

lect 24 Partial wave method (Stationary state method)

(1)

Now we need to solve the Schrödinger Eq

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

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

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

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

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

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

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

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

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

then

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

On the other hand, we would like directly solve

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

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

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

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

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

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

examples:

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

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

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

Asymptotic expansion:

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

as $kr \rightarrow +\infty$,

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

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

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The boundary condition can be represented as

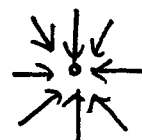
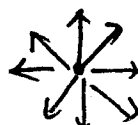
$$\psi(r) \xrightarrow{r \rightarrow \infty} \sum_l \sqrt{4\pi(2l+1)} i^l j_l(kr) + i^{l+1} k f_l h_l(kr)$$

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

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

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

particle number conservation



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

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

This 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

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

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

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

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

⑦ Discussion:

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

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

② The sign of the phase shift δ_ℓ

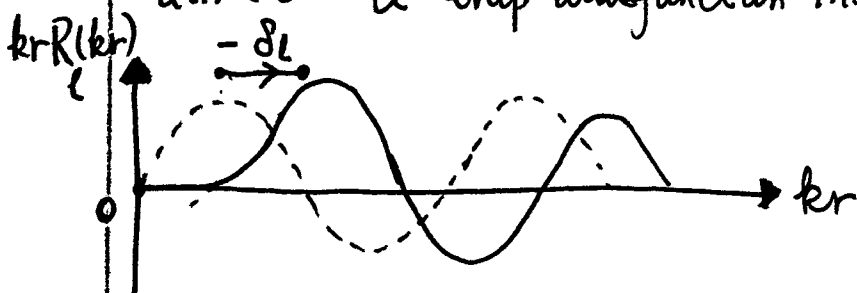
$$\frac{1}{r^2} \left(\frac{d}{dr} r^2 \frac{d}{dr} R_\ell \right) + \left[k^2 - \frac{\ell(\ell+1)}{r^2} - u(r) \right] R_\ell = 0$$

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

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

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

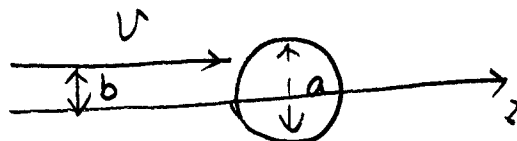
$u(r) < 0$ it trap wavefunction inside $\delta_\ell > 0$.



* 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_l , is important.

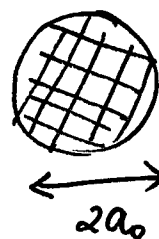
Thus $L = l\hbar \sim m v b \sim m v a$



$l \sim \frac{mv}{\hbar} a = \frac{a}{\lambda}$, 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:

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

$$R_l(kr) = \begin{cases} 0 & r < a \\ \cos \delta_l j_l(kr) - \sin \delta_l n_l(kr) & r > a \end{cases}$$

this form is the same as $\frac{j_l(kr) + i e^{i\delta_l} \sin \delta_l h_l(kr)}{1 + i e^{i\delta_l} \sin \delta_l}$ up to

a phase factor. check! $\checkmark j_l + i e^{i\delta_l} \sin \delta_l (j_l + i n_l)$

$$= (1 + i e^{i\delta_l} \sin \delta_l) j_l - e^{i\delta_l} \sin \delta_l n_l = e^{i\delta_l} [\cos \delta_l j_l - \sin \delta_l n_l]$$

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Continuity at $r=a \Rightarrow \chi_0 = kr = ka$

$$R(ka)=0 \Rightarrow \cos \delta_l(k) j_l(ka) = \sin \delta_l(k) n_l(ka)$$

$$\Rightarrow \tan \delta_l(k) = \frac{j_l(ka)}{n_l(ka)}$$

Low energy limit: $ka \rightarrow 0$:

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

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

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

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