Scattering Theory

Lec.2

Partial waves:

As we mentioned, the incident wavefunction is represented or characterized by wavevector $\vec{k}$ which alligned to be parallel to z- axis. The scattered wavefunction by $\vec{k'}$ which is in same magnitude as k.

The direction of k' is specified with angle θ (explained previously) and azimuthal angle φ about z-axis.

Eq(15) suggests that for spherically symmetric scattering potential $V(r)$ the scattering amplitude $f(k, k')$ is:

$$f(\theta, \varphi) = f(\theta) \quad \text{-----} \quad (22)$$

So, for incident particle wavefunction

$$\psi_0(r) = \sqrt{n}\, e^{ikr} = \sqrt{n}\, e^{ikr\cos\theta} \quad \text{-----} \quad (23)$$

and the total wavefunction

$$\psi(r) = \sqrt{n}\left[e^{ikr\cos\theta} + \frac{e^{ikr}}{r} f(\theta) \right] \quad \text{---- (24)}$$

Eq (23, and 24) shows neither ψ_0 (incident) nor ψ (total) wave functions depend on φ (Azimuthal angle).

For large values of r (outside scattering region) both ψ_0 and ψ satisfy free-space shrödinger equation

$$(\nabla^2 + k^2)\psi = 0 \quad \text{-------- } (*)$$

The general solution of above in spherical polar coordinates (but not depends on φ)

$$\psi(r,\theta) = \sum_{l} R_l(r)\, P_l(\cos\theta) \quad \text{--- (25)}$$

and, from previous lectures.

the Legendre function $P_\ell(\cos\theta)$ is related with spherical harmonics

$$P_\ell(\cos\theta) = \sqrt{\frac{4\pi}{2\ell+1}}\; Y_{\ell,0}(\theta,\varphi) \quad \text{---- (26)}$$

with combination of Eq (25, 26) we obtain:

$$r^2 \frac{d^2R_\ell}{dr^2} + 2r\frac{dR_\ell}{dr} + \left[k^2r^2 - \ell(\ell+1)\right]R_\ell = 0 \quad \text{---- (27)}$$

The solution (independent) to (27) is the spherical Bessel function $j_\ell(kr)$ and $y_\ell(kr)$

$$j_\ell(z) = z^\ell\left(\frac{-1}{z}\frac{d}{dz}\right)^\ell\left(\frac{\sin z}{z}\right),$$

and

--- (28)

$$y_\ell(z) = -z^\ell\left(-\frac{1}{z}\frac{d}{dz}\right)^\ell\left(\frac{\cos z}{z}\right) \quad \text{--- (29)}$$

For or near $z \to 0$, j_ℓ are well-behaved and $y_\ell(z)$ become regular.

$$j_\ell(z) \longrightarrow \frac{\sin(z - \ell\pi/2)}{z}$$

and

$$y_\ell(z) \longrightarrow \frac{\cos(z - \ell\pi/2)}{z} \quad \text{----- (30)}$$

So

$$e^{ikr\cos\theta} = \sum_\ell a_\ell \, j_\ell(kr) \, P_\ell(\cos\theta)$$

a_ℓ : constant.

Legendre functions are orthonormal:

$$\int_{-1}^{1} P_n(\mu) P_m(\mu) \, d\mu = \frac{\delta_{nm}}{n + 1/2} \quad \text{--- (31)}$$

By inversion of above integral:

$$a_\ell \, j_\ell(kr) = (\ell + 1/2) \int_{-1}^{1} e^{ikr\mu} P_\ell(\mu) \, d\mu$$

$$j_\ell(y) = \frac{(-i)^\ell}{2} \int_{-1}^{1} e^{iy\mu} P_\ell(\mu) \, d\mu .$$

$$\ell = 0, 1, 2, 3, ----$$

$$a_\ell = i^\ell (2\ell + 1)$$

So,

$$\psi_0(r) = \sqrt{n} \, e^{ikr\cos\theta} = \sqrt{n} \sum_\ell i^\ell (2\ell+1) \, j_\ell(kr) \, P_\ell(\cos\theta)$$

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Equation (32) is important equation because it shows how the incident plan waves decompose into a series of spherical waves which termed as (partial waves).

Then the most general expression for total wavefunction outside scattering region is:

$$\psi(r) = \sqrt{n} \sum_{\ell} \left[A_\ell \, j_\ell(kr) + B_\ell \, y_\ell(kr) \right] P_\ell(\cos\theta) \quad \text{----- (33)}$$

A and B are constants.

In the large r- limit equation 33 will be:

$$\psi(r) = \sqrt{n} \sum_{\ell} \left[A_\ell \frac{\sin(kr - \ell\frac{\pi}{2})}{kr} - B_\ell \frac{\cos(kr - \ell\frac{\pi}{2})}{kr} \right] P_\ell(\cos\theta) \quad \text{----- (34)}$$

Equation (34) also can be written as:

$$\psi(r) = \sqrt{n} \sum_{\ell} \left[C_\ell \frac{\sin(kr - \ell\frac{\pi}{2} + \delta_\ell)}{kr} \right] P_\ell(\cos\theta),$$

where sin and cos functions are combined to give a sin function which is phase-shifted by δ_ℓ, where:

$$A_\ell = C_\ell \cos\delta_\ell$$

and $$B_\ell = -C_\ell \sin\delta_\ell$$

$$\psi(r) \simeq \sqrt{n} \sum_{\ell} C_\ell \left[\frac{e^{i(kr - \frac{\ell\pi}{2} + \delta_\ell)} - e^{-i(kr - \frac{\ell\pi}{2} + \delta_\ell)}}{2ikr} \right] P_\ell(\cos\theta), \quad \text{--- (35)}$$

Also, in the large-r, limit (combining 23 and 24)

$$\frac{\psi(r) - \psi_0(r)}{\sqrt{n}} = \frac{e^{ikr}}{r} f(\theta) \quad \text{---- (36)}$$

Equation (36) shows:

That the right hand side is only contains the outgoing spherical waves. This implies that the coefficient of incoming spherical waves in large r- limit expansion $\psi(r)$ and $\psi_0(r)$ must be same. Equation 35 and 36 follows:

$$C_\ell = (2\ell+1)\, e^{i(\delta_\ell + \ell\pi/2)} \qquad \text{---} (37)$$

from above equations

$$f(\theta) = \sum_{\ell=0}^{\infty} (2\ell+1)\, \frac{e^{i\delta_\ell}}{k} \sin\delta_\ell\, P_\ell(\cos\theta), \qquad \text{-----} (38)$$

From 12

$$\frac{d\sigma}{d\Omega} = |f(\theta)|^2$$

The differential scattering cross-section is equal to squared of scattering angle.

so, the total cross-section is:

$$\sigma_{tot} = \int |f(\theta)|^2 \, d\Omega$$

$$= \frac{1}{k^2} \oint d\varphi \int_{-1}^{1} d\mu \sum_{\ell} \sum_{\ell'} (2\ell+1)(2\ell'+1)\, e^{i(\delta_\ell - \delta_{\ell'})}$$

$$* \sin\delta_\ell \sin\delta_{\ell'} \, P_\ell(\mu) P_{\ell'}(\mu), \quad \text{----} (39)$$

where $\mu = \cos\theta$

after evaluate of integral

$$\boxed{\sigma_{tot} = \frac{4\pi}{k^2} \sum_{\ell} (2\ell+1) \sin^2\delta_\ell ,} \quad \text{---} \ 40$$

Phase shift:

For spherically symmetric potential $V(r)$ which vanishes for $r > a$, where $\underline{\underline{a}}$ is nominated as a rang of the potential. For $r > a$, the wavefunction $\psi(r)$ satified the free-space of sch. equation of equation ⊛

$$(\nabla^2 + k^2)\psi = 0,$$

The most general solution which is consistent with no incoming spherial-waves is

$$\psi(r) = \sqrt{n} \sum_{\ell=0}^{\infty} i^{\ell} (2\ell+1) R_\ell(r) P_\ell(\cos\theta) \quad \text{---- (41)}$$

where

$$R_\ell(r) = e^{i\delta_\ell} \left[\cos\delta_\ell \, j_\ell(kr) - \sin\delta_\ell \, y_\ell(kr) \right]$$

the logarithmic derivative of the lth radial wave-function, $R_l(r)$ outside the region of the potential is given by:

$$\alpha_{l+} = ka\left[\frac{\cos\delta_l\, j_l'(ka) - \sin\delta_l\, y_l'(ka)}{\cos\delta_l\, j_l(ka) - \sin\delta_l\, y_l(ka)}\right] \quad \text{----(42)}$$

$$j_l' = \frac{dj_l}{dx}, \text{---}$$

we can also inverted it to

$$\tan\delta_l = \frac{ka\, j_l'(ka) - \alpha_{l+}\, j_l(ka)}{ka\, y_l'(ka) - \alpha_{l+}\, y_l(ka)}$$

for $r<a$ ---43

$$\psi(r) = \sqrt{n}\sum_l^{\infty} i^l (2l+1) R_l(r)\, P_l(\cos\theta) \quad \text{----(44)}$$

Equation 43 is the general solution for schrödinger equation inside the range of the potential $(r<a)$ which doesn't depends on φ

and

$$R_\ell(r) = \frac{u_\ell(r)}{r}$$

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

The boundary condition

$$u_\ell(r) = 0$$

shows that the radial wavefunction is well-behaved at the origion.

So, a well behaved solution of the above equation from $r=0$, integrate out to $r=a$, also form logarithmic derivative

$$\alpha_\ell = \frac{1}{(u_\ell/r)} \left.\frac{d(u_\ell/r)}{dr}\right|_{r=a}$$

But as you know

ψ and its derivative should be continuous for physically acceptible wavefunction, so

$$\alpha_{l+} = \alpha_{l-}$$

and the phase shift can be determined from (43).

Scattering by Hard sphere:

let as assume scattering by hard sphere, for which the potential is (∞) for $r<a$, and (0) for $r>a$, which implies $U_\ell = 0$ for all ℓ.

$$B_{\ell_-} = B_{\ell_+} = \infty \quad (\text{for all } \ell)$$

$$\tan\delta_\ell = \frac{j_\ell(ka)}{y_\ell(ka)}$$

for $\ell = 0$ (s-wave), Last equation will be

$$\tan\delta_0 = \frac{\sin(ka)/ka}{-\cos(ka)/ka}$$

$$= -\tan(ka)$$

from above equations

$$\delta_0 = -ka$$

The S- wave radial function

$$R_0 = e^{-ika} \frac{[\cos(ka)\sin(kr) - \sin(ka)\cos(kr)]}{kr}$$

$$= e^{-ika} \frac{\sin[k(r-a)]}{kr}$$

The corresponding radial wavefunction for the incident wave takes the form

$$R_0(r) = \frac{\sin(kr)}{kr}$$

$$\tan \delta_\ell = \frac{-(ka)^{2\ell+1}}{(2\ell+1)[(2\ell-1)!!]^2}$$

So, for low energy only S- wave is important

$$\frac{d\sigma}{d\Omega} = \frac{\sin^2 ka}{k^2} \simeq a^2$$

for $ka \ll 1$

$$\sigma_{tot} = \int \frac{d\sigma}{d\Omega} d\Omega = 4\pi a^2$$

Low energy scattering:

Example

Consider scattering by finite potential well, characterized by $V = V_0$ for $r < a$, and $V = 0$ for $r \geq a$. Here, V_0 is constant. The potential is repulsive for $V_0 > 0$, and attractive for $V_0 < 0$.

The outside wavefunction is given by:

$$R_0(r) = e^{i\delta_0}\left[\cos\delta_0\, j_0(kr) - \sin\delta_0\, y_0(kr)\right]$$

$$= \frac{e^{i\delta_0} \sin(kr+\delta_0)}{kr} \qquad \text{---- (45)}$$

The inside wavefunction

$$R_0 = B\,\frac{\sin(k'r)}{r},$$

B : is constant

$$E - V_0 = \frac{\hbar^2 k'^2}{2m}$$

For $E > V_0$, equation (45) is applies.
However, for $E < V_0$, we have

$$R_0(r) = B\,\frac{\sinh(\kappa r)}{r}$$

$$V_0 - E = \frac{\hbar^2 \kappa^2}{2m}$$

and its radial derivative

$$\tan(ka + \delta_0) = \frac{k}{\bar{k}}\tan(\bar{k}a)$$

for $E > V_0$

for $E > V_0$

$$\tan(ka + \delta_0) = \frac{k}{\kappa}\tanh(\kappa a)$$

for $E < V_0$

Now: Consider attractive potential for which $E > V_0$, suppose $|V_0| \gg E$

$$ka + \delta_0 \simeq \frac{k}{\bar{k}}\tan(\bar{k}a)$$

$$\delta_0 \simeq ka\left[\frac{\tan(\bar{k}a)}{\bar{k}a} - 1\right]$$

The scattering cross-section will be:

$$\sigma_{tot} = \frac{4\pi}{k^2} \sin^2 \delta_0$$

$$= 4\pi a^2 \left[\frac{\tan(k'a)}{k'a} - 1 \right]^2 \quad \text{---} (46)$$

$$k'a = \sqrt{k^2a^2 + \frac{2m|V_0|a^2}{\hbar^2}}$$

for small value of ka

$$\boxed{k'a \simeq \sqrt{\frac{2m|V_0|a^2}{\hbar^2}}}$$

The total cross-section (for S-wave) is independent of the energy of incident particles.

Note For ($k'a \simeq 4.49$) at which $\delta \longrightarrow \pi$, and the scattering cross-section (46) vanishes. In fact, the σ is not exactly zero, because contributions from $\ell > 0$ partial waves. It follows that for certain values of (V_0 and k) which gives almost perfect transmission of incident wave. This effect is called " Ramsauer-Townsend " effect.