Quantum Theory of Scattering

Topics already covered: Laboratory and centre of mass frames, basic assumptions, probability densities for incident and scattered waves, scattering amplitude, differential and total scattering cross-section, expansion formula for plane waves, partial wave analysis, optical theorem

Topic 1: Phase Shift in Scattering Process In presence of a target represented by a spherically symmetric potential, $V(r)$, the radial part of the Schrödinger equation for a particle of mass m and energy E is given by,

$$\left[\frac{d^2}{dr^2}+\frac{2}{r}\frac{d}{dr}+\left\{k^2-u(r)-\frac{l(l+1)}{r^2}\right\}\right]R_{kl}(r)=0 \tag{1}$$

where, $k^2=\frac{2mE}{\hbar^2}$ and, $u(r)=\frac{2mV(r)}{\hbar^2}$. Putting $R_{kl}(r)=\frac{Q_{kl}(r)}{r}$ in equation(1), we find

$$\left[\frac{d^2}{dr^2}+\left\{k^2-\frac{l(l+1)}{r^2}\right\}\right]P_{kl}(r)=0 \tag{2}$$

and also for $u(r)=0$, we consider $R_{kl}=\frac{P_{kl}(r)}{r}$ and therefore equation(1) can be written as

$$\left[\frac{d^2}{dr^2}+\left\{k^2-u(r)-\frac{l(l+1)}{r^2}\right\}\right]Q_{kl}(r)=0 \tag{3}$$

Subtracting equation(3) from equation(2) and integrating within the limit 0 to infinity, we find

$$\begin{aligned}&\int_0^\infty\left\{P\frac{d^2Q}{dr^2}-Q\frac{d^2P}{dr^2}\right\}dr-\int_0^\infty Pu(r)Qdr=0\\ \Rightarrow&\left[P\frac{dQ}{dr}-Q\frac{dP}{dr}\right]_{r=0}^\infty=\int_0^\infty Pu(r)Q\ dr\end{aligned} \tag{4}$$

Now P_{kl} and Q_{kl} for $r\to 0$ is a finite quantity. For the shake of mathematical simplicity, we can set it as zero. For $r\to\infty$, $P_{kl}=\frac{\sin\left(kr-\frac{l\pi}{2}\right)}{k}$ and $Q_{kl}(r)=c_l\frac{\sin\left(kr-\frac{l\pi}{2}+\delta_l\right)}{k}$ so that,

$$\begin{aligned}P_{kl}\frac{dQ_{kl}}{dr}-Q_{kl}\frac{dP_{kl}}{dr}&=\frac{c_l}{k}\left[\sin\left(kr-\frac{l\pi}{2}\right)\cos\left(kr-\frac{l\pi}{2}+\delta_l\right)-\sin\left(kr-\frac{l\pi}{2}+\delta_l\right)\cos\left(kr-\frac{l\pi}{2}\right)\right]\\&=\frac{c_l}{k}\sin\left(-\delta_l\right)\end{aligned}$$

which implies

$$\boxed{\sin\delta_l=-\frac{k}{c_l}\int_0^\infty P_{kl}(r)\left[\frac{2m}{\hbar^2}V(r)\right]Q_{kl}(r)dr} \tag{5}$$

where, δ_l represents the phase shift between the incident $[P_{kl}(r)]$ and scattered waves $[\frac{Q_{kl}(r)}{c_l}]$ due to the presence of the scaterrer or the target mimicked by the potential $V(r)$. Now if (i) The projectile or the incident wave is very fast so that the limit of interaction is very small and/or (ii) The range of the potential is short, one can easily replace the scattered wave function by the incident wave and thus the phase shift is given by,

$$\boxed{\sin\delta_l=-k\int_0^\infty u(r)[rj_l(kr)]^2dr} \tag{6}$$

where, we have considered $P_{kl}(r)=\frac{Q_{kl}(r)}{c_l}=rj_l(kr)$; $j_l(kr)$ being the spherical Bessel function.

Topic 2: The Born Approximation We begin with a time independent formation of scattering process and we assume that the Hamiltonian can be written as,

$$H = H_0 + V = \frac{p^2}{2m} + V$$

In absence of the scatterer, V should be zero and the energy eigen state would just be free particle state designated by $|p\rangle$. The presence of V causes the energy eigenstate to be different from a free particle state. However, if the scattering process is to be elastic *i.e.* no change in energy, we are interested in obtaining a solution of a full Hamiltonian Schrödinger equation with the same energy eigen ket of H_0 so that,

$$H_0|\phi\rangle = E|\phi\rangle \tag{7}$$

and we want to solve the basic Schrödinger equation,

$$(H_0 + V)|\psi\rangle = E|\psi\rangle \tag{8}$$

Both H_0 and $(H_0 + V)$ execute continuous energy spectrum *i.e.* a free particle having energy E. We look for a solution of equation(8) such that for $V \to 0$ we find $|\psi\rangle \to |\phi\rangle$ where $|\psi\rangle$ is the solution of the free particle with the same energy eigenvalue. The desired solution is,

$$|\psi\rangle = \frac{1}{E - H_0} V|\psi\rangle + |\phi\rangle \tag{9}$$

But there is a problem in equation which arises because of the singular nature of the $\frac{1}{E-H_0}$ operator. To avoid this singularity, the solution of equation(8), the solution is done by making the energy slightly complex, *i.e.*

$$\boxed{|\psi^{\pm}\rangle = \frac{1}{E - H_0 \pm i\epsilon} V|\psi^{\pm}\rangle + |\phi\rangle} \tag{10}$$

This equation is termed as Lippman Schrödinger integral equation. This is a Ket equation independent of particle representation. Let us now confine ourselves to the position basis by multiplying $\langle\vec{r}|$ from the left,

$$\langle\vec{r}|\psi^{\pm}\rangle = \langle\vec{r}|\phi\rangle + \left\langle \vec{r} \left| \frac{1}{E - H_0 \pm i\epsilon} V \right| \psi\pm \right\rangle \tag{11}$$

Now using the completeness theorem, $\int |\vec{r}\rangle\langle\vec{r}| d^3\vec{r} = 1$, we have

$$\langle\vec{r}|\psi^{\pm}\rangle = \langle\vec{r}|\phi\rangle + \int d^3\vec{r}' \left\langle \vec{r} \left| \frac{1}{E - H_0 \pm i\epsilon} \right| \vec{r}' \right\rangle \langle\vec{r}'|V|\psi^{\pm}\rangle \tag{12}$$

This is an integral equation of scattering because the unknown Ket $|\psi^{\pm}\rangle$ appears under the integral sign. Now if $|\phi\rangle$ stands for a plane wave with momentum $\vec{p}$, we can write,

$$\langle\vec{r}|\phi\rangle = \phi(r) = \frac{1}{(2\pi\hbar)^{3/2}} e^{i\frac{\vec{p}.\vec{r}}{\hbar}} \quad \texttt{and} \quad \left\langle \vec{r} \left| \frac{1}{E - H_0 \pm i\epsilon} \right| \vec{r}' \right\rangle = -\frac{2m}{\hbar^2} \left[\frac{e^{\pm ik|\vec{r}-\vec{r}'|}}{4\pi|\vec{r}-\vec{r}'|} \right] \quad \texttt{<see Appendix>}$$

so that

$$\langle\vec{r}|\psi^{\pm}\rangle = \langle\vec{r}|\phi\rangle - \frac{2m}{\hbar^2} \int d^3\vec{r}' \frac{e^{\pm ik|\vec{r}-\vec{r}'}}{4\pi|\vec{r}-\vec{r}'|} \langle\vec{r}'|V|\psi^{\pm}\rangle \tag{13}$$

Now note that

$$\langle \vec{r}^{\,\prime}|V|\psi^+\rangle \;=\; \int \langle \vec{r}^{\,\prime}|V|\vec{r}^{\,\prime\prime}\rangle\langle \vec{r}^{\,\prime\prime}|\psi^+\rangle \; d^3\vec{r}^{\,\prime\prime} = \int V(\vec{r}^{\,\prime\prime})\langle \vec{r}^{\,\prime\prime}|\psi^+\rangle\delta(\vec{r}-\vec{r}^{\,\prime\prime}) \; d^3\vec{r}^{\,\prime\prime} = V(\vec{r}^{\,\prime})\psi^+(\vec{r}^{\,\prime})$$

Thus,

$$\boxed{\langle \vec{r}^{\,\prime}|\psi^+\rangle \;=\; \langle \vec{r}|\phi\rangle \;-\; \int \; d^3\vec{r}^{\,\prime} \; \frac{e^{ik|\vec{r}-\vec{r}^{\,\prime}|}}{4\pi|\vec{r}-\vec{r}^{\,\prime}|} \; v(\vec{r}^{\,\prime})\psi^+(\vec{r}^{\,\prime})} \tag{14}$$

where, $v(\vec{r}^{\,\prime}) = \frac{2mV(\vec{r}^{\,\prime})}{\hbar^2}$. Now let us assume that the detector is placed far away from the scatterer so that $|\vec{r}-\vec{r}^{\,\prime}| \simeq \; |\vec{r}|$ i.e. $|\vec{r}| \; >> \; |\vec{r}^{\,\prime}|$ so that

$$k|\vec{r}-\vec{r}^{\,\prime}| = k\sqrt{r^2+(r^{\prime})^2-2\vec{r}.\vec{r}^{\,\prime}} = kr\sqrt{1+\left(\frac{r^{\prime}}{r}\right)^2 - 2\frac{\vec{r}.\vec{r}^{\,\prime}}{r^2}} \simeq kr\left[1-2\;\frac{\vec{r}.\vec{r}^{\,\prime}}{r^2}\right]^{1/2}$$

Expanding the binomial series and retaining upto the 2nd term, we get

$$k|\vec{r}-\vec{r}^{\,\prime}| \simeq kr\left[1-\frac{\vec{r}.\vec{r}^{\,\prime}}{r^2}\right] = kr - k\hat{r}.\vec{r}^{\,\prime} = kr - \vec{k}^{\prime}.\vec{r}^{\,\prime} \qquad [\because \vec{k}^{\prime} = k\hat{r}]$$

Thus,

$$\langle \vec{r}|\psi^+\rangle \;=\; \langle \vec{r}|\phi\rangle - \frac{1}{4\pi}\frac{e^{ikr}}{r} \int \; d^3\vec{r}^{\,\prime} \; e^{-i\vec{k}^{\prime}.\vec{r}^{\,\prime}} \; v(\vec{r}^{\,\prime})\psi^+(\vec{r}^{\,\prime})$$

$$\Rightarrow \boxed{\psi^+(\vec{r}) \;=\; \phi(\vec{r}) \;+\; \frac{e^{ikr}}{r}\left[-\frac{1}{4\pi}\;\int\; d^3\vec{r}^{\,\prime} \; e^{-i\vec{k}^{\prime}.\vec{r}^{\,\prime}} \; v(\vec{r}^{\,\prime})\psi^+(\vec{r}^{\,\prime})\right]} \tag{15}$$

Comparing equation (15) with the scattering equation,

$$\psi(\vec{r}) \;\xrightarrow{r\to\infty}\; \phi(\vec{r}) \;+\; f(\theta)\;\frac{e^{ikr}}{r}$$

We can write the expression for the scattering amplitude as,

$$\boxed{f_k(\theta) \;=\; -\frac{1}{4\pi}\;\int\; d^3\vec{r}^{\,\prime}\; e^{-i\vec{k}^{\prime}.\vec{r}^{\,\prime}} \; v(\vec{r}^{\,\prime})\psi^+(\vec{r}^{\,\prime})} \tag{16}$$

Using the Born approximation, one can replace the scattered wave function by the incident wave so that the scattering amplitude becomes,

$$f_k(\theta) = \; -\frac{1}{4\pi}\int \; d^3\vec{r}^{\,\prime} \; e^{-i\vec{k}^{\prime}.\vec{r}^{\,\prime}} \; u(\vec{r}^{\,\prime}) \; e^{i\vec{k}.\vec{r}^{\,\prime}} \;=\; -\frac{2m}{4\pi\hbar^2}\;\int\; d^3\vec{r}^{\,\prime}\; e^{-i\vec{q}.\vec{r}^{\,\prime}} \; V(\vec{r}^{\,\prime})$$

where, $\vec{q} = \vec{k}^{\prime} - \vec{k}$ is defined as the momentum transfer during collision process. Further expressing $d^3\vec{r}^{\,\prime} = r^{\prime 2}dr^{\prime}\sin\theta d\theta d\phi$ (where $0 \le r^{\prime} \le \infty$, $0 \le \theta \le \pi$, $0 \le \phi \le 2\pi$) and performig the integration over θ and ϕ co-ordinates, we find

$$f_k(\theta) = -\frac{m}{\hbar^2}\int_{r=0}^{\infty}\int_{\theta=0}^{\pi} r^2 \; dr \; e^{iq\cos\theta} \; V(r)\sin\theta \; d\theta = -\frac{m}{\hbar^2}\int_{r=0}^{\infty} r^2\left[\frac{e^{-iqr}-e^{iqr}}{iqr}\right]V(r)dr$$

$$\Rightarrow \boxed{f_k(\theta) = \frac{2m}{q\hbar^2}\int_{r=0}^{\infty} r \; V(r)\sin\; qr \; dr} \tag{17}$$

Appendix

$$\left\langle \vec{r} \left| \frac{1}{E - H_0 \pm i\epsilon} \right| \vec{r}' \right\rangle = \int\int d^3\vec{p}'\ d^3\vec{p}''\, \langle \vec{r}|\vec{p}'\rangle \left\langle \vec{p}' \left| \frac{1}{E - H_0 \pm i\epsilon} \right| \vec{p}'' \right\rangle \langle \vec{p}''|\vec{r}'\rangle$$
$$= \frac{1}{(2\pi\hbar)^3} \int\int d^3\vec{p}'\ d^3\vec{p}'' \left\langle \vec{p}' \left| \frac{1}{E - H_0 \pm i\epsilon} \right| \vec{p}'' \right\rangle e^{\frac{i}{\hbar}(\vec{p}'.\vec{r}' - \vec{p}''.\vec{r}')}$$

Now since, $\left\langle \vec{p}' \left| \frac{1}{E-H_0 \pm i\epsilon} \right| \vec{p}'' \right\rangle = \frac{1}{E - \frac{(p'')^2}{2m} \pm i\epsilon} \langle \vec{p}'|\vec{p}''\rangle = \frac{1}{E - \frac{(p'')^2}{2m} \pm i\epsilon} \delta(\vec{p}'' - \vec{p}')$

$$\left\langle \vec{r} \left| \frac{1}{E - H_0 \pm i\epsilon} \right| \vec{r}' \right\rangle = \frac{1}{(2\pi\hbar)^3} \int d^3\vec{p}'\, e^{\frac{i}{\hbar}\vec{p}'.(\vec{r} - \vec{r}')} \left[\frac{1}{E - \frac{(p')^2}{2m} - i\epsilon} \right]$$

Putting $E = \frac{\hbar^2 k^2}{2m}$, $\frac{\vec{p}'}{\hbar} = \kappa$, $d^3\vec{p}' = (p')^2\ dp' \sin\theta\ d\theta\ d\phi$ and integrating over the angle ϕ we find

$$\left\langle \vec{r} \left| \frac{1}{E - H_0 \pm i\epsilon} \right| \vec{r}' \right\rangle = \frac{m}{2\pi^2\hbar^2} \int_{\kappa=0}^{\infty} \frac{\kappa^2}{k^2 - \kappa^2 \pm i\epsilon}\, d\kappa \int_{\theta=0}^{\pi} e^{i\kappa|\vec{r}-\vec{r}'|\cos\theta} \sin\theta\ d\theta$$
$$= \frac{m}{2\pi^2\hbar^2} \int_{\kappa=0}^{\infty} \frac{\kappa^2}{k^2 - \kappa^2 \pm i\epsilon}\, d\kappa \int_{z=-1}^{+1} e^{i\kappa|\vec{r}-\vec{r}'|z}\ dz$$
$$= \frac{m}{\pi^2\hbar^2} \int_{\kappa=0}^{\infty} \frac{\kappa \sin(\kappa|\vec{r} - \vec{r}'|)}{k^2 - \kappa^2 \pm i\epsilon}\, d\kappa$$
$$= -\frac{2m}{\hbar^2} \left[\frac{e^{\pm ik|\vec{r}-\vec{r}'|}}{4\pi|\vec{r} - \vec{r}'|} \right]$$

The integration over κ can be done using the standard method of complex contour integration.

Assignment

1. Using partial wave analysis, show that for a beam of low energy particles scattered by a rigid sphere, the scattering cross-section is four times the geometrical cross-section of the sphere.

2. Using Born approximation, find the scattering amplitude and total scattering cross-section for scattering of a particle of mass m by the following potential:

   (a) Square well potential: $V(r) = -V_0$ for $r < a$ and 0 elsewhere
   (b) Exponential potential: $V(r) = -V_0 \exp\left[-\frac{r}{a}\right]$
   (c) Pure/Screened Coulomb potential: $V(r) = -V_0 \frac{e^{-\mu r}}{r}$
   (d) Gaussian potential: $V(r) = -V_0 \exp\left[-\left(\frac{r}{a}\right)^2\right]$
   (e) $V(r) = -V_0 r^2 \exp\left[-\left(\frac{r}{a}\right)^2\right]$

Reference

1. Modern Quantum Mechanics, J. J. Sakurai, Cambridge University Press

2. Quantum Mechanics, B. H. Bransden and C. Joachin, Dorling Kimberley

3. Quantum Mechanics, A. K. Ghatak and S. Lokanathan, Kluwer Academic Publishers