Scattering

Partial Wave Analysis

Formalism

Suppose we have a spherical symmetric potential $V(r)$, then the Schrodinger equation is

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

the general solution is

$$\psi_l(r,\theta,\phi) = R_l(r)Y_l^m(\theta,\phi)$$

introduce a new variable $u_l(r) = rR_l(r)$, then we have

$$\left(-\frac{\hbar^2}{2m}\frac{d^2}{dr^2} + \frac{l(l+1)\hbar^2}{2mr^2} + V(r)\right)u_l(r) = Eu_l(r)$$

in which $E = \dfrac{\hbar^2 k^2}{2m}$.

<u>For the very far away region</u>, both the potential and the centrifugal contribution are negligible, we got

$$\frac{d^2}{dr^2}u_l(r) = -k^2 u_l(r)$$
$$u_l(r) = Ce^{ikr} + De^{-ikr}$$

we just take the first term, which is an outgoing spherical wave, then

$$R_l(r) \sim \frac{e^{ikr}}{r}$$

it is consistent with the expectation.

<u>For the intermediate region</u>, where the potential can be ignored but the centrifugal term cannot, we got

$$\left(-\frac{d^2}{dr^2} + \frac{l(l+1)}{r^2}\right)u_l(r) = k^2 u_l(r)$$
$$u_l(r) = Ar\cdot j_l(kr) + Br\cdot n_l(kr)$$
$$R_l(r) = A\cdot j_l(kr) + B\cdot n_l(kr)$$

To get the form like e^{ikr}, change to use spherical Hankel functions

$$h_l^1(x) \equiv j_l(x) + in_l(x),\ h_l^2(x) \equiv j_l(x) - in_l(x)$$

We want an outgoing wave, so take the first kind of the Hankel function, then the wave function in the region with $V(r) \approx 0$ can be written as

$$\psi(r,\theta,\phi) = A\left\{e^{ikz} + \sum_{l,m=0} C_{l,m} \cdot h_l^1(kr) \cdot Y_l^m(\theta,\phi)\right\}$$

Considering our potential is spherical symmetric, so we take the $m = 0$ term only, then

$$Y_l^{m=0}(\theta,\phi) = \sqrt{\frac{2l+1}{4\pi}} P_l(\cos\theta)$$

Then rewrite the wave function (in the exterior region) as

$$\psi(r,\theta) = A\left\{e^{ikz} + k\sum_{l=0} i^{l+1}(2l+1) \cdot a_l \cdot h_l^1(kr) \cdot P_l(\cos\theta)\right\}$$

When $r \to \infty$, we have

$$h_l^1(kr) \to (-i)^{l+1} \cdot \frac{e^{ikr}}{kr}$$

$$\psi(r,\theta) \to A\left\{e^{ikz} + f(\theta)\frac{e^{ikr}}{r}\right\}$$

in which the scattering amplitude is

$$f(\theta) = \sum_{l=0} (2l+1) \cdot a_l \cdot P_l(\cos\theta)$$

The differential cross section is

$$\frac{d\sigma}{d\Omega} = |f(\theta)|^2 = \sum_{l,l'} (2l+1)(2l'+1) \cdot a_l^* a_{l'} \cdot P_l(\cos\theta) P_{l'}(\cos\theta)$$

the total cross section is

$$\sigma = 4\pi \sum_{l=0} (2l+1)|a_l|^2$$

Strategy

For consistency, we rewrite the incident wave as

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

then the wave function in the exterior region is

$$\psi(r,\theta) = A\sum_{l=0} i^l (2l+1)\left[j_l(kr) + ik \cdot a_l \cdot h_l^1(kr)\right] P_l(\cos\theta)$$

Phase Shifts

Firstly consider the free particle situation without potential, we should have

$$\psi_l = Ai^l(2l+1)\cdot j_l(kr)\cdot P_l(\cos\theta) \approx A\frac{2l+1}{2ikr}\left[e^{ikr}-(-1)^l e^{-ikr}\right]P_l(\cos\theta)$$

in which the second term (incoming wave) comes from the incident plane wave.
Then consider the angular momentum conservation, each partial wave (with specific l) scatters independently, so the influence of potential will just be the extra phases in each l-mode as

$$\psi_l \approx A\frac{2l+1}{2ikr}\left[e^{i(kr+2\delta_l)}-(-1)^l e^{-ikr}\right]P_l(\cos\theta)$$

$$\psi_l = A\cdot i^l(2l+1)R_l(r)\cdot P_l(\cos\theta)$$

it can also be written as the previous form with a_l as

$$\psi_l \approx A\left\{\frac{2l+1}{2ikr}\left[e^{ikr}-(-1)^l e^{-ikr}\right]+\frac{2l+1}{r}a_l e^{ikr}\right\}P_l(\cos\theta)$$

$$a_l = \frac{1}{k}e^{i\delta_l}\sin(\delta_l)$$

Then the scattering amplitude and the cross section can be written as

$$f(\theta) = \frac{1}{k}\sum_{l=0}(2l+1)e^{i\delta_l}\sin(\delta_l)\cdot P_l(\cos\theta)$$

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

To determine the Phase Shift

Define

$$\beta_l \equiv \left(\frac{r}{R_l}\frac{dR_l}{dr}\right)_{r=R}$$

where $r = R$ is the boundary between interior and exterior.
Then for the interior region, this beta can be calculated with Schrodinger equation, while for the exterior region it is related to the phase shift as

$$\tan\delta_l = \frac{kR\cdot j_l'(kR)-\beta_l\cdot j_l(kR)}{kR\cdot n_l'(kR)-\beta_l\cdot n_l(kR)}$$

Born Approximation

We have the general solution to the Schrodinger equation takes the form

$$\psi^+(\vec{r}) = e^{i\vec{k}\cdot\vec{r}} - \frac{1}{4\pi}\frac{1}{\hbar^2/2m}\int d^3r'\,\frac{e^{ik|\vec{r}-\vec{r}'|}}{|\vec{r}-\vec{r}'|}V(\vec{r}')\psi^+(\vec{r}')$$

in which the + represents the forward evolving wave function.
When $r \longrightarrow \infty$,

$$e^{ik|\vec{r}-\vec{r}'|} \approx e^{ik(r-\hat{r}\cdot\vec{r}')}$$
$$\frac{1}{|\vec{r}-\vec{r}'|} \approx \frac{1}{r}$$

then we have

$$\psi^+(\vec{r}) = e^{i\vec{k}\cdot\vec{r}} - \frac{1}{4\pi}\frac{2m}{\hbar^2}\frac{e^{ikr}}{r}\int d^3r'\, e^{-ik\hat{r}\cdot\vec{r}'}V(\vec{r}')\psi^+(\vec{r}')$$

Considering the scattered wave function can be written as

$$\psi(\vec{r}) = e^{i\vec{k}\cdot\vec{r}} + f(\theta,\phi)\frac{e^{ikr}}{r}$$

we got the expression of the scattering amplitude as

$$f(\theta,\phi) = -\frac{1}{4\pi}\frac{2m}{\hbar^2}\int d^3r'\, e^{-ik\hat{r}\cdot\vec{r}'}V(\vec{r}')\psi^+(\vec{r}')$$

The **first order Born approximation** takes

$$\psi^+(\vec{r}') \approx e^{i\vec{k}\cdot\vec{r}'}$$

Then we got

$$f^1(\theta,\phi) = -\frac{1}{4\pi}\frac{2m}{\hbar^2}\int d^3r'\, e^{i(\vec{k}-k\hat{r})\cdot\vec{r}'}V(\vec{r}')$$

the second order Born approximation can be found in Eq.(6.86) in Sakurai.

To further simplify it, we set the momentum transfer $\vec{q} = \vec{k} - k\hat{r}$, and $|\vec{q}| = 2k\sin\frac{\theta}{2}$, θ is the angle between $\hat{r}$ and $\vec{k}$, in which $\vec{k}$ is the input momentum direction, $\hat{r}$ is the output momentum direction.
Then the integral can be evaluated as

$$f^1(\theta,\phi) = -\frac{1}{4\pi}\frac{2m}{\hbar^2}V(\vec{q})$$
$$V(\vec{q}) = \int d^3r'\, e^{i\vec{q}\cdot\vec{r}'}V(\vec{r}')$$

The differential cross section can be written as

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

When is the Born approximation applicable?

Short answer is as long as the second order perturbation is smaller than the first order, or

$$|\frac{1}{4\pi}\frac{2m}{\hbar^2}\int d^3r'\,\frac{e^{ik|\vec{r}-\vec{r}'|}}{|\vec{r}-\vec{r}'|}V(\vec{r}')\psi^+(\vec{r}')| \ll 1$$

For low energy scattering with $kr \ll 1$, a is the effective radius of the potential,

$$\sim \frac{1}{4\pi}\frac{2m}{\hbar^2}\frac{1}{a}V_0\left(\frac{4}{3}\pi a^3\right) \ll 1$$

$$V_0 \ll \frac{\hbar^2}{2ma^2}$$

For high energy scattering with $kr \gg 1$,

$$V_0 \ll \frac{\hbar^2}{2ma^2}\frac{ka}{\ln(ka)}$$

if $k \to \infty$, Born approximation is always good.

Optical Theorem

Hand-waving proof:

$$|\psi\rangle = S|\phi\rangle$$
$$S^\dagger S = I$$
$$S = I + iT$$

then

$$\left(I - iT^\dagger\right)(I + iT) = I + i\left(T - T^\dagger\right) + T^\dagger T = I$$
$$-i\left(T - T^\dagger\right) = T^\dagger T$$
$$2\Im[T_{ii}] = \sum_n |T_{in}^\dagger|^2$$

Useful application

$$\Im[f(\vec{k}, \vec{k})] = \Im[f(\theta = 0)] = \frac{k}{4\pi}\sigma_{\text{tot}}$$