Chapter III: Theory of Elastic Scattering
Classical theory

Observations of elastic scattering of atoms and molecules can be accounted for to a large extent by classical mechanics. Classically, scattering of a beam of particles passing through a material medium can be calculated by considering the orbits of representative particles in the beam. Suppose a parallel beam of particles of uniform intensity and of infinite lateral extent to be incident on a single scattering center which is supposed to be associated with a particle of infinite mass. Let \( E \) be the initial kinetic energy of the incident particle and \( V(r) \) the spherically symmetric potential energy due to the centre of force. After scattering the particle moves in a direction making an angle \( \theta \) with the incident direction. The perpendicular drawn from the scattering center to the initial direction of motion of a particle in the beam is known as impact parameter \( b \). For each value of \( b \) there will be a definite value of the angle of scattering \( \Theta \).

The deflection function \( \Theta \) is defined by \( \Theta = |\Theta| \). From the consideration of energy and momentum conservation the expression for the classical deflection function can be written as,

\[
\Theta (b, E) = \pi - 2b \int_0^\infty \frac{d\nu}{n^2 [F_c(n)]^{1/2}} \quad \cdots \cdots (1)
\]

where

\[
F_c(n) = 1 - V(n)/E - b^2/n^2 \quad \cdots \cdots (2)
\]

\( \Theta \) is positive for net repulsive and negative for attractive trajectories.
We assume that the potential $V(r)$ consists of a long-range attractive part, an attractive well and a short range repulsive part. For this type of potential a typical curve can be drawn (Fig. 1) showing the dependence of the deflection function upon the reduced impact parameter $b^* = b/\sigma$ for a definite value of the reduced collision energy $E^* = E/\epsilon$ where $\epsilon$ is the depth of the attractive well and $\sigma$ is a characteristic length. The positive region of the curve is associated with domination of repulsion and the negative region with predominance of the attractive forces.

The number of particles scattered in a direction $\theta$ per unit time per unit incident intensity can be written as

$$\frac{d\sigma(\theta)}{d\Omega} = \sum_{i=1}^{3} b_i \sin \theta \left| \frac{\partial \theta}{\partial b_i} \right|$$

where the summation is over the three possible branches of the deflection function contributing to the scattering angle $\theta$. $d\Omega$ is the solid angle subtended at the scattering centre between the two cones of semi vertical angle $\theta$ and $\theta + d\theta$.

The quantity in eqn(3) has the dimension of area and is known as the differential cross section for elastic scattering of the incident beam by the scattering centre. It is seen from the classical description whenever $\sin \theta = 0$, provided $d\theta/db$ is finite, a pole occurs in the scattering at the appropriate angle. This is called 'glory effect'. Another singularity as well as discontinuity occurs at $\theta = \theta_r$ where $d\theta/db = 0$ which is called
Fig. 1. (a) Dependence of the deflection function upon the reduced impact parameter $b^*$ for L-J (12;6) potential for a reduced relative kinetic energy $E^*$.

(b) The corresponding dependence of the semiclassical reduced phase $\eta^*$ upon the reduced impact parameter $b^*$ for the same case.
'rainbow effect'. It is seen from the fig.1 that for $\theta > \theta_r$ only one region of the deflection function contributes to the scattering while three regions contribute for $\theta < \theta_r$ i.e., three values of $b$ correspond to a given value of $|\Theta|$.

The total elastic cross section $\sigma$ of the incident particle of a given velocity is defined as the total number of particles scattered elastically by the scattering centre per unit time from a beam of unit intensity i.e., such that one incident particle crosses unit area per unit time.

$$\sigma = 2\pi \int_0^\pi \sin \theta \frac{d\sigma(\theta)}{d\Omega} d\theta \quad \ldots \ldots \ (4)$$

In practice the number scattered through an angle greater than some small angle $\theta_0$ can be measured. If the lower limit of $\theta$ in expression (4) is replaced by $\theta_0$, we shall get the 'incomplete' or 'apparent' total cross section.

However classical theory cannot explain some unphysical singularities in differential cross sections and divergence in the low angle scattering due to inverse power potential. Experimentally we get also some oscillations in total and differential cross sections which cannot be explained by classical theory. So to interpret all the important features of scattering, quantum theory is essential.
Quantum theory

Suppose a beam of particles of mass $m$, velocity $v$ and energy $E = \frac{p^2 + m^2}{2m}$ be incident on a scattering centre along the positive direction of the $z$-axis and the scattering field is central i.e., it can be represented by a potential $V(r)$, a function of $r$ only. The origin of coordinates is taken at the scattering centre and the $z$-axis taken as the polar axis of the spherical polar coordinates.

The Schrödinger equation representing the beam can now be written as

$$
\nabla^2 \psi + \frac{2m}{\hbar^2} \left[ E - \frac{\hbar^2 V(r)}{m} \right] \psi = 0
$$

or,

$$
\left[ \nabla^2 + k^2 - U(r) \right] \psi = 0 \quad \ldots \ldots (5)
$$

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

The stream of incident particles can be represented by the plane wave $\exp(ikz)$ where $k$ is equal to $\sqrt{2mE}/\hbar$. The scattered particles may be represented by a spherical wave diverging from the scattering centre and with an amplitude inversely proportional to the distance. Therefore, to get a solution of the wave equation (5) we can take the asymptotic form for large $r$

$$
\psi \sim e^{ikz} + \frac{e^{ikr}}{r} f(\theta) \quad \ldots \ldots (6)
$$

Now our problem is to find the function $f(\theta)$ which can be calculated using Rayleigh - Faxon - Holtzmark method of partial waves.
In field free space the Schrödinger wave equation can be written as
\[
\left( \nabla^2 + k^2 \right) \psi = 0 \tag{7}
\]
and the solution of this equation will be of the form
\[
\psi = e^{i k z} = \sum_{l=0}^{\infty} \frac{A_l u_l(r)}{k r} P_l(\cos \theta) \tag{8}
\]
where
\[
\frac{d^2 u_l}{dr^2} + \left[ k^2 - \frac{l(l+1)}{r^2} \right] u_l = 0 \tag{9}
\]
\(l\) is the orbital angular momentum and \(P_l(\cos \theta)\) is the Legendre function. Equation (9) is a well known equation in mathematical physics and solution of this equation in terms of Bessel function can be written as
\[
\frac{u_l(r)}{kr} = \left( \frac{\pi}{2kr} \right)^{1/2} J_{l+1/2}(kr) \tag{10}
\]
The constant \(A_l\) in eqn. (8) is equal to \((2l+1)i^l\) and eqn. (8) becomes
\[
e^{i k z} = \sum_{l=0}^{\infty} (2l+1)i^l \frac{u_l(r)}{kr} P_l(\cos \theta) \tag{10}
\]
with
\[
u_l(r) \sim \sin \left( kr - \frac{1}{2} i \ell \pi \right)
\]
We shall now find out solution of eqn.(5) that has the asymptotic form of an incident plane wave and a spherical scattered
wave. \( \psi \) can be written as a harmonic expansion as

\[
\psi = \sum_{\ell=0}^{\infty} B_{\ell} \frac{\psi_{\ell}(r)}{kr} P_{\ell}(\cos \theta) \quad \cdots \quad (11)
\]

where

\[
\frac{d^2 \psi_{\ell}}{dr^2} + \left( k^2 - \frac{\delta(r)}{r^2} - \frac{\ell(\ell+1)}{r^2} \right) \psi_{\ell} = 0 \quad \cdots \quad (12)
\]

We must choose solutions for \( \psi_{\ell} \) in equation (12) which vanish at origin. If \( \delta(r) \rightarrow 0 \) for large \( r \)

\[\psi_{\ell}(r) \sim \sin \left( kr - \frac{1}{2} \ell \pi + \eta_{\ell} \right)\]

where \( \eta_{\ell} \) is a phase constant.

So at large value of \( r \) the effect of scattering potential \( V(r) \) is to introduce a change of phase in the asymptotic form of the radial functions.

If \( \psi \) of eqn. (11) is to have asymptotic form (6) we have, for all \( \ell \),

\[
D_{\ell} r^{-1} e^{ikr} \sim \frac{\left[ B_{\ell} \sin \left( kr - \frac{1}{2} \ell \pi + \eta_{\ell} \right) - (2\ell+1) i^{\ell} \sin \left( kr - \frac{\ell \pi}{2} \right) \right]}{kr}
\]

\[
= \frac{\exp\left[ i \left( kr - \frac{1}{2} \ell \pi \right) \right]}{2ikr} \left[ B_{\ell} e^{i\eta_{\ell}} - (2\ell+1) i^{\ell} \right]
\]

\[
- \frac{\exp\left[ -i \left( kr - \frac{1}{2} \ell \pi \right) \right]}{2ikr} \left[ B_{\ell} e^{-i\eta_{\ell}} - (2\ell+1) i^{\ell} \right]
\]

\[\cdots \cdots (13)\]

where \( D_{\ell} \) is a constant. If the asymptotic form includes outgoing
spherical waves only, the second term in eqn.(13) must vanish and we get

\[ B_\ell = (2\ell + 1)i^{\ell}e^{i\eta_\ell} \quad \ldots \quad (14) \]

Substitution for \( B_\ell \) in equation (11) gives the wave function

\[ \Psi = \sum_{\ell=0}^{\infty} (2\ell + 1)i^{\ell}e^{i\eta_\ell} j_\ell(r) P_\ell(\cos \theta) / kr \quad \ldots \quad (15) \]

The amplitude of the scattered wave is obtained in terms of phase shift \( \eta_\ell(k) \) as

\[ f(\theta) = \sum_{\ell=0}^{\infty} D_\ell P_\ell(\cos \theta) \]

\[ = \frac{1}{2ik} \sum_{\ell=0}^{\infty} (2\ell + 1)(e^{2i\eta_\ell - 1}) P_\ell(\cos \theta) \quad \ldots \quad (16) \]

The differential cross section for elastic scattering at an angle \( \theta \) is then given by

\[ I(\theta) = \frac{d\sigma(\theta)}{d\Omega} = \frac{1}{4k^2} \left\{ \left[ \sum_{\ell}(2\ell + 1) \sin 2\eta_\ell P_\ell(\cos \theta) \right]^2 \right. \]

\[ + \left. \left[ \sum_{\ell}(2\ell + 1)(\cos 2\eta_\ell - 1) P_\ell(\cos \theta) \right]^2 \right\} \quad \ldots \quad (17) \]

and the total cross section is given by

\[ \sigma = \frac{4\pi}{k^2} \int_0^{2\pi} \sin \theta \left| f(\theta) \right|^2 d\theta \]

\[ = 4\pi \sum_{\ell=0}^{\infty} \left( 2\ell + 1 \right) \sin^2 \eta_\ell \quad \ldots \quad (18) \]
The exact quantum treatment of elastic scattering requires generally a large number of numerical integration of the radial wave equations which are very laborious although this has been done for many cases. If some approximations can be introduced suitably, then the computational labour of evaluating wave functions, phase shift or cross section becomes much less. So these approximation methods for radial wave function or phase shift are widely used by many workers.

**JWKB Approximation**

Jeffreys - Wentzel - Kramers - Brillouin approximation or asymptotic approximation for the radial wave function is valid only in the limit of very slowly varying potential.

\[
\frac{d}{dr} \left[ \ln V(r) \right] \ll k r
\]  \hspace{1cm} \cdots \cdots (19)

which means that the de Broglie wavelength is small enough so that the fractional change in \(V(r)\) over a wavelength is negligible. With this assumption the radial differential equation may be simplified and the usual 'semiclassical' radial wave functions are written in two forms expressing the asymptotic behaviour on the two sides of the classical turning point \(r_0\).

\[
\psi_\ell (r) \sim \frac{1}{2} \left[ \frac{p_\infty}{|p_r|} \right]^{1/2} \exp \left[ - \frac{1}{\hbar} \int_{r_0}^r |p_r| dr \right], \quad r < r_0 \quad \cdots \cdots (20a)
\]

\[
\psi_\ell (r) \sim \left[ \frac{p_\infty}{|p_r|} \right]^{1/2} \sin \left[ \frac{1}{\hbar} \int_{r_0}^r p_r dr + \frac{\pi}{4} \right], \quad r > r_0 \quad \cdots \cdots (20b)
\]
being the local radial momentum given by
\[ \hat{p}_r = \hbar k_r = \hbar / \lambda_r = \left[ 2m(E - V_{\text{eff}}(r))^2 \right]^{1/2} \]
where the effective potential is defined by
\[ V_{\text{eff}}(r) = V(r) + \left( \ell + \frac{1}{2} \right) \frac{\hbar^2}{2m r^2} \]
(21)

\( p_\infty = \hbar k \) is the incident momentum and \( k_r = \frac{k}{\mathcal{F}_C(r)} \) is the local wave number.

\[ \mathcal{F}_C(r) = 1 - \frac{V(r)}{k} - \left( \ell + \frac{1}{2} \right)^2 \frac{k^2 r^2}{k^2 r^2} \]
\[ = 1 - \frac{V(r)}{E - b^2 / r^2} \]
\[ = 1 - \frac{V_{\text{eff}}}{E} \]
(22)

where \( b = \left( \ell + \frac{1}{2} \right) / k \).

The classical turning point \( r_0 \) is defined by the outermost zero of \( \mathcal{F}_C(r) \) i.e., the value of \( r \) for which \( \mathcal{F}_C(r) = 0 \).
Therefore equation (20b) can be expressed in the following form suitable for numerical computation
\[ u_\ell(r) = \left[ \mathcal{F}_C(r) \right]^{-1/2} \sin \left[ \int_{r_0}^r \left[ \mathcal{F}_C(r) \right]^{1/2} dr + \frac{\pi}{4} \right] \]
(23)

The JWKB-approximated phase shifts may be obtained directly from the asymptotic form of the radial wave function by comparing the expression
\[ \sin \left[ k \int_{r_0}^R \left[ \mathcal{F}_C(r) \right]^{1/2} dr + \frac{\pi}{4} \right] \]
and
\[ \sin \left[ kr - \frac{\ell \pi}{2} + \eta_\ell \right] \]
in the limit of large \( R \).
Then we have

\[ \eta_l = \lim_{R \to \infty} \frac{k}{r_o} \left[ \int_{r_o}^{R} \frac{F_0(\xi)}{\xi} d\xi \right] + \frac{\pi}{\xi} (l + \frac{1}{2}) \]

\[ = \frac{\pi}{\xi} (l + \frac{1}{2}) + k r_o + \frac{1}{r_o} \int_{0}^{\infty} \left[ F_0(\xi) \xi \right] d\xi \]

For computational purposes this may be written in the form

\[ \eta_l = \frac{\pi}{2} (l + \frac{1}{2}) + k r_o \left\{ \int_{0}^{1} \left[ F_0(\xi) \xi \right] d\xi \right\} \]

where \( \xi = r_o / r \).

Since eqn (25) involves only a quadrature, whereas the exact solution requires direct numerical integration of the second order differential equation the JWKB phase shift calculation is much faster. For high energies i.e., above the critical energy for classical orbiting the JWKB phase shifts are sufficiently accurate. The JWKB approximation imposes no restriction on the size of phase shift but the absolute uncertainty increases with the magnitude of \( \eta_l \).

**Born Approximation**

To treat the scattering of a beam of particles by a field \( V(r) \) we can obtain an approximate formula which is only valid for fast particles but which can be evaluated with much less labour than the exact formula given by eqn (16).

Here also we have to solve the wave equation (5) where \( \psi \) has the asymptotic form (6). We shall use the theorem that the most
general bounded solution of the equation
\[ \nabla^2 \psi + k^2 \psi = F(x, y, z) \]
where \( F(x, y, z) = F(r) \) is a known function, which has a particular integral behaving asymptotically like an outgoing spherical wave, is
\[ \psi = G(x, y, z) - \frac{1}{4\pi} \int \frac{\exp(i k |\vec{r} - \vec{r}'|)}{|\vec{r} - \vec{r}'|} F(\vec{r}') d\tau'. \]
where \( G \) is the general solution of
\[ \nabla^2 G + k^2 G = 0. \]
So the solution \( \psi \) of eqn(5) will satisfy the integral equation
\[ \psi = G - \frac{1}{4\pi} \int \frac{\exp(i k |\vec{r} - \vec{r}'|)}{|\vec{r} - \vec{r}'|} u(\vec{r}') \psi(\vec{r}') d\tau' \]
(26)
The expression on the right side of eqn (26) represents an outgoing wave. Thus in order that \( \psi \) may have the form (6)
\[ G = e^{ikz}. \]
Let \( \hat{n} \) be unit vector in the direction of \( \vec{r} \), then
\[ |\vec{r} - \vec{r}'| = r - \hat{n} \cdot \vec{r}' + \text{terms of order } 1/r. \]
Hence from (26)
\[ \psi \sim e^{ikz} - r e^{ik \cdot \hat{n} \cdot \vec{r}' - \frac{1}{4\pi} \int e^{-i k \hat{n} \cdot \vec{r}'} u(\vec{r}') \psi(\vec{r}') d\tau'. \]
(27)
Eqns. (26) and (27) are exact. We now assume that the wave is not much diffracted by the scattering centre and then $\psi (\vec{r}')$ in the integral in (27) can be replaced by the unperturbed wave function $\exp \left( i\vec{k}\cdot\vec{z}' \right)$. This approximation is valid only for fast particles.

We then obtain from (6) and (27) dropping the dashes

$$f(\theta) = -\frac{1}{4\pi} \int e^{i\vec{p} \cdot \left( \vec{n}_0 - \vec{n} \right)} \psi(\vec{r}) d\tau \quad \ldots \quad (28)$$

where $\vec{n}_0$ is unit vector along the Z-axis.

This method is known as Born approximation which is a first order approximation method. The method can be continued to higher approximation by an iterative procedure.

The angular integration in (28) can be done taking $\vec{n}_0 - \vec{n}$ as polar axis and writing $\vec{K} = k \left( \vec{n}_0 - \vec{n} \right)$ and $K = 2k \sin \frac{1}{2} \theta$. we obtain

$$f(\theta) = -\frac{2m}{\hbar^2} \int_0^\infty \frac{\sin K\rho}{K\rho} V(r) r^2 dr \quad \ldots \quad (29)$$

where $K\rho$ is the change in momentum due to scattering. The scattering amplitude given by Born approximation is always real whereas exact scattering amplitude is complex. Eqn. (29) can be written in the form (16) using the harmonic expansion

$$\frac{\sin K\rho}{K\rho} = \frac{\pi}{2Kr} \sum_{\ell=0}^\infty (2\ell+1) P_{\ell}(\cos \theta) \left[ J_{\ell+\frac{1}{2}}(Kr) \right]^2.$$
so that
\[
f(\theta) = -\frac{\pi m}{\hbar^2 k} \sum_{\ell=0}^{\infty} (2\ell+1) P_{\ell}(\cos \theta) \int_0^\infty \left[ J_{\ell+\frac{1}{2}}(k\nu) \right]^2 v(\nu) \nu \, d\nu.
\]

which reduces to the form (16) if
\[
e^{2i\eta_l} - 1 = -\frac{2i\pi m}{\hbar^2} \int_0^\infty \left[ J_{\ell+\frac{1}{2}}(k\nu) \right]^2 v(\nu) \nu \, d\nu \quad \cdots (30)
\]

In the Born approximation the interaction potential is assumed to be a small perturbation. Under this condition \( \eta_l \) should be small so that \( e^{2i\eta_l} - 1 \) can be approximated by \( 2i\eta_l \). Then
\[
\eta_B = \eta_l = -\frac{\pi m}{\hbar^2} \int_0^\infty \left[ J_{\ell+\frac{1}{2}}(k\nu) \right]^2 v(\nu) \nu \, d\nu \quad \cdots (31)
\]

So Born's approximation is equivalent to the use of phases given by (31) in (16). For small values of \( \eta_l \) the agreement between Born approximation and exact calculation is fairly good.

For large \( \ell \), the main contribution to the integral arises from the region outside the first zero of the Bessel function, \( r_0 \) and replacing the rapidly oscillatory part of the integrand by its mean value beyond \( r_0 \), we obtain
\[
\eta_B = -\frac{m}{\hbar^2} \int_b^\infty \frac{v(\nu) \, d\nu}{(1 - \ell^2/k^2 \nu^2)^{1/2}} \quad \cdots (32)
\]
Jeffrey obtained the same expression for phase shift by another route and so this expression for phase shift is sometimes called Jeffreys-Born phase shift. For an inverse sixth power potential \( V(r) \sim \frac{c^{(6)}}{r^s} \), Jeffreys-Born approximation for higher order phases may be written as
\[
\eta_{JB} = \frac{3\pi}{16} \frac{m_c c^{(6)}}{\hbar^2} \frac{k^4}{(\ell + \frac{1}{2})^5} \quad \cdots \quad (33)
\]

**Semi-classical Theory**

The semi-classical approximation may be considered to be defined by a set of mathematical approximations introduced into equation (16). Semi-classical approximation techniques always add some insight into the physics which helps to draw some inferences and make some predictions which would not be possible otherwise.

1. The phase shift \( \eta_\ell \) is replaced by its JWKB-approximation value given by eqn (24). For understanding the relation between quantum and classical results, the most important property of the JWKB phase shift is its simple relation to the classical deflection function \( \Theta(\ell) \)

\[
\Theta(\ell) = 2d\eta_\ell / d\ell.
\]

2. The Legendre polynomial is replaced by the asymptotic expression valid for large \( \ell \). For \( \sin \theta > 1/\ell \)

\[
P_\ell (\cos \theta) \approx \left[ \frac{1}{2} (\ell + \frac{1}{2}) \pi \sin \theta \right]^{-1/2} \sin \left[ (\ell + \frac{1}{2}) \theta + \frac{\pi}{4} \right] \quad \cdots \quad (34)
\]
For $\sin \theta \leq 1/l$,

$$P_\ell (\cos \theta) \simeq (\cos \theta)^\ell J_\nu \left[ (\ell + \frac{1}{2}) \theta \right] \quad \ldots \ldots \quad (35)$$

These formulae overlap slightly, so that the whole range of $\theta$ is covered. This approximation requires for its validity that many $\ell$-values contribute to the scattering at a given angle or that the major contribution comes from $\ell$-values large compared to unity. However formulae (34) and (35) are good approximations even at rather small $\ell$.

(3) The summation of scattering amplitudes in eqn (16) is replaced by an integral over $\ell$. This approximation requires for its validity that many partial waves should contribute to the scattering and that the phase shift should vary slowly and smoothly with $\ell$. $(\ell + 1/2)$ is replaced by $\ell$. If we consider angles not too close to 0 or $\pi$, with the above approximations using eqn.(34) we can write the semi-classical scattering amplitude as

$$f_{\text{sc}}(\theta) = \frac{-1}{k(2\pi \sin \theta)^{1/2}} \int_0^\infty d\ell \ell^{1/2} \left[ e^{iB_1(\ell)} - e^{iB_2(\ell)} \right] \quad \ldots \ldots \quad (36)$$

where $B_1(\ell) = 2\eta_\ell + \ell\theta + \pi/4$ and $B_2(\ell) = 2\eta_\ell - \ell\theta - \pi/4$ ...(37)

The terms in the integrand are rapidly oscillating and for the most part destructively interfere. So the integral for scattering amplitude is evaluated by the method of stationary phase. Here we take the values of $\ell$, say $L$, for which one or the other of the $B$s are stationary. When $(B_1')_L = (dB_1/d\ell)_L = 0$, only
significant contribution to the integral comes from the region near $L$. Writing $B^\prime_1 = 0$ in eqn (37) we get

$$\eta_L^\prime = (\frac{d\eta}{dl})_L = -\frac{1}{2} \Theta_L.$$  

When $B^\prime_2 = 0$, $\eta_L^\prime = \frac{1}{2} \Theta_L$. We have seen previously that for net repulsive trajectories $\Theta = -\Theta$ and for net attractive trajectories $\Theta = -\Theta$. Thus for the contributions from the attractive branch of the deflection function we have $\eta_L^\prime = \frac{1}{2} \Theta_L$ corresponding to $B^\prime_1 = 0$ and for repulsive branch we have also $\eta_L^\prime = \frac{1}{2} \Theta_L$ corresponding to $B^\prime_2 = 0$.

Equation (36) can be expressed as the sum of three terms

$$f_{sc}^{\prime} (\Theta) = f_a (\Theta) + f_b (\Theta) + f_c (\Theta)$$

where $a$, $b$ and $c$ refer to the three regions of $L$, outermost attractive, inner attractive and inner repulsive region respectively. For $\Theta$ greater than the rainbow angle there will be one region of stationary phase.

**Rainbow Scattering**

In general $\Theta_r$ may be either positive or negative. But for the atomic and molecular scattering problem $\Theta_r$ and $(d\eta/dl)_r$ are always negative. Now from the definition of rainbow angle

$$\left(\frac{d^2 \eta}{dl^2}\right)_r = \frac{1}{2} \left(\frac{d \Theta}{dl}\right)_r = 0 \quad \cdots \quad (38)$$

and

$$\left(\frac{d^3 \eta}{dl^3}\right)_r = \frac{1}{2} \left(\frac{d^2 \Theta}{dl^2}\right)_r \equiv q_r \quad \cdots \quad (39)$$

where $q$ is always positive.
The scattering amplitude near the rainbow angle can be expressed as
\[ f_{\#}(\theta) = f_{\#}(\theta) + f_{c}(\theta), \quad \ldots \ldots \quad (40) \]

\( f_{\#}(\theta) \) gives the combined contribution of \( f_{\#}(\theta) \) and \( f_{c}(\theta) \) to the scattering amplitude. The repulsive contribution is given by
\[ f_{c}(\theta) = \left[ I_{c}(\theta) \right]^{1/2} e^{i\gamma_{c}}, \quad \ldots \ldots \quad (41) \]

where \( \gamma_{c} = 2\eta_{L_{c}} - L_{c}\theta - \pi/2 \).

To evaluate \( f_{\#} \) which is associated with the attractive branch of the deflection function we must use the function \( B_{1} \) of eqn(36):

Near a rainbow angle, the deflection function may be expanded in the form
\[ \Theta(l) = \Theta_{\#} + q_{r}(l-l_{r})^{2}, \quad \ldots \ldots \quad (42) \]

Then the phase shift near \( l_{r} \) will be given by the expression
\[ \eta_{l} = \eta_{\#} - \frac{1}{2} \theta_{\#} (l-l_{r}) + \frac{1}{6} q_{r} (l-l_{r})^{3} \quad \ldots \ldots \quad (43) \]

Therefore from eqns.(43) and (37) we can write
\[ B_{1} = 2\eta_{\#} - \theta_{\#} (l-l_{r}) + \frac{1}{3} q_{r} (l-l_{r})^{3} + l\theta + \frac{\pi}{4} \]
\[ \equiv B_{1}(l_{r}) + \Delta B_{1}, \quad \ldots \ldots \quad (44) \]

where \( B_{1}(l_{r}) \equiv 2\eta_{\#} + l_{r}\theta_{\#} + \pi/4 \).
and \[ \Delta B_1 = \frac{1}{3} q r (l-l r)^3 + (\theta - \theta r)(l-l r) + l r (\theta - \theta r) \]

so that
\[
\frac{f_r (\theta)}{r} \approx -\frac{1}{k} \left[ \frac{r}{2 \pi \sin \theta} \right]^{1/2} e^{i B_1 (r)} \int_{-\infty}^{\infty} e^{-i \Delta B_1} d(l-l r)
\]
\[
= \frac{1}{k} \left[ \frac{r}{2 \pi \sin \theta} \right]^{1/2} e^{i \delta - \frac{1}{3} r 2 \pi Ai(x)}
\]
\[
= \left[ I_r (\theta) \right]^{1/2} e^{i \delta} \]  \[ \ldots \ldots \ldots (45) \]

where \( \delta = 2 q r + l r \theta - 3 \pi / 4 \), \( \chi = q_r^{-1/3}(\theta - \theta r) \)

and \[ I_r (\theta) = \frac{1}{k^2} \frac{2 \pi l r}{\sin \theta} q_r^{-2/3} Ai \left[ q_r^{-1/3}(\theta - \theta r) \right] \]

\( Ai(\chi) \) is the Airy function.

The principal maximum of \( Ai(\chi) \) occurs at \( \chi \approx 1 \), so \( I_r (\theta) \)
becomes maximum at an angle \( \theta = \theta_r - q_r^{1/3} \) which is smaller than
rainbow angle given by classical theory. This low resolution
rainbow peak is spread over an appreciable angular range.

Variation of Airy function with \( x \) explains the oscillatory
behaviour of the cross section on the bright side of rainbow
( \( \chi < 0 \) i.e. \( \theta < \theta_r \) ) and the rapid fall off on the dark side
( \( \chi > 0 \) i.e. \( \theta > \theta_r \) ).

Now the total semiclassical scattering amplitude is
\[ f (\theta) \approx \left[ I_c (\theta) \right]^{1/2} e^{i \gamma_c} + \left[ I_r (\theta) \right]^{1/2} e^{i \delta} \]  \[ \ldots \ldots (46) \]
The differential cross section is given by

\[ I(\theta) = I_c(\theta) + I_r(\theta) + 2 (I_c I_r) \cos (S - \gamma) \quad \ldots (47) \]

The last term in eqn. (47) which is due to the interference of repulsive and attractive branch of \( f(\theta) \) gives the high frequency oscillations in differential cross sections. The cross section oscillates between the limits \( I_{\text{max}}(\theta) \) and \( I_{\text{min}}(\theta) \) given by

\[ I_{\text{max}} = \left[ I_r^{1/2} + I_c^{1/2} \right]^2 \quad \text{and} \quad I_{\text{min}} = \left[ I_r^{1/2} - I_c^{1/2} \right]^2, \quad (48) \]

Wavelength of this high frequency oscillations in the neighbourhood of the broad rainbow maximum is

\[ \Delta \theta = \frac{\pi}{\delta (S - \gamma_c) / d\theta} = \frac{2\pi}{\ell_r + \ell_c} \quad \ldots (49) \]

At angles appreciably larger than the rainbow angle the amplitude of the oscillations decreases and at least nearly monotonic behaviour characteristic of noninterfering scattering is obtained. On the low angle side of the rainbow, the three contributions always produce interference.

**Glory Scattering**

If the deflection function passes through zero or an even multiple of \( \pi \) the classical scattering possesses a singularity in the forward direction. Similarly if it passes through an odd
multiple of $\pi$ the backward scattering is singular. These are known as forward and backward 'glory' scattering respectively.

At a backward glory the deflection function near $\pi$ may be approximated by the expression

$$\Theta(\ell) = \pi + \alpha(\ell - l_g)$$

The classical scattering at an angle $\theta$ close to $\pi$ is now the sum of equal contributions from $\Theta = \theta$ and $2\pi - \theta$ and is given by

$$I_c(\theta) = 2 \kappa^2 l_g |a|^{-1}(\pi - \theta)^{-1}$$

where $\kappa = \chi^{-1}$. Provided $\pi - \theta$ is not too small the semi-classical approximation in this case may be obtained by evaluating the amplitudes at $\Theta(\ell) = \theta$ and $\Theta(\ell) = 2\pi - \theta$ separately by the method of stationary phase and then combining them with appropriate phases. But when $\theta$ is very close to $\pi$ this method fails due to two reasons. First, the contributing parts of the scattering amplitude integral are not separated, but overlap. Second, the sinusoidal approximation (34) for the Legendre function must be replaced by the Bessel function approximation (35).

We may integrate (50) to obtain a suitable approximate expression for the phase shift for those values of $\ell$ that contribute most to a glory

$$\eta_l = \frac{1}{2} \pi (\ell - l_g) + \frac{1}{4} a (\ell - l_g)^2 + \eta_d$$

... (52)
The scattering amplitude becomes
\[ f_{sc} = (\chi/2i) \exp\left(2i\eta q - \pi ilq\right) \int_0^\infty (2l+1) \exp\left[\frac{1}{2} ia(l-lq)^2\right] \]
\[ \times J_0(l\sin\theta) \, dl, \quad \ldots \ldots (53) \]

The integral in (53) may be evaluated by using an integral representation for \( J_0(x) \),
\[ J_0(x) = \frac{1}{2\pi} \int_0^{2\pi} e^{ix\cos\theta} \, d\theta, \quad \ldots \ldots (54) \]
inverting the order of integration and extending the lower limit of the \( l \)-integral to \(-\infty\), which is permissible when \( aLq^2 \) is much greater than unity. We then find
\[ f_{sc} = \chi(lq + \frac{1}{2})(2\pi/a)^{1/2} e^{i\varphi'} J_0(lq\sin\theta). \quad \ldots \ldots (55) \]

where the phase constant \( \varphi' \) is given by the formula
\[ \varphi' = 2\pi q - \pi lq - \pi/4 \quad \ldots \ldots (56) \]

For a forward glory the result is the same except that the term \( \pi lq \) in (56) is missing. In case there are no other amplitudes interfering with (55), the glory cross section is given by the formula
\[ I_{sc}(\theta) = A^2 \left(lq + \frac{1}{2}\right)^2 (2\pi/4!^2) J_0^2(lq\sin\theta) \quad \ldots \ldots (57) \]
At finite values of $\theta$ the cross section oscillates, which can occur due to interference between the two contributions from $\theta < \pi$ and $\theta > \pi$. When $\sin \theta \to 0$, the singularity in the classical cross section is replaced by a finite peak in the forward or backward direction of magnitude

$$I_{sc} (\text{peak}) = \frac{\lambda^2}{2} \left( \frac{\ell_0}{\ell} + \frac{1}{2} \right)^2 \left( \frac{2\pi}{|a|} \right). \quad (58)$$

As the mean value of $J_0^2(\kappa)$ is $1/\pi \kappa$ we see that the mean value of $I_{sc}$ agrees with the classical value (51).

**Total Elastic Cross Section**

Here we have analysed the interference pattern in the angular distribution arising from the glory effect. But there is an important feature of glory scattering which is manifested in the energy or velocity dependence of total elastic cross section.

Massey and Mohr first developed an approximation formula for the total elastic cross section appropriate for heavy-particle scattering according to an inverse $\kappa^5$ power potential. The usual cross section can be written as the sum of two terms, $Q_{JM} = Q_< + Q_>$. The first term corresponds to that region of angular momentum $0 \leq L \leq L$ in which phase shifts are large and random where $rph$-approximation is applicable. The second term corresponds to the region $L > L$ where phase shifts are small but non-random and for which $JB$-approximation is valid. The division is arbitrarily made at $L = L$ such that $|\eta_{JB}(L)| = 1/2$.
For the rph region

\[ Q_\lt = \frac{8\pi}{k^2} \sum_{l=0}^{L} \left( l + \frac{1}{2} \right) \frac{1}{2} \approx \frac{2\pi L^2}{k^2} \] .... (59)

and for the JB-region we have

\[ Q_\gt \approx \frac{8\pi}{k^2} \int_{L}^{\infty} (l + \frac{1}{2}) \text{Sin}^2 \eta_{JB} \approx \int_{L}^{\infty} l \eta_{JB}^2 \] .... (60)

replacing \( l + \frac{1}{2} \) by \( l \), the sum by an integral and \( \text{Sin} \eta_{JB} \) by \( \eta_{JB} \).

For potential of the form \( v(r) \sim -\frac{C^{(s)}}{r^s} \), substituting for \( \eta_{JB} \) we get

\[ Q_\gt \approx \frac{\pi}{(s-2)} \frac{L^2}{k^2} \] .... (61)

Utilising the cut-off condition

\[ L = \left[ \frac{2mC^{(s)}}{\hbar^2} \int f^{(s)} \right]^{1/(s-1)} \] .... (62)

where \( f^{(s)} \) is a known function of \( s \).

Thus the MM cross section becomes

\[ Q_{MM} = \frac{C^{(s)}}{\hbar^2} \left[ f^{(s)} \right]^{2/(s-1)} \] .... (63)

where

\[ p_{MM}(s) = \pi \left( \frac{2s-3}{s-2} \right) \left[ 2f^{(s)} \right]^{2/(s-1)} \] .... (64)
Eqn. (63) gives the velocity dependence of the total cross section.

Landau and Lifshitz approximation treatment is more accurate, in which the entire $Q$ sum is replaced by an integral, and JB phases are used throughout.

$$\frac{3}{k^2} \int_0^\infty d\ell \sin^2 \eta J_B$$

Then we can get equation analogous to eqn (63) as

$$Q_{LL} = \frac{3}{k^2} \left[ \frac{c^{(s)}}{k v} \right]^{2/ (s-1)}$$

where

$$\psi_{LL}(s) = \pi^2 \left[ 2 f^{(s)} \right]^{2/ (s-1)} \sin \left( \frac{\eta}{\sin \left( \frac{\pi}{s-1} \right) \sin \left( \frac{2}{s-1} \right) } \right)$$

We have seen that for a realistic potential possessing a minimum the classical deflection function $\Theta(h)$ passes through zero at the glory impact parameter $b_0$. Thus the phase shift curve $\eta^{(L)}$ exhibits a broad maximum around $\eta_{m}(L)$ as shown in fig. 1. Near this region a significant fraction of nonrandom phases are present and they give rise to a non-negligible increment $\Delta Q$ to the cross section given by eqn. (63). The maximum phase $\eta_{m}$ increases with a decrease in $k$, and if the attractive well is deep enough $\eta_{m}(k)$ can pass through multiples of $\pi/2$ giving rise alternately to positive and negative incremental contribution $\Delta Q/\bar{Q}$ to the rph approximated portion of the
MM total cross section. So \( Q_\nu \) shows an undulatory velocity dependence. The positions and magnitudes of the maxima and minima are determined by \( n_m(k) \). So for a given potential if the dependence of \( n_m \) on wave number can be evaluated by some method, the extrema velocities and amplitudes can be found out.

The inverse problem

In the scattering problem usually the potential is assumed to be given and the scattering cross section is calculated from it. In the inverse scattering problem one assumes that the cross section is experimentally determined and the potential is to be found. The problem is to decide what set of measurements allows the construction of a unique potential. Within the limitations of classical mechanics Firsov and Keller et al have solved the problem on the assumption that a unique spherically symmetric monotonic repulsive potential exists which tends to zero as \( r \to \infty \).

They show that \( V(\nu) \) may be determined for \( \nu > \nu_0 \) if the observed differential cross section is known for all \( \theta \) in \([0, \pi]\) at energy \( E \). Here \( \theta \) is a monotonic function of \( b \) then from eqn. (3) we can write

\[
b^2(\theta) = 2\int_{\theta}^{\pi} d\phi \sin \phi \frac{d\sigma(\phi)}{d\Omega}, \quad \ldots \quad (67)
\]

In this case the deflection angle must be equal to \( \pi \) when the impact parameter is zero.
The problem now is to determine the potential from \( b(\theta) \) or from \( \Theta(b) \).

Let us write
\[
\upsilon(\tau) = 1 - \frac{V(\tau)}{E}
\]
in equation (1) and introduce
\[
\chi = \frac{1}{r^2 \upsilon}
\]
as a new variable of integration. Then we have
\[
\frac{1}{2} \left[ \pi - \Theta(\upsilon) \right] = \int_0^\upsilon d\chi \; q(\chi) (\upsilon - \chi)^{1/2}
\]
where
\[
q(\chi) = -\frac{\sqrt{\chi}}{\pi} \frac{d\tau}{d\chi} = \frac{r \upsilon^{3/2}}{2\upsilon + \upsilon d\upsilon/d\tau}
\]
and \( \upsilon = b^{-2} \).

According to (68), the function \( g \) is an Euler transform of \( i/2 (\pi - \Theta) \). By its inversion we get
\[
q(\chi) = \frac{1}{2} \chi^{-1/2} - \frac{1}{2\pi} \int_0^\chi d\upsilon \; \frac{\Theta'(\upsilon)}{\sqrt{\chi - \upsilon}}
\]
\[
= \frac{1}{2} \chi^{-1/2} - \frac{1}{2\pi} \int_0^{\Theta(\chi)} \frac{d\theta}{\sqrt{\chi - \upsilon(\theta)}}
\]
because \( \Theta(0) = 0 \). The upper limit \( \Theta(\chi) \) of the integral in (69) is determined by \( \chi = \upsilon(\theta) \). Now the function \( \upsilon(\tau) \) is obtained by
\[
-\frac{\sqrt{\chi}}{q(\chi)} = \tau \frac{d\chi}{d\tau} = -\chi \left( 2 + \tau \frac{d\chi}{d\tau} \frac{d\ln \upsilon}{d\chi} \right)
\]
so that
\[
\frac{d \ln \nu}{d \chi} = - \frac{1}{\pi \sqrt{\chi}} \int_0^\pi \frac{\theta(\chi')}{\sqrt{\chi - \chi' \sin^2 \theta}} d\theta
\]

Because \( \nu \to 1 \) as \( r \to \infty \), that is \( \chi \to 0 \),
\[
\nu = \exp \left\{ - \frac{1}{\pi} \int_0^\infty \frac{\theta(\chi')}{\sqrt{\chi - \chi' \sin^2 \theta}} d\theta \right\}
\]

If we invert the order of integrations then \( \chi' \) integral can be carried out. Then
\[
\nu = \exp \left\{ - \frac{2}{\pi} \int_0^\pi \theta(\chi') \sin^{-1} \left[ \sqrt{\chi \cos \theta} \right] d\theta \right\}
\]

The procedure is thus to find \( b(\theta) \) by using eqn. (67) from the differential cross section and then to compute \( \nu \) by means of (70) in terms of \( \chi \). \( r \) can then be determined as a function of \( \chi \),
\[
r = \frac{1}{\sqrt{\chi \nu}}
\]

This is inserted in \( \psi(\chi) \) and \( V(r) \) is given by \( V = E (1 - \nu) \).

By this inversion procedure, at a given energy, the potential can be obtained only down to the distance of closest approach.

Exact quantum mechanical solution of the inversion problem exist essentially for two cases. In the first case the phase
shifts for all \( l \) values (orbital angular momentum, or impact parameter) at one energy are known and in the second case the phase shifts for one value of \( l \) and for all energies are known. In the latter case the information concerning the bound states of the potential is also required. In the first case only certain classes of potentials can be inverted in a unique manner. Solutions for both cases appear to be unusable for practical purposes, especially for collisions of heavy particles due to the many contributing partial waves.