

Lect 24 Partial wave method (stationary state method)

Now we need to solve the Schrödinger Eq

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

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

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

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

$$= \sum_{l=0}^{\infty} \sqrt{4\pi(2l+1)} i^l j_l(kr) Y_{l0}(\theta)$$

$$\xrightarrow{kr \rightarrow \infty} \sum_{l=0}^{\infty} \sqrt{4\pi(2l+1)} i^l \frac{1}{2ikr} [e^{i(kr - \frac{l\pi}{2})} - e^{-i(kr - \frac{l\pi}{2})}] Y_{l0}$$

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

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

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

then

$$\psi(\vec{r}) \xrightarrow{r \rightarrow \infty} \sum_l \left[\sqrt{\frac{4\pi(2l+1)}{}} i^l j_e(kr) + \frac{f_e}{r} e^{ikr} \right] Y_{el}(\theta).$$

On the other hand, we would like directly solve

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

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

$$\text{with } E = \frac{\hbar^2 k^2}{2m} \quad \text{and} \quad U(r) = \frac{2mV(r)}{\hbar^2}.$$

At $r \rightarrow \infty$, $U(r) \rightarrow 0$, and $R_l(r)$ should be the solution of

the free space: as a superposition of incident wave and scattering wave.

Background knowledge: $j_e(kr)$, $n_e(kr)$, $h_e(kr)$

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

$$j_e(p) = (-)^l p^l \left(\frac{1}{p} \frac{d}{dp} \right)^l \frac{\sin p}{p}$$

$$n_e(p) = (-)^{l+1} p^l \left(\frac{1}{p} \frac{d}{dp} \right)^l \frac{\cos p}{p}$$

$$h_e(p) = j_e(p) + i n_e(p)$$

examples:

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

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

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

Asymptotic expansion:

$$kr \rightarrow 0 : \quad j_e(kr) \rightarrow \frac{(kr)^l}{(2l+1)!!}, \quad n_e(kr) \rightarrow -\frac{(2l-1)!!}{(kr)^{l+1}}$$

as $kr \rightarrow +\infty$,

$$j_e(kr) \xrightarrow{r \rightarrow \infty} \frac{1}{kr} \sin(kr - \frac{l\pi}{2}), \quad n_e(kr) \xrightarrow{r \rightarrow \infty} \frac{-1}{kr} \cos(kr - \frac{l\pi}{2}),$$

$$h_e(kr) \xrightarrow{r \rightarrow \infty} \frac{1}{ikr} e^{i(kr - \frac{l\pi}{2})}.$$

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The boundary condition can be represented as

$$\psi(r) \xrightarrow{r \rightarrow \infty} \sum_l \sqrt{4\pi(2l+1)} i^l j_e(kr) + i^{l+1} k f_e h_e(kr)$$

$$= \sum_l \sqrt{4\pi(2l+1)} i^l \left[j_e(kr) + \frac{i k f_e}{\sqrt{4\pi(2l+1)}} h_e(kr) \right]$$

denote $\frac{\alpha_e}{2} = \frac{ikf_e}{\sqrt{4\pi(2l+1)}}$, then $j_e(kr) + \frac{\alpha_e}{2} h_e(kr)$

$$\rightarrow \frac{1}{2ikr} [(1 + \alpha_e) e^{i(kr - \frac{l\pi}{2})} - e^{-i(kr - \frac{l\pi}{2})}]$$

particle number conservation



$$\Rightarrow |1 + \alpha_e| = 1, \text{ parameterize } 1 + \alpha_e = e^{2i\delta_e} \Rightarrow \alpha_e = e^{i\delta_e} (e^{i\delta_e} - e^{-i\delta_e}) = e^{i\delta_e} 2i \sin \delta_e$$

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

This is the form of boundary condition. In l -th channel, the information

is determined by " δ_e ". By comparing with the actual solution of $R_e(r)$,

we can obtain δ_e . Then from δ_e , we have

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

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

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

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

④ Discussion:

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

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

② The sign of the phase shift δ_ℓ

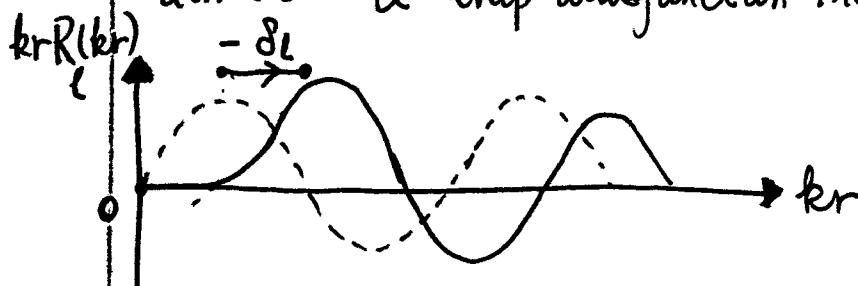
$$\frac{1}{r^2} \left(\frac{d}{dr} r^2 \frac{d}{dr} R_\ell \right) + \left(k^2 - \frac{\ell(\ell+1)}{r^2} - U(r) \right) R_\ell = 0$$

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

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

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

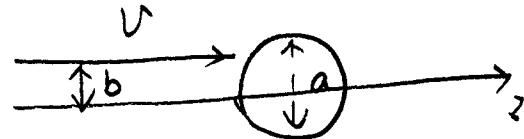
$U(r) < 0$ it trap wavefunction inside $\delta_\ell > 0$.



* how many partial waves are needed?

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

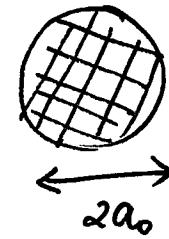
$$\text{Thus } l = l\hbar \sim mvb \sim mva$$



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

Example: hard sphere scattering.

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



Solving the Radial equation:

$$\left(\frac{1}{r^2} \left(\frac{d}{dr} r^2 \frac{d}{dr} R_e \right) + \left(k^2 - \frac{l(l+1)}{r^2} - \frac{2m}{\hbar^2} V(r) \right) R_e \right) = 0$$

$$R_e(kr) = \begin{cases} 0 & r < a \\ \cos \delta_e j_e(kr) - \sin \delta_e n_e(kr) & r > a \end{cases}$$

this form is the same as $j_e(kr) + i e^{i \delta_e} \sin \delta_e n_e(kr)$ up to a phase factor. check!

$$\begin{aligned} & j_e + i e^{i \delta_e} \sin \delta_e (j_e + i n_e) \\ &= (1 + i e^{i \delta_e} \sin \delta_e) j_e - e^{i \delta_e} \sin \delta_e n_e = e^{i \delta_e} [\cos \delta_e j_e - \sin \delta_e n_e] \end{aligned}$$

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

$$R(ka) = 0 \Rightarrow \cos \delta_e(k) j_e(ka) = \sin \delta_e(k) n_e(ka)$$

$$\Rightarrow \tan \delta_e(k) = \frac{j_e(ka)}{n_e(ka)}$$

Low energy limit: $ka \rightarrow 0$:

$$j_e(ka) \xrightarrow{ka \rightarrow 0} \frac{(ka)^l}{(2l+1)!!} \quad n_e(ka) \xrightarrow{ka \rightarrow 0} -\frac{(2l-1)!!}{x^{l+1}}$$

$$\tan \delta_e(k) \xrightarrow{ka \rightarrow 0} -\frac{(ka)^{2l+1}}{[(2l-1)!!]^2 (2l+1)}.$$

only the S-wave is important, we have

$$\boxed{\delta_0(k) \sim -\frac{(ka)}{x} < 0}$$

$$\sigma_t \approx \frac{4\pi}{k^2} \sin^2 \delta_0 \approx 4\pi a^2, \text{ which is 4 times larger}$$

than the cross section.
classical