Partial waves (cont'd)

Stationary states with well-defined angular momentum

$$\varphi^{(0)}_{k,\ell,m} = \sqrt{\frac{2k^2}{\pi}}\, j_\ell(kr)\, Y_\ell^m(\theta,\varphi) \qquad \text{(free particle)}$$

In this basis,

$$e^{ikz} = \sum_{\ell=0}^{\infty} i^\ell \sqrt{4\pi(2\ell+1)}\, Y_\ell^0(\theta)\, j_\ell(kr)$$

Angular dependence is encoded in spherical harmonic $Y_\ell^m(\theta,\varphi)$

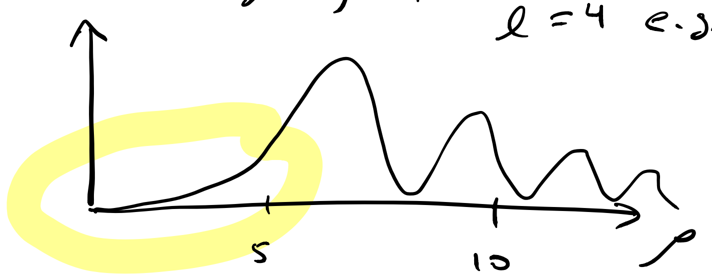
- Probability of finding particle in solid angle $d\Omega_0$ about direction (θ_0,φ_0) between r and $r+dr$

$$r^2 j_\ell^2(kr)\, |Y_\ell^m(\theta_0,\varphi_0)|^2\, dr\, d\Omega_0$$

$$j_\ell(\rho) \sim \frac{\rho^\ell}{(2\ell+1)!!} \quad \text{as } \rho \to 0$$

Let's plot $\rho^2 j_\ell^2(\rho)$

$\ell = 4$ e.g.



remains close to zero for $\rho \ll \sqrt{\ell(\ell+1)}$

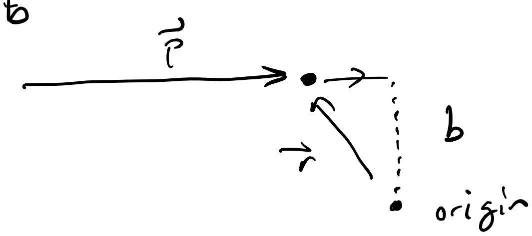
i.e. $r < \frac{1}{k}\sqrt{\ell(\ell+1)}$

In a sphere centered at origin of radius

$$b_\ell(k) = \frac{1}{k}\sqrt{\ell(\ell+1)}$$

a particle in some state $|\varphi^{(0)}_{k,\ell,m}\rangle$ is practically unaffected by what happens in this region.

In classical mechanics, there is an "impact parameter" b



angular momentum $\mathcal{L}$

$$b = \frac{|\mathcal{L}|}{|p|}$$

we replace $|\mathcal{L}| \to \hbar\sqrt{\ell(\ell+1)}$

$|p| \to \hbar k$

(semi-classical interpretation)

Asymptotic behavior

As $\rho \to \infty$

$$j_\ell(\rho) \to \frac{1}{\rho}\sin\left(\rho - \frac{\ell\pi}{2}\right)$$

so

$$\varphi^{(0)}_{k,\ell,m} \to \sqrt{\frac{2k^2}{\pi}}\, Y_\ell^m(\theta,\varphi)\, \frac{e^{-ikr}e^{i\ell\frac{\pi}{2}} - e^{ikr}e^{-i\ell\frac{\pi}{2}}}{2ikr}$$

ingoing wave   outgoing wave

amplitudes have phase difference of $\ell\pi$

If we have a wave packet of free spherical waves, some ℓ, m. At first we have incoming wave, becomes distorted gives rise to outgoing wave w/ shift $\ell\pi$.

Let's expand plane wave in terms of free spherical waves.

$$\langle \vec{r} \,|\, 0,0,k \rangle = \left(\frac{1}{2\pi}\right)^{3/2} e^{ikz} = \left(\frac{1}{2\pi}\right)^{3/2} e^{ikr\cos\theta}$$

$$|0,0,k\rangle = \int_0^\infty dk' \sum_{\ell=0}^{\infty} \sum_{m=-\ell}^{\ell} |\varphi^{(0)}_{k',\ell,m}\rangle \langle \varphi^{(0)}_{k',\ell,m} | 0,0,k\rangle$$

$$= \sum_{\ell=0}^{\infty} c_{k,\ell} \, |\varphi^{(0)}_{k,\ell,0}\rangle$$

orthogonal if eigenvalues are different $\propto \delta(k-k')$

we've also used $L_z |0,0,k\rangle = 0$

they are both eigenstates ($|0,0,k\rangle$, $|\varphi_{k,\ell,m}\rangle$) of L_z

scalar product is prop. to δ_{m0}

$$e^{ikz} = \sum_{\ell=0}^{\infty} i^\ell \sqrt{4\pi(2\ell+1)}\, Y_\ell^0(\theta)\, j_\ell(kr)$$

The spherical harmonic Y_ℓ^0 is proportional to $P_\ell(\cos\theta)$ (Legendre polynomial)

$$Y_\ell^0(\theta) = \sqrt{\frac{2\ell+1}{4\pi}}\, P_\ell(\cos\theta)$$

$$\Rightarrow e^{ikz} = \sum_{\ell=0}^{\infty} i^\ell (2\ell+1)\, j_\ell(kr)\, P_\ell(\cos\theta)$$

Partial waves in a potential

Assume $V(r)$ is a central potential.

$$\varphi_{k,\ell,m}(\vec{r}) = \underbrace{\frac{1}{r} u_{k,\ell}(r)}_{R_{k,\ell}(r)} Y_\ell^m(\theta,\varphi)$$

(Note dropped (0) superscript)

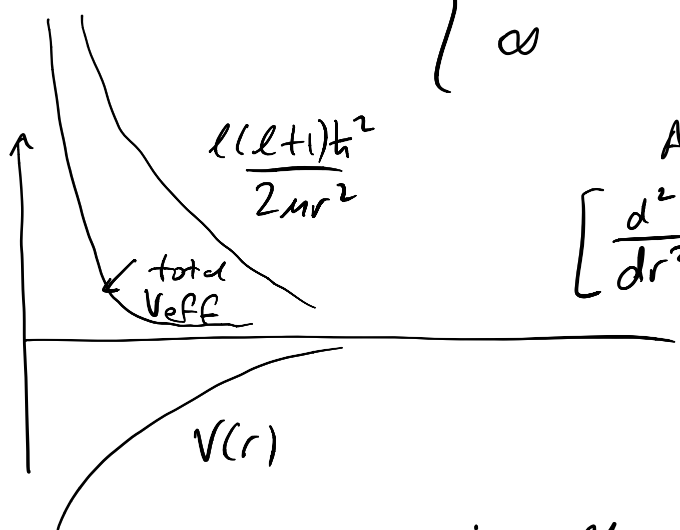
From Schrödinger equation:

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

subject to the constraint that $u_{k,\ell}(r=0)=0$

This looks like a 1-d problem with effective potential

$$V_{eff}(r) = \begin{cases} V(r) + \dfrac{\ell(\ell+1)\hbar^2}{2\mu r^2} & r>0 \\ \infty & r<0 \end{cases}$$



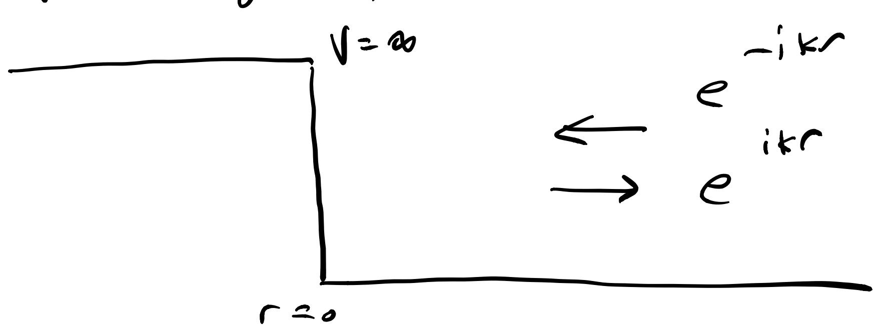
As $r\to\infty$

$$\left[\frac{d^2}{dr^2} + k^2\right]u_{k,\ell}(r) = 0$$

As $r\to\infty$, solution is $u_{k,\ell}(r) = Ae^{ikr} + Be^{-ikr}$

we also have to satisfy $u_{k,\ell}(0)=0$ this constrains A and B.

In 1-D language, like incident plane wave from right, and "reflected" wave from left



there is no "transmitted" wave since $V = \infty$.

$\Rightarrow |A| = |B|$ (refl. and incident must be equal)

$$u_{k,\ell}(r) \underset{r\to\infty}{\sim} |A| \left[e^{ikr} e^{i\varphi_A} + e^{-ikr} e^{i\varphi_B} \right]$$

$$= C \sin(kr - \beta_\ell)$$

β_ℓ is a phase, can be determined since $u_{k,\ell}(0) = 0$.

If $V = 0$, we found $\beta_\ell = \frac{\ell\pi}{2}$

we can write

$$u_{k,\ell}(r) \underset{r\to\infty}{\sim} C \sin\left(kr - \frac{\ell\pi}{2} + \delta_\ell\right)$$

the term δ_ℓ is the phase shift of the partial wave $\varphi_{k,\ell,m}(r)$. Depends on k (energy)

we can write the asymptotic behavior as

$$\varphi_{k,\ell,m}(\vec{r}) \underset{r\to\infty}{\sim} C \frac{\sin\left(kr - \frac{\ell\pi}{2} + \delta_\ell\right)}{r} Y_\ell^m(\theta,\varphi)$$

$$= C Y_\ell^m(\theta,\varphi) \frac{\underbrace{e^{-ikr} e^{i\left(\frac{\ell\pi}{2} - \delta_\ell\right)}}_{\text{incoming wave}} - \underbrace{e^{ikr} e^{-i\left(\frac{\ell\pi}{2} - \delta_\ell\right)}}_{\text{outgoing wave}}}{2ir}$$

Again looks like a free spherical wave, w/ phase shift.

Define a new partial wave $\tilde{\varphi}_{k,\ell,m}(\vec{r}) = e^{i\delta_\ell}\varphi_{k,\ell,m}(\vec{r})$

better identification w/ what we saw in free-case:

$$\tilde{\varphi}_{k,\ell,m}(\vec{r}) \underset{r\to\infty}{\sim} Y_\ell^m(\theta,\varphi)\,\frac{e^{-ikr}e^{i\ell\frac{\pi}{2}} - e^{ikr}e^{-i\ell\frac{\pi}{2}}e^{2i\delta_\ell}}{2ikr}$$

Same incoming wave as in free particle case (apart from normalization)

when potential transforms it into outgoing wave. It has accumulated a phase shift $2\delta_\ell$ relative to free outgoing wave (if $V=0$).

$e^{2i\delta_\ell}$ summarizes the effect of the potential on particle w/ angular momentum ℓ.

★ δ_ℓ depends on the energy

If $V(r)$ has a finite range $V(r) = 0$ if $r > r_0$ the spherical wave $\varphi^{(0)}_{k,\ell,m}$ barely penetrates the sphere of radius $b_\ell(k)$ around origin.

i.e. the potential has essentially no effect on waves for which $b_\ell(k) \gg r_0$

like incoming wave turning back before reaching the zone of influence of $V(r)$.

At each energy, there is a critical value l_M of the angular momentum, given by

$$\sqrt{l_M(l_M+1)} \simeq k r_0$$

The phase shift δ_l is significant only if $l \lessapprox l_M$.

For shorter-range potentials and lower incident energy, only non-zero phase shifts will be for the lower l values.

s-wave scattering ($l=0$) at very low energy.

s + p-wave at higher etc..

e.g. useful for collision w/ ultra-cold atoms (s-wave scattering)

Cross-section in terms of phase shifts

$V_k^{diff}(\vec{r})$ involves partial waves w/ same energy $\frac{\hbar^2 k^2}{2M}$.

$V_k^{diff}(\vec{r})$ is independent of φ (azimuthal symmetry)

$$V_k^{diff}(\vec{r}) = \sum_{l=0}^{\infty} C_l \tilde{\varphi}_{k,l,0}(\vec{r})$$

If $V(r)=0$, $\psi_k^{diff}(\vec{r})$ reduces to plane wave e^{ikz} and the partial waves become free spherical waves $\varphi^{(0)}_{k,\ell,m}(\vec{r})$

$$e^{ikz} = \sum_{\ell=0}^{\infty} i^\ell \sqrt{4\pi(2\ell+1)}\, j_\ell(kr)\, Y_\ell^0(\theta)$$

If $V(r) \neq 0$ we have a scattered wave and a plane wave.

$\tilde{\varphi}_{k,\ell,0}(\vec{r})$ and $\varphi^{(0)}_{k,\ell,0}(r)$ differ in asymptotic behavior only in presence of outgoing wave, which has same radial dependence.

we expect that

$$\psi_k^{diff}(\vec{r}) = \sum_{\ell=0}^{\infty} i^\ell \sqrt{4\pi(2\ell+1)}\, \tilde{\varphi}_{k,\ell,0}(r)$$

Let's check that this form is of the type

$$\psi_k^{diff}(r) \sim e^{ikz} + f_k(\theta,\varphi)\frac{e^{ikr}}{r}$$

$$\sum_{\ell=0}^{\infty} i^\ell \sqrt{4\pi(2\ell+1)}\, \tilde{\varphi}_{k,\ell,0}(\vec{r}) \underset{r\to\infty}{\sim} -\sum_{\ell=0}^{\infty} i^\ell \sqrt{4\pi(2\ell+1)}\, Y_\ell^0 \times \frac{1}{2ikr}\left[e^{-ikr}e^{i\ell\frac{\pi}{2}} + e^{ikr}e^{-i\ell\frac{\pi}{2}}e^{2i\delta_\ell}\right]$$

$$e^{2i\delta_\ell} = 1 + 2i\, e^{i\delta_\ell}\sin\delta_\ell$$

$$\hookrightarrow -\sum_{\ell=0}^{\infty} i^\ell \sqrt{4\pi(2\ell+1)}\, Y_\ell^0(\theta) \times \left[\frac{e^{-ikr} e^{\frac{i\ell\pi}{2}} - e^{ikr} e^{-\frac{i\ell\pi}{2}}}{2ikr} - \frac{e^{ikr}}{r}\frac{1}{k} e^{-\frac{i\pi\ell}{2}} e^{i\delta_\ell} \sin\delta_\ell \right]$$

this is asymptotic exp. of plane wave e^{ikz}

Thus as $r \to \infty$

$$= e^{ikz} + f_k(\theta) \frac{e^{ikr}}{r}$$

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

The differential scattering cross-section is then

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

The total cross-section is

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

to determine $\sigma(\theta)$ or σ in theory requires knowledge of all phase shifts $\delta_\ell\ \forall \ell$.

these can be calculated e.g. if potential $V(r)$ is known (numerical techniques, etc.) separately for each ℓ.

Partial-wave method more useful if there are only a small # of non-zero phase shifts.

For a finite-range potential $V(r)$,

$\delta_\ell \sim 0$ for $\ell > \ell_M$. (see prev. notes)

Remark :

If $V(r)$ is unknown, one can look at the angular dependence of cross-section to deduce potential.

e.g. isotropic $\rightarrow$ s-wave

θ-dependence $\Rightarrow$ phase shifts other than s-wave are nonzero.

You can find model for $V(r)$ which reproduces the measured $\sigma(\theta)$.

Remark 2 :

There are "scattering resonances" as a function of energy $\sigma(E)$

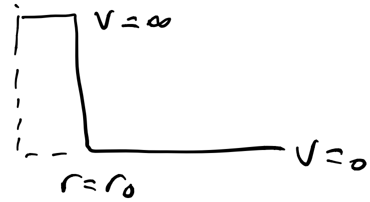
If phase shift $\delta_\ell = \frac{\pi}{2}$ for some ℓ and some energy $E = E_0$, then contribution to σ reaches its upper limit, cross-section shows a peak.

This is analogous to transmission coefficient of e.g. 1D square potential which had resonances.

Examples

Low-energy scattering by a hard sphere potential

$$V(r) = \begin{cases} 0 & r > r_0 \\ \infty & r < r_0 \end{cases}$$



The incident energy is assumed small

$k r_0 << 1$

then we can neglect all phase shifts except for s-wave (HW problem to prove this)

$$f_k(\theta) = \frac{1}{k} e^{i\delta_0(k)} \sin \delta_0(k) \sqrt{4\pi}\, Y_0^0$$

$$= \frac{1}{k} e^{i\delta_0(k)} \sin\delta_0(k)$$

$$|f_k(\theta)|^2 = \sigma(\theta) = \frac{1}{k^2} \sin^2 \delta_0(k)$$

$$\sigma = \frac{4\pi}{k^2} \sin^2 \delta_0(k)$$

How can we determine $\delta_0(k)$?

For $r > r_0$ $\left[\frac{d^2}{dr^2} + k^2\right] u_{k,0}(r) = 0$

with $u_{k,0}(r_0) = 0$ since $V(r_0) = \infty$.

$$u_{k,0} = \begin{cases} C \sin\left[k(r-r_0)\right] & \text{for } r > r_0 \\ 0 & r < r_0 \end{cases}$$

$$u_{k,0}(r) \underset{r\to\infty}{\sim} \sin(kr+\delta_0)$$

thus $\delta_0(k) = -kr_0$

$$\sigma = \frac{4\pi}{k^2}\sin^2 kr_0, \quad \text{since } kr_0 \ll 1, \quad \simeq 4\pi r_0^2$$

Classically we would find πr_0^2

this phenomenon is analogous to diffraction of a light wave.