Lect 5. Partial wave method

In the center-force field, $\vec{L}$ is conserved. We can seperate the scattering amplitude in each partile wave channel. We choose $(H, \vec{L}, l_z)$ as the complete set of conserved quantities. We want to solve

$$\left[-\frac{\hbar^2}{2m}\nabla^2 + V(r)\right]\psi = E\psi,$$ under the scattering boundry condition of $$\psi(r) \xrightarrow{r\to+\infty} e^{ikz} + f(\theta)\frac{e^{ikr}}{r}.$$

Partial wave means, we decompose this boundry condition into different channel of l. The incoming wave can be decomposed as

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

$j_l(kr)$ is l-th spheric Bessel function, which is the solution of the radial part of Laplace equation in the spheric coordinate system:

$$\frac{d^2R(\rho)}{d\rho^2} + \frac{2}{\rho}\frac{dR(\rho)}{d\rho} + \left[1 - \frac{l(l+1)}{\rho^2}\right]R(\rho) = 0$$

where $\rho = kr$.

The scattering wave can be decomposed $f(\theta)=\sum_l f_l\, Y_{l0}(\theta)$, thus in the l-th partial wave channel, the bounday condition ⟶

$$\left[\sqrt{4\pi(2l+1)}\; i^l\, j_l(kr) \qquad + \frac{f_l\, e^{ikr}}{r}\right] Y_{l0}(\theta) \quad .$$

On the other hand, we can solve the radial equation

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

$$\Rightarrow \left[\frac{1}{r^2}\frac{d}{dr}(r^2\frac{d}{dr} + k^2 - \frac{l(l+1)}{r^2} - U(r)\right] R_l = 0\,, \quad \text{where } E=\frac{\hbar^2 k^2}{2m}, \quad U(r)=\frac{2mV(r)}{\hbar^2}$$

at $kr\to+\infty$, $U(r)\to 0$. Thus ingeneral R_l can be expanded as a linear superposition of incoming wave + scattering outgoing wave.

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In the spherical coordination, incoming wave is $j_l(kr)$,
out going wave is $h_l(kr)$.

Rember that there are two linearly independent solutions to

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

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

examples:

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

$$j_1(kr)=\frac{\sin kr}{(kr)^2}-\frac{\cos kr}{kr} \qquad n_1(kr) = -\frac{\cos kr}{(kr)^2}-\frac{\sin kr}{kr}$$

$\overset{\frac{(kr)^l}{(2l+1)!!}}{j_l(kr)}$ is regular at $kr \to 0$, $\overset{-(2l-1)!!/(kr)^{l+1}}{n_l(kr)}$ diverges at $kr \to 0$.

On the other hand as $kr \to +\infty$, they behave as

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

From j_l and n_l, we can combine into propagating waves as

$$h_l(kr) = j_l(kr) + i n_l(kr) \xrightarrow{kr\to+\infty} \frac{1}{ikr} e^{i(kr - l\pi/2)}$$

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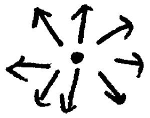
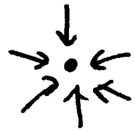
So let us express the solution from solving the radial equation as

$$R_l(kr) \xrightarrow{kr\to+\infty} \sqrt{4\pi(2l+1)}\, i^l \left[j_l(kr) + \overset{\text{coefficent}}{\frac{a_l}{2}} h_l(kr) \right]$$

$$= \sqrt{4\pi(2l+1)}\, i^l \frac{1}{2ikr} \left[\underbrace{(1+a_l) e^{i(kr - l\pi/2)}} - \underbrace{e^{-[i(kr - \frac{l\pi}{2})]}} \right]$$





$\Rightarrow \quad |1+a_l| = 1 \quad \Rightarrow$ let us paramterize $\quad 1 + a_l = e^{2i\delta_l}$

$$\Rightarrow a_l = e^{i\delta_l}(e^{i\delta_l} - e^{-i\delta_l})$$

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

$$\Rightarrow \boxed{R_l(kr) \xrightarrow{kr\to+\infty} \sqrt{4\pi(2l+1)}\, i^l e^{i\delta_l} \frac{1}{kr} \sin(kr - \frac{l\pi}{2} + \delta_l)}$$

What we get from solving the radial equation. The net effect of scattering potential is the phase shift δ_l. For free space, $\delta_l = 0$.

Compare $\underset{\nearrow \text{ from solving radial Eq}}{R_\ell(kr)} \xrightarrow{kr\to+\infty} \sqrt{4\pi(2\ell+1)}\,\frac{i^\ell e^{i\delta_\ell}}{kr}\sin(kr-\frac{\ell\pi}{2}+\delta_\ell)$ ★

and $\longrightarrow \sqrt{4\pi(2\ell+1)}\, i^\ell j_\ell(kr) + \frac{f_\ell e^{ikr}}{r}$

from general argument

★ → goes back to $R_\ell(kr) \xrightarrow{kr\to+\infty} \sqrt{4\pi(2\ell+1)}\, i^\ell[j_\ell(kr) + ie^{i\delta_\ell}\sin\delta_\ell\, h_\ell(kr)]$

$$h_\ell(kr) \xrightarrow{kr\to+\infty} \frac{1}{ikr}e^{i(kr-\ell\pi/2)}$$

$$\Rightarrow \sqrt{4\pi(2\ell+1)}\, i^\ell \underbrace{\qquad}_{ie^{i\delta_\ell}\sin\delta_\ell} \frac{1}{ikr}e^{i(kr-\ell\pi/2)} = \frac{f_\ell}{r}e^{ikr}$$

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

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

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

★ As long as we can get the phase shift δ_ℓ, we know the cross section. Scattering problem is reduced into solving radial equation with the proper boundry condition of $R_\ell(kr) \xrightarrow{r\to+\infty} \frac{i^\ell e^{i\delta_\ell}}{kr}\sin(kr-\frac{\ell\pi}{2}+\delta_\ell$

Dis ussion:

✻ optical theorem:

$$f(\theta) = \sum_l f_l \, Y_{l0}(\theta) = \sum_l \frac{e^{i\delta_l}}{k} \sin\delta_l \sqrt{4\pi(2l+1)} \; Y_{l0}(\theta)$$

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

✻ The sign of the phase shift δ_l. Consider the radial Eq.

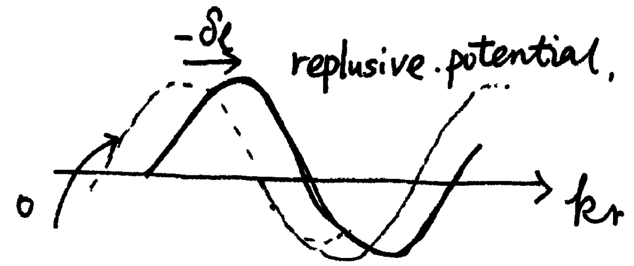
$$\frac{1}{r^2}\left(\frac{d}{dr} r^2 \frac{d}{dr} R_l\right) + \left[k^2 - \frac{l(l+1)}{r^2} - U(r)\right] R_l = 0$$

$$R_l \xrightarrow{kr \to +\infty} \frac{1}{kr} \sin\left(kr - \frac{l\pi}{2} + \delta_l\right) \quad \text{where } k = \sqrt{\frac{2mE}{\hbar^2}}.$$

at $U(r) = 0$, we have $\delta_l = 0$.

If $U(r) \underset{<}{>} 0$, it means that in the region of $U(r)$, there are $\underset{\text{more}}{\text{less}}$ oscillatin occur $\Rightarrow$ $\delta_l < 0$. (repulsive potential)

$\delta_l > 0$ (attractive potential).



replusive potential, Wave function is pushed outside.

$\delta_l < 0$.

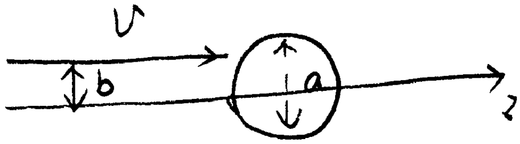
$\sin(kr - \frac{l\pi}{2})$
for $\delta_l = 0$

Similarly. wave function is pushed inside for attractive pottential,

$\delta_l > 0$.

★ 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.

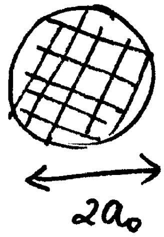


Thus $L = l\hbar \sim mvb \sim mva$

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

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

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

this form is the same as $\underline{j_l(kr) + i e^{i\delta_l} \sin\delta_l\, h_l(kr)}$ up to a phase factor. check! $= j_l + i e^{i\delta_l} \sin\delta_l (j_l + i n_l)$

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

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

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

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

Low energy limit: $ka \to 0$:

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

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

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.