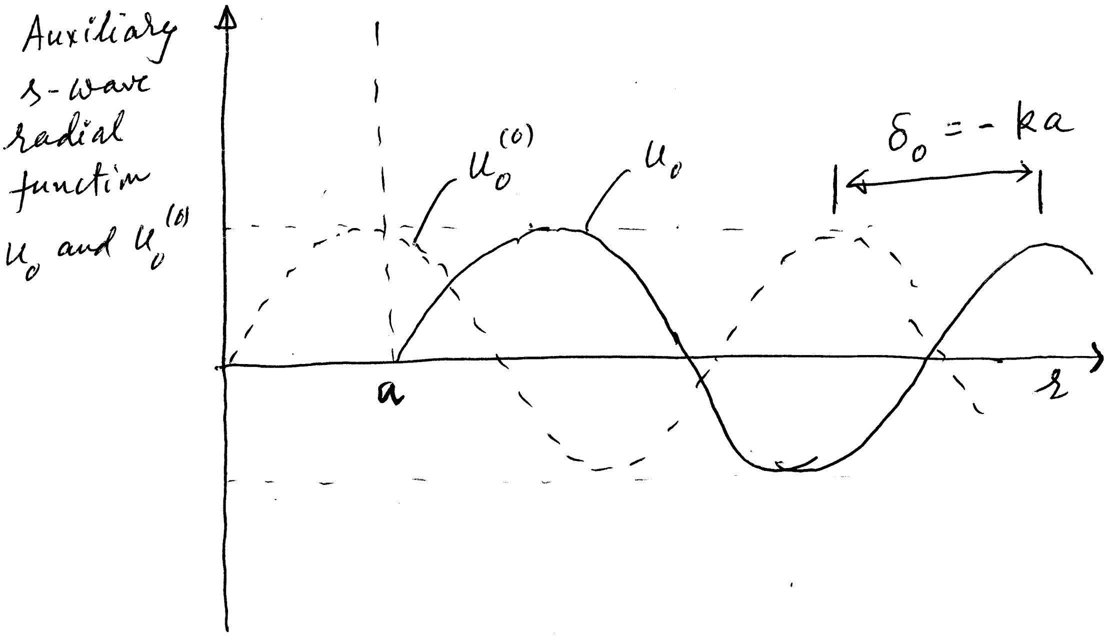
Therefore, the hard-sphere radial wave function is (in the s-wave)

$$R_0(r) = \begin{cases} 0 & r \le a \\ \dfrac{\sin k(r-a)}{kr} \end{cases}$$

while the s-wave radial wave function in the absence of the potential is

$$R_0^{(0)}(r) = j_0(kr) = \frac{\sin kr}{kr}. \quad (\text{for all } r)$$

In the figure below we have plotted $u_0^{(0)} \equiv kr R_0^{(0)}(r)$ and $u_0(r) = kr R_0(r)$



Low-energy limit of δ_ℓ

First we note that $\delta_0 = -ka$ exactly for all k, i.e., for all energies. Now, for all ℓ, including $\ell = 0$, we have

$$\tan \delta_\ell = \frac{j_\ell(ka)}{n_\ell(ka)}$$

exactly. For low energies $ka \ll 1$. Therefore,

$$j_\ell(ka) \simeq \frac{(ka)^\ell}{(2\ell+1)!!}$$

$$n_\ell(ka) \simeq -\frac{(2\ell-1)!!}{(ka)^{\ell+1}}$$

Therefore

$$\underset{(ka \ll 1)}{\tan \delta_\ell \simeq} \; -\frac{(ka)^{2\ell+1}}{(2\ell+1)!!\,(2\ell-1)!!} \quad \cdots\cdots (5)$$

Explicitly, low-energy phase shifts for the first few partial waves are given by

$$\tan \delta_0 \simeq -ka = \delta_0$$

$$\tan \delta_1 \simeq -\frac{(ka)^3}{3} \approx \delta_1$$

$$\tan \delta_2 \simeq -\frac{(ka)^5}{30} \approx \delta_2$$

We see that

$$\frac{\delta_1}{\delta_0} << 1, \quad \frac{\delta_2}{\delta_1} << 1$$

i.e., at low-energy the phase shifts for higher partial waves becomes progressively smaller so that the dominant contribution to the scattering comes from the s-wave.

Now, we can calculate the elastic scattering cross-section at low energy:

$$\sigma = \frac{4\pi}{k^2} \sum_{l=0}^{\infty} (2l+1) \sin^2 \delta_l$$

$$\simeq \frac{4\pi}{k^2} \sin^2 \delta_0$$

$$\simeq \frac{4\pi}{k^2} k^2 a^2 \qquad \left| \begin{array}{l} \delta_0 = -ka \text{ (small)} \\ \therefore \sin \delta_0 \approx \delta_0 = -ka \end{array} \right.$$

$$= 4\pi a^2,$$

which is four times the geometric cross section of the sphere.

High energy limit of the phase shifts

At high energies we have $ka >> 1$. ~~Also~~ Now,

$$j_\ell(ka) \underset{ka>>1}{\sim} \frac{\sin(ka - \ell\pi/2)}{ka}$$

$$n_\ell(ka) \underset{ka>>1}{\sim} -\frac{\cos(ka - \ell\pi/2)}{ka}$$

Therefore, in the high-energy limit, we have

$$\tan\delta_\ell(k) \simeq -\tan(ka - \ell\pi/2)$$

i.e.,

$$\delta_\ell(k) \simeq -ka + \tfrac{1}{2}\ell\pi \quad (ka>>1). \qquad (6)$$

At high energy, many ℓ-values contribute. We have appreciable contribution to the scattering cross sections from partial waves starting from $\ell=0$ up to a maximum of about $\ell_{max} \simeq ka$.

The integrated elastic cross-section is then

$$\sigma_{el} \simeq \frac{4\pi}{k^2} \sum_{l=0}^{l_{max}}{}' (2l+1) \sin^2 \delta_l$$

$$= \frac{4\pi}{k^2} \left[\sin^2 ka + 3 \sin^2 (\pi/2 - ka) + 5 \sin^2 (2\pi/2 - ka) + \cdots \right]$$

$$= \frac{4\pi}{k^2} \left[\sin^2 ka + 3 \cos^2 ka + 5 \sin^2 ka + 7 \cos^2 ka + \cdots \right]$$

$$\simeq \frac{4\pi}{k^2} \left(1 + 2 + 3 + \cdots + l_{max} \right)$$

$$= \frac{4\pi}{k^2} \; \frac{l_{max} (l_{max} + 1)}{2}$$

$$\simeq \frac{4\pi}{k^2} \cdot \frac{l_{max}^2}{2}$$

$$= \frac{2\pi}{k^2} l_{max}^2$$

$$= \frac{2\pi}{k^2} \cdot k^2 a^2$$

$$= 2\pi a^2 ,$$

which is twice the geometric cross-section of the sphere.

Ex Scattering by a square-well potential.

Consider the attractive square-well potential of depth V_0 and range a, i.e.,

$$V(r) = \begin{cases} -V_0 & r \leq a \\ 0 & r > a. \end{cases}$$

The plot of $V(r)$ is shown in the figure below

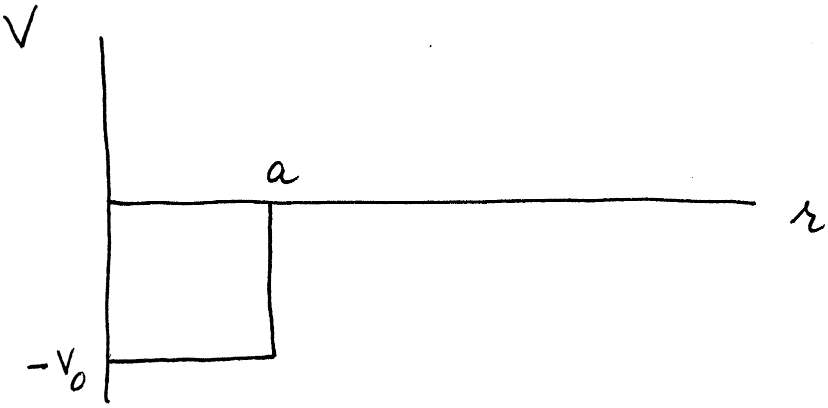


Fig: Square-well potential

The radial Schrödinger equation in the interior $(r<a)$ and exterior $(r>a)$ regions are

$$\frac{d^2 R_l}{dr^2} + \frac{2}{r}\frac{dR_l}{dr} + \left(k^2 - \frac{l(l+1)}{r^2} - U\right) R_l = 0; \quad r<a \quad \cdots (1)$$

and

$$\frac{d^2 R_l}{dr^2} + \frac{2}{r}\frac{dR_l}{dr} + \left(k^2 - \frac{l(l+1)}{r^2}\right) R_l = 0; \quad r>a. \quad \cdots (2)$$

Here

$$k^2 = \frac{2mE}{\hbar^2}$$

$$U = \frac{2mV}{\hbar^2}.$$

We now define another parameter K (capital 'kay')

as

$$K^2 = k^2 + U_0 = \frac{2m}{\hbar^2}(E + V_0).$$

Eq (1) can now be written as

$$\left[\frac{d^2}{dR^2} + \frac{2}{r}\frac{d}{dr} + K^2 - \frac{l(l+1)}{r^2}\right] R_l(r) = 0 \,; \quad r < ka \qquad (3)$$

The solution of this equation which is regular at the origin is $j_l(Kr)$. Therefore, inside the well ($r<a$), the radial wavefunction is

$$R_l(r) = N j_l(Kr) \,; \quad r < a \qquad \text{- - - - -} \quad (4)$$

where N is an arbitrary constant. Outside the well ($r>a$) the radial wave function is a solution of Eq. (2). We have

$$R_l(r) = c_l j_l(kr) + d_l n_l(kr) \,; \quad r > a \quad . \, (5)$$

which is a linear combination of $j_l(kr)$ and $n_l(kr)$.

We 'normalize' the radial wavefunction as

$$R_\ell(r) \underset{r\to\infty}{\sim} \frac{\sin(kr - \ell\pi/2 + \delta_\ell)}{kr}$$

Therefore, we must choose

$$c_\ell = \cos\delta_\ell$$

$$d_\ell = -\sin\delta_\ell$$

in Eq. (5). Therefore, we write

$$R_\ell(r) = \cos\delta_\ell \, j_\ell(kr) - \sin\delta_\ell \, n_\ell(kr). \quad \cdots (6)$$

$$(r > a).$$

Thus, the radial wavefunction for all r is given by

$$R_\ell(r) = \begin{cases} N j_\ell(Kr) \; ; & r < a \\ \cos\delta_\ell \, j_\ell(kr) - \sin\delta_\ell \, n_\ell(kr) \; ; & r > a. \end{cases}$$

$$\cdots (7).$$

The phase shift

The wavefunction and its derivative must match at $x = a$, i.e.,

$$N_\ell\, j_\ell(Ka) = \cos\delta_\ell\, j_\ell(ka) - \sin\delta_\ell\, n_\ell(ka) \quad \cdots\cdots (8)$$

$$N_\ell\, K j_\ell'(Ka) = \cos\delta_\ell\, k j_\ell'(ka) - \sin\delta_\ell\, k n_\ell'(ka) \quad \cdots (9)$$

where the prime represents derivative with respect to the argument. Dividing (9) by (8) we have

$$\frac{K j_\ell'(Ka)}{j_\ell(Ka)} = \frac{k\cos\delta_\ell\, j_\ell'(ka) - k\sin\delta_\ell\, n_\ell'(ka)}{\cos\delta_\ell\, j_\ell(ka) - \sin\delta_\ell\, n_\ell(ka)}$$

$$= \frac{k j_\ell'(ka) - k\tan\delta_\ell\, n_\ell'(ka)}{j_\ell(ka) - \tan\delta_\ell\, n_\ell(ka)}$$

or $K j_\ell'(Ka) j_\ell(ka) - \tan\delta_\ell\, K j_\ell'(Ka)\, n_\ell(ka)$

$$= k j_\ell(Ka) j_\ell'(ka) - k\tan\delta_\ell\, j_\ell(Ka)\, n_\ell'(ka)$$

or,

$$\tan\delta_\ell \left[k j_\ell(Ka)\, n_\ell'(ka) - K j_\ell'(Ka)\, n_\ell(ka) \right]$$

$$= k j_\ell(Ka)\, j_\ell'(ka) - K j_\ell'(Ka)\, j_\ell(ka)$$

or,

$$\tan\delta_\ell = \frac{k j_\ell'(ka) j_\ell(Ka) - K j_\ell(ka) j_\ell'(Ka)}{k n_\ell'(ka) j_\ell(Ka) - K n_\ell(ka) j_\ell'(Ka)} \quad \cdots (8)$$

<u>Low-energy limit of the phase shift.</u>

For low energy, $ka \ll 1$. Therefore

$$j_\ell(ka) \xrightarrow[ka \ll 1]{} \frac{(ka)^\ell}{(2\ell+1)!!}$$

$$n_\ell(ka) \xrightarrow[ka \ll 1]{} -\frac{(2\ell-1)!!}{(ka)^{\ell+1}}$$

$\therefore$

$$j_\ell'(ka) \xrightarrow[ka \ll 1]{} \frac{\ell\,(ka)^{\ell-1}}{(2\ell+1)!!}$$

$$n_\ell'(ka) \xrightarrow[ka \ll 1]{} \frac{(\ell+1)(2\ell-1)!!}{(ka)^{\ell+2}}$$

Therefore, in the low-energy limit we have

$$\tan\delta_\ell \simeq \frac{k\,\frac{\ell(ka)^{\ell-1}}{(2\ell+1)!!}\,j_\ell(Ka) - K\,\frac{(ka)^\ell}{(2\ell+1)!!}\,j_\ell'(Ka)}{k\,\frac{(\ell+1)(2\ell-1)!!}{(ka)^{\ell+2}}\,j_\ell(Ka) + K\,\frac{(2\ell-1)!!}{(ka)^{\ell+1}}\,j_\ell'(Ka)}$$

or,

$$\tan\delta_\ell \simeq \frac{1}{(2\ell+1)!!\,(2\ell-1)!!}\cdot\frac{\ell(ka)^{\ell-1}j_\ell(Ka) - Ka\,(ka)^{\ell-1}j_\ell'(Ka)}{\frac{(\ell+1)j_\ell(Ka)}{(ka)^{\ell+2}} + Ka\,\frac{1}{(ka)^{\ell+2}}\,j_\ell'(Ka)}$$

or,

$$\tan\delta_\ell \simeq \frac{(ka)^{2\ell+1}}{(2\ell+1)!!\,(2\ell-1)!!}\cdot\frac{\ell j_\ell(Ka) - Ka\,j_\ell'(Ka)}{(\ell+1)j_\ell(Ka) + Ka\,j_\ell'(Ka)}. \quad \text{---(9)}$$

From this we deduce the important result that at low-energy the phase shifts are given by

$$\tan\delta_\ell \approx (ka)^{2\ell+1}$$

i.e., low partial waves dominate. Although this result has been deduced for the square-well potential, it is generally true for any smooth potential.

From Eq. (9) we also notice that at a certain energy the denominator may vanish at a certain partial wave l. The phase shift δ_l then becomes equal to $\pi/2$. In that case the partial cross section $\sigma_{el,l}$ for the l^{th} partial wave is maximum. This is known as resonance scattering in the l^{th} partial wave.

If there is no resonance, the s-wave dominates the other wave.

s-wave phase shift

For s-wave, the exact formula for the phase shift can easily be expressed in terms of elementary trigonometric functions. Substituting $l=0$ in Eq. (8) we get

$$\tan\delta_0 = \frac{k\, j_0'(ka)\, j_0(Ka) - K\, j_0(ka)\, j_0'(Ka)}{k\, n_0'(ka)\, j_0(Ka) - K\, n_0(ka)\, j_0'(Ka)}$$

Multiply both the numerator and the denominator by a.

$$\tan\delta_0 = \frac{ka\, j_0'(ka)\, j_0(Ka) - Ka\, j_0(ka)\, j_0'(Ka)}{ka\, n_0'(ka)\, j_0(Ka) - Ka\, n_0(ka)\, j_0'(Ka)} \qquad (10)$$

Now

$$j_0(x) = \frac{\sin x}{x}, \qquad j_0'(x) = \frac{\cos x}{x} - \frac{\sin x}{x^2}$$

$$n_0(x) = -\frac{\cos kx}{x}, \qquad n_0'(x) = \frac{\sin x}{x} + \frac{\cos x}{x^2}.$$

$$\therefore \quad x\, j_0'(x) = \cos x - \frac{\sin x}{x} \qquad \cdots\cdots (11)$$

$$x\, n_0'(x) = \sin x + \frac{\cos x}{x} \qquad \cdots\cdots (12)$$

Substitute Eqs. (11) and (12) in Eq. (10).

We get

$$\tan\delta_0 = \frac{\left(\cos ka - \frac{\sin \cancel{ka}}{\cancel{ka}}\right)\frac{\sin Ka}{Ka} - \left(\cos Ka - \frac{\sin \cancel{Ka}}{\cancel{Ka}}\right)\frac{\sin ka}{ka}}{\left(\sin ka + \frac{\cos \cancel{ka}}{\cancel{ka}}\right)\frac{\sin Ka}{Ka} + \frac{\cos ka}{ka}\left(\cos Ka - \frac{\sin \cancel{Ka}}{\cancel{Ka}}\right)}$$

$$= \frac{\frac{\cos ka \sin Ka}{Ka} - \frac{\cos Ka \sin ka}{ka}}{\frac{\sin ka \sin Ka}{Ka} + \frac{\cos ka \cos Ka}{ka}}$$

$$= \frac{ka \cos ka \sin Ka - Ka \cos Ka \sin ka}{ka \sin ka \sin Ka + Ka \cos ka \cos Ka}$$

cancel a

$$= \frac{k \cos ka \sin Ka - K \cos Ka \sin ka}{k \sin ka \sin Ka + K \cos ka \cos Ka}$$

Divide both numerator and denominator by $\cos ka \cos Ka$

$$= \frac{k \tan Ka - K \tan ka}{k \tan ka \tan Ka + K}$$

Divide numerator and denominator by K

$$\tan\delta_0 = \frac{-\tan ka + \frac{k}{K}\tan Ka}{1 + \frac{k}{K}\tan ka \tan Ka}$$

$$= \frac{\tan(-ka) + \frac{k}{K}\tan Ka}{1 - \frac{k}{K}\tan(-ka)\tan Ka}$$

Let

$$\tan X = \frac{k}{K}\tan Ka$$

therefore

$$\tan\delta_0 = \frac{\tan(-ka) + \tan X}{1 - \tan(-ka)\tan X} \qquad \text{.....}(13).$$

Use the trigonometric identity

$$\tan(A+B) = \frac{\tan A + \tan B}{1 - \tan A \tan B}$$

$\therefore$

$$\tan\delta_0 = \tan(-ka + X)$$

or $\quad \delta_0 = -ka + X$

or, $$\boxed{\delta_0 = -ka + \tan^{-1}\left(\frac{k}{K}\tan Ka\right)} \quad \cdots\cdots (14)$$

This equation for δ_0 is exact.

Low-energy limit of the s-wave phase shift.

In the low-energy limit (i.e., $ka \ll 1$) we can obtain an approximate formula for the s-wave phase shift δ_0 either from Eq. (9) or from Eq. (14).

Substituting $l = 0$ in Eq. (9) we get

$$\tan\delta_0 \simeq (ka)\,\frac{-Ka\,j_0'(Ka)}{j_0(Ka) + Ka\,j_0'(Ka)}$$

$(ka \ll 1)$

Using Eq. (11)

$$\tan\delta_0 \simeq ka\,\frac{-\left(\cos Ka - \frac{\sin Ka}{Ka}\right)}{\frac{\sin \cancel{Ka}}{\cancel{Ka}} + \cos Ka - \frac{\sin \cancel{Ka}}{\cancel{Ka}}}$$

or $$\tan\delta_0 \simeq -ka\underbrace{\left(1 - \frac{\tan Ka}{Ka}\right)}_{-\text{ve for } Ka < \pi/2} \quad \cdots\cdots (15)$$

Suppose the term within the brackets in the above equation is finite, i.e., $Ka \neq \pi/2, 3\pi/2, 5\pi/2 \ldots$ etc. Then since ka is very small, $\tan\delta_0$ is very small too. Therefore,

$$\tan\delta_0 \simeq \delta_0 \simeq -ka\left(1-\frac{\tan Ka}{Ka}\right)$$

Hence the s-wave cross-section is

$$\sigma_0 = \frac{4\pi}{k^2}\sin^2\delta_0 \qquad \Big|\ \sin\delta_0 \approx \delta_0$$

$$= \frac{4\pi}{k^2} k^2a^2\left(1-\frac{\tan Ka}{Ka}\right)^2$$

i.e.,

$$\sigma_0 = 4\pi a^2\left(1-\frac{\tan Ka}{Ka}\right)^2 \quad \text{------} (16)$$

Next, what might happen if the potential strength is large enough so that

$$Ka = \pi/2$$

i.e.

$$\left(\sqrt{U_0+k^2}\right)a = \pi/2$$

Since k is small

$$\sqrt{U_0}\,a = \pi/2.$$

At this strength, the potential can just support a bound state, with negligible binding energy.

Now, starting from a weak potential, if we gradually increase the strength of the potential (keeping k fixed) $\tan\delta_0$ gradually increases starting from a very small value. When Ka approaches $\pi/2$ from below ($Ka \to \pi/2^-$) $\tan Ka \to \infty$, i.e., $\tan\delta_0 \to \infty$, i.e., $\delta_0 \to \pi/2$. The potential now is just able to support a bound state with almost zero energy (i.e., bound state energy $= -\epsilon$ with ϵ very small). The scattering cross-section is now

$$\sigma_{sc} = \frac{4}{k^2}\sin^2\delta_0 = \frac{4\pi}{k^2} \to \infty \text{ as } k \to 0.$$

So there is a resonance in the elastic cross section if the potential can support a bound state with almost zero energy. At resonance, the elastic cross-section increases to the unitarity limit $4\pi/k^2$.

Next, keeping R fixed, if we keep on increasing the strength of the potential δ_0 would increase and become greater than $\pi/2$, but the cross-section would fall. If we increase the potential strength so that Ka approaches $3\pi/2$, the potential is now just able to support a second bound state at zero energy while the first bound state is now much deeper.

With $Ka \to 3\pi/2^-$, $\tan Ka \to \infty$, so that again $\tan\delta_0 \to \infty$. Now $\delta_0 = 3\pi/2$, so that $\sin\delta_0 = -1$. We have again a resonance with cross section reaching the unitarity limit.

Thus, at small incid^t energies, we can have resonance in the elastic cross section if the potential can <u>just</u> support one bound state, two bound states, and so on.