Lect 24 Partial wave method (Stationary state method)

Now we need to solve the Schrödinger Eq

$\left[-\frac{\hbar^2}{2m}\nabla^2 + V(r)\right]\psi = E\psi$ under the scattering boundary condition

$\psi(r) \xrightarrow{r\to+\infty} e^{ikz} + f(\theta)\frac{e^{ikr}}{r}$, and then determine $f(\theta)$.

Partial wave means that we can decompose this boundary condition into different channels of l, and solve the Schrödinger Eq in each channel separately.

incident wave

$$\boxed{\begin{aligned} e^{ikz} = e^{ikr\cos\theta} &= \sum_{l=0}^{\infty}(2l+1)\, i^l\, j_l(kr)\, P_l(\cos\theta) \\ &= \sum_{l=0}^{\infty}\sqrt{4\pi(2l+1)}\, i^l\, j_l(kr)\, Y_{l0}(\theta) \\ &\xrightarrow{kr\to\infty} \sum_{l=0}^{\infty}\sqrt{4\pi(2l+1)}\, i^l\, \frac{1}{2ikr}\left[e^{i(kr-\frac{l\pi}{2})} - e^{-i(kr-\frac{l\pi}{2})}\right] Y_{l0} \end{aligned}}$$

$j_l(kr)$ is the l-th spheric Bessel function, i.e the solution of the radial part of Laplace Eq in the spheric coordinate system

$$\frac{d^2R(\rho)}{d\rho^2} + \frac{2}{\rho}\frac{dR(\rho)}{d\rho} + \left(1 - \frac{l(l+1)}{\rho^2}\right)R(\rho) = 0, \text{ where } \rho = kr.$$

The scattering wave can be decomposed $f(\theta) = \sum_l f_l\, Y_{l0}(\theta)$.

then $\psi(\vec{r}) \xrightarrow{r\to\infty} \sum_l \left[\sqrt{4\pi(2l+1)}\, i^l j_l(kr) + \frac{f_l}{r} e^{ikr}\right] Y_{l0}(\theta)$.

On the other hand, we would like directly solve

$$\left[-\frac{\hbar^2}{2m}\nabla^2 + V(r)\right]\psi(r) = E\psi, \quad \text{with } \psi = \sum_{l=0}^{\infty} R_l(kr)\, Y_{l0}(\theta)$$

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

with $E = \frac{\hbar^2 k^2}{2m}$ and $u(r) = \frac{2m V(r)}{\hbar^2}$.

At $r\to\infty$, $u(r) \Rightarrow 0$, and $R_l(r)$ should be the solution of the free space: as a superposition of incident wave and scattering wave.

Background knowledge: $j_l(kr)$, $n_l(kr)$, $h_l(kr)$

$$\left[\frac{d^2}{dr^2} + \frac{2}{r}\frac{d}{dr} + k^2 - \frac{l(l+1)}{r^2}\right] R_l(r) = 0 \quad \text{set } \rho = kr$$

$$\left.\begin{aligned} j_l(\rho) &= (-)^l \rho^l \left(\frac{1}{\rho}\frac{d}{d\rho}\right)^l \frac{\sin\rho}{\rho} \\ n_l(\rho) &= (-)^{l+1} \rho^l \left(\frac{1}{\rho}\frac{d}{d\rho}\right)^l \frac{\cos\rho}{\rho} \\ h_l(\rho) &= j_l(\rho) + i\, n_l(\rho) \end{aligned}\right\}$$

examples:

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

$j_1(kr) = \frac{\sin kr}{(kr)^2} - \frac{\cos kr}{kr}$

$n_1(kr) = -\frac{\cos kr}{(kr)^2} - \frac{\sin kr}{kr}$

Asymptotic expansion:

$kr \to 0$: $j_l(kr) \to \frac{(kr)^l}{(2l+1)!!}$, $n_l(kr) \to -\frac{(2l-1)!!}{(kr)^{l+1}}$

as $kr \to +\infty$,

$$j_l(kr) \xrightarrow{r\to\infty} \frac{1}{kr}\sin\left(kr-\frac{l\pi}{2}\right), \quad n_l(kr) \xrightarrow{r\to\infty} \frac{-1}{kr}\cos\left(kr-\frac{l\pi}{2}\right),$$

$$h_l(kr) \xrightarrow{r\to\infty} \frac{1}{ikr} e^{i\left(kr-\frac{l\pi}{2}\right)}.$$

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The boundary condition can be represented as

$$\psi(r) \xrightarrow{r\to\infty} \sum_l \sqrt{4\pi(2l+1)}\; i^l j_l(kr) + i^{l+1} k f_l \, h_l(kr)$$

$$= \sum_l \sqrt{4\pi(2l+1)}\; i^l \left[j_l(kr) + \frac{i k f_l}{\sqrt{4\pi(2l+1)}} h_l(kr) \right]$$

denote $\frac{a_l}{2} = \frac{ikf_l}{\sqrt{4\pi(2l+1)}}$, then $j_l(kr) + \frac{a_l}{2} h_l(kr)$

$$\to \frac{1}{2ikr}\left[(1+a_l)\, e^{i\left(kr-\frac{l\pi}{2}\right)} - e^{-i\left(kr-\frac{l\pi}{2}\right)}\right]$$

particle number conservation

$\Rightarrow |1+a_l| = 1$, parameterize $1+a_l = e^{2i\delta_l} \Rightarrow a_l = e^{i\delta_l}\left(e^{i\delta_l} - e^{-i\delta_l}\right)$

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

$$\Rightarrow \boxed{\psi(r) \xrightarrow{r\to\infty} \sum_l \sqrt{4\pi(2l+1)}\; i^l e^{i\delta_l} \frac{1}{kr}\sin\left(kr - \frac{l\pi}{2} + \delta_l\right) Y_{l0}(\theta)}$$

This ~~the~~ is the form of boundary condition. In l-th channel, the information is determined by "δ_l". By comparing with the actual solution of $R_l(r)$, we can obtain δ_l. Then from δ_l, we have

$$\frac{ik f_\ell}{\sqrt{4\pi(2\ell+1)}} = \frac{a_\ell}{2} = e^{i\delta_\ell}\, i \sin\delta_\ell \Rightarrow \boxed{f_\ell = \frac{1}{k} e^{i\delta_\ell} \sin\delta_\ell \sqrt{4\pi(2\ell+1)}}$$

$$\sigma(\theta) = |f(\theta)|^2 = \frac{4\pi}{k^2}\left|\sum_{\ell=0}^{\infty} \sqrt{2\ell+1}\, e^{i\delta_\ell} \sin\delta_\ell\, Y_{\ell 0}(\theta)\right|^2$$

$$\boxed{\sigma_t = \int d\Omega\, \sigma(\theta) = \frac{4\pi}{k^2} \sum_{\ell=0}^{\infty} (2\ell+1) \sin^2\delta_\ell \,.}$$

In summary, scattering problem is reduced to solving radial Eq with the proper boundary condition $R_\ell(kr) \xrightarrow{r\to+\infty} \frac{i^\ell e^{i\delta_\ell}}{kr} \sin(kr - \frac{\ell\pi}{2} + \delta_\ell)$.

Discussion:

① optical theorem: $f(\theta) = \sum_\ell f_\ell Y_{\ell 0}(\theta) = \sum_\ell \frac{e^{i\delta_\ell}}{k} \sin\delta_\ell \sqrt{2\ell+1}\, P_\ell(\cos\theta)$

$$\mathrm{Im}\, f(0) = \frac{1}{k} \sum_{\ell=0}^{\infty} \sin^2\delta_\ell (2\ell+1) = \frac{k}{4\pi} \sigma_t \Rightarrow \boxed{\sigma_t = \frac{4\pi}{k^2} \mathrm{Im}\, f(0)}$$

② The sign of the phase shift δ_ℓ

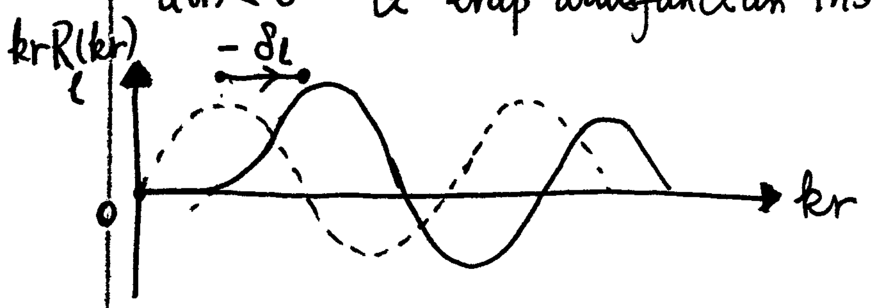
$$\frac{1}{r^2}\left(\frac{d}{dr} r^2 \frac{d}{dr} R_\ell\right) + \left[k^2 - \frac{\ell(\ell+1)}{r^2} - u(r)\right] R_\ell = 0$$

$$R_\ell \xrightarrow{kr\to+\infty} \frac{1}{kr} \sin(kr - \frac{\ell\pi}{2} + \delta_\ell)$$

if $u(r) = 0$, we have $\delta_\ell = 0$.

$u(r) > 0$, it push wavefunction outside $\delta_\ell < 0$,

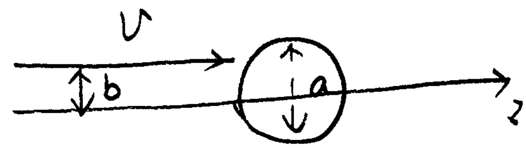
$u(r) < 0$ it trap wavefunction inside $\delta_\ell > 0$.



★ how many partial waves are needed?

Say, let us assume the range of force is a. Only where the distance $b \le a$, the scattering effect, i.e. δ_ℓ, is important.

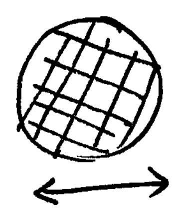
Thus $L = \ell\hbar \sim mvb \sim mva$



$$\ell \sim \frac{mv}{\hbar} a = \frac{a}{\lambdabar}$$, where $\lambdabar$ is the de Broglie wave length of the incoming particle.

Example: hard sphere scattering.

$$V(r) = \begin{cases} \infty & r < a_0 \\ 0 & r > a_0 \end{cases}$$



Sloving the Radial equation:

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

$$R_\ell(kr) = \begin{cases} 0 & r < a \\ \cos\delta_\ell\, j_\ell(kr) - \sin\delta_\ell\, n_\ell(kr) & r > a \end{cases}$$

this form is the same as $\underline{j_\ell(kr) + i e^{i\delta_\ell} \sin\delta_\ell\, h_\ell(kr)}$ up to a phase factor. check! $= j_\ell + i e^{i\delta_\ell} \sin\delta_\ell (j_\ell + i n_\ell)$

$$= (1 + i e^{i\delta_\ell} \sin\delta_\ell) j_\ell - e^{i\delta_\ell} \sin\delta\, n_\ell = e^{i\delta_\ell}[\cos\delta_\ell\, j - \sin\delta_\ell\, n]$$

Continuity at $r = a \Rightarrow x_0 = kr = ka$

$$R(ka) = 0 \Rightarrow \cos\delta_\ell(k)\, j_\ell(ka) = \sin\delta_\ell(k)\, n_\ell(ka)$$

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

Low energy limit: $ka \to 0$:

$$j_\ell(ka) \xrightarrow{ka\to 0} \frac{(ka)^\ell}{(2\ell+1)!!} \qquad n_\ell(ka) \xrightarrow{ka\to 0} -\frac{(2\ell-1)!!}{x^{\ell+1}}$$

$$\tan\delta_\ell(k) \xrightarrow{ka\to 0} -\frac{(ka)^{2\ell+1}}{[(2\ell-1)!!]^2(2\ell+1)} .$$

only the S-wave is important, we have $\boxed{\delta_0(k) \sim -(ka) < 0}$

$\sigma_t \approx \frac{4\pi}{k^2}\sin^2\delta_0 \approx 4\pi a^2$, which is 4 times larger than the classical cross section.