Partial wave approximation

For a spherically-symmetric potential the basis of plane waves is "unnatural"

We will now switch to the spherical waves

New basis: free particles with fixed angular momentum

$$\langle \hat{H} \rangle = E = \frac{\hbar^2 k^2}{2m} \quad \langle \hat{L}^2 \rangle = \hbar^2 \ell(\ell+1) \quad \langle \hat{L}_z \rangle = \hbar m$$

$$\psi_{k\ell m}(x) = \underbrace{C_{k\ell m}}_{\text{normalization}} R_{k\ell}(r) Y_{\ell m}(\theta, \varphi)$$

Free particle Schrodinger eqn:

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

dimentionless units $\rho \Rightarrow kr$

$$R_\ell''(\rho) + \frac{2}{\rho} R_\ell(\rho) + R_\ell(\rho) - \frac{\ell(\ell+1)}{\rho^2} R_\ell(\rho) = 0$$

Solution: spherical Bessel functions

$$R_\ell(\rho) = a_\ell j_\ell(\rho) + b_\ell n_\ell(\rho)$$

$$j_\ell(\rho) = \left(\frac{\pi}{2\rho}\right)^{1/2} J_{\ell+1/2}(\rho)$$ Bessel functions (regular at $\rho = 0$)

$$n_\ell(\rho) = \left(\frac{\pi}{2\rho}\right)^{1/2} N_{\ell+1/2}(\rho)$$ Neumann function (singular at $\rho = 0$)

Properties of the spherical Bessel functions

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

$$j_0(\rho) = \frac{\sin\rho}{\rho} \qquad j_1(\rho) = \frac{\sin\rho}{\rho^2} - \frac{\cos\rho}{\rho}$$

$$n_\ell(\rho) = -(-\rho)^\ell \left(\frac{1}{\rho}\frac{d}{d\rho}\right)^\ell \left(\frac{\cos\rho}{\rho}\right)$$

$$n_0(\rho) = \frac{\cos\rho}{\rho} \qquad n_1(\rho) = -\frac{\cos\rho}{\rho^2} - \frac{\sin\rho}{\rho}$$

small ρ:

$$j_\ell(\rho) \xrightarrow{\rho\to 0} \frac{\rho^\ell}{(2\ell+1)!!} \qquad n_\ell(\rho) \xrightarrow{\rho\to 0} \frac{(2\ell-1)!!}{\rho^{\ell+1}}$$

large ρ:

$$j_\ell(\rho) \xrightarrow{\rho\to\infty} \frac{1}{\rho}\sin(\rho - \pi\ell/2)$$

$$n_\ell(\rho) \xrightarrow{\rho\to\infty} -\frac{1}{\rho}\cos(\rho - \pi\ell/2)$$

Often it is more convenient to use Hankel functions

$$h_\ell^{(\pm)} = j_\ell(\rho) \pm i\, n_\ell(\rho) \xrightarrow{\rho\to\infty} (-i)^{\pm(\ell+1)} \frac{e^{\pm i\rho}}{\rho}$$

Wave - functions defined at the origin

$$\psi_{\ell m}(\vec{r}) \sim j_\ell(kr)\, Y_{\ell m}(\theta,\varphi)$$

since $\int_0^\infty r^2 dr\, j_\ell(kr)\, j_{\ell'}(k'r) = \frac{\pi}{2k^2}\delta(k-k')\delta(\ell-\ell')$

and $\int |\psi_{\ell m}(\vec{r})|^2 d^3\vec{r} = 1$

$$\psi_{\ell m}(\vec{r}) \equiv \langle \vec{r} | \hat{k}, \ell, m \rangle = \frac{i^\ell}{\hbar}\left(\frac{2mk}{\pi}\right)^{1/2} j_\ell(kr)\, Y_{\ell m}(\theta,\varphi)$$

Connection to the plane wave basis

$$e^{ikz} = \sum_\ell (2\ell+1)\, i^\ell\, j_\ell(kr)\, P_\ell(z/r)$$

or, more generally,

$$e^{i\vec{k}\vec{r}} = \sum_\ell (2\ell+1)\, i^\ell\, j_\ell(kr)\, P_\ell(\hat{k}\cdot\hat{r})$$

Let's now consider scattering from a spherically symmetric potential $V(r)$ that is local (i.e. $V(r)=0$ for $r>R$)

Outside the potential range $V=0 \Rightarrow$

$$\psi = A_\ell(kr)\, Y_{\ell m}(\theta,\varphi)$$

where $A_\ell(kr)$ is a linear combination of:

$j_\ell(kr)$, $n_\ell(kr)$ "standing waves"

$h_\ell^\pm(kr) \rightrightarrows (-1)^{\pm(\ell+1)} \frac{e^{\pm ikr}}{r}$ "running waves"

If $V=0$ $A_\ell \equiv j_\ell$ – regular wave (no singularity at $r=0$)

$$A_\ell = \frac{1}{2}\left(h_\ell^+(kr) + h_\ell^-(kr)\right)$$

General form of the solution for $r > R$

$$A_\ell(\rho) = \frac{c}{2}\left[h_\ell^-(kr) + e^{2i\delta_\ell} h_\ell^+(kr) \right]$$

- Rotational symmetry $\longrightarrow$ angular momentum is conserved for each component

$$(\ell m)_{incoming} \longrightarrow (\ell m)_{outgoing}$$

no mixing

- Unitarity $\longrightarrow$ probability is conserved

$e^{2i\delta_\ell}$ is purely phase factor ($\delta_\ell \in \mathbb{R}$)

Scattering properties of V are completely determined by the phase shifts δ_ℓ of partial waves

4a $\longrightarrow$

To make this connection, we need to solve the Schrodinger eqn for $r < R$

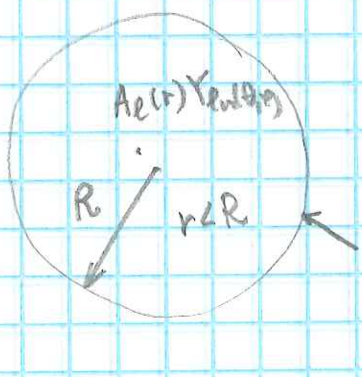
$$\psi_\ell(\vec{r}) = A_\ell(r)\, Y_{\ell m}(\theta,\varphi) = \frac{u_\ell(r)}{r} Y_{\ell m}(\theta,\varphi)$$

Boundary condition

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

$$-\frac{\hbar^2 \nabla^2}{2m_e}\psi + V\psi = E\psi$$

$$u_\ell'' + \left(k^2 - \frac{2m_e}{\hbar^2}V - \frac{\ell(\ell+1)}{r^2}\right)u_\ell = 0$$



$$\frac{c}{2}\left(h_\ell^-(\rho) + e^{2i\delta_\ell} h_\ell(\rho)\right] =$$

$$= c\, e^{2\delta_\ell}\left(j_\ell(\rho)\cos\delta_\ell - n_\ell(\rho)\sin\delta_\ell \right)$$

on the boundary $\longrightarrow$ match logarithmic derivatives

$$\beta_\ell = \frac{d(\ln A_\ell(r))}{d(\ln r)} = \frac{r}{A_\ell(r)}\frac{dA_\ell(r)}{dr}$$

Connection between plane-wave formalism and partial wave formalism

Plane wave for $r \to \infty$ — no φ dependence

$$\psi(\vec{r}) = \frac{1}{(2\pi\hbar)^{3/2}}\left[e^{ikz} + f(\theta)\frac{e^{ikr}}{r}\right] \qquad \boxed{i^l = e^{i\pi l/2}}$$

$$e^{ikz} = \sum_l (2l+1)\, i^l j_l(kr)\, P_l(\cos\theta)$$

and $j_l(kr) \xrightarrow{r\to\infty} \dfrac{e^{i(kr-\pi l/2)} - e^{-i(kr-\pi l/2)}}{2ikr}$

Define $f(\theta) = \sum_l (2l+1) f_l(\theta) P_l(\cos\theta)$

Then

$$\psi(\vec{r}) = \sum_{l=0}^{\infty}(2l+1)P_l(\cos\theta)\left[f_l(\theta)\frac{e^{ikr}}{r} + \frac{e^{ikr}}{2ikr} - \frac{e^{-ikr+i\pi l}}{2ikr}\right]$$

$$= \sum_{l=0}^{\infty}(2l+1)P_l(\cos\theta)\frac{1}{2ik}\left[\frac{e^{ikr}}{r}\left[1+2ikf_l(\theta)\right] - \frac{e^{-ikr+i\pi l}}{r}\right]$$

$$= \sum_{l=0}^{\infty}(2l+1)P_l(\cos\theta)\frac{1}{2ik}\left[\underbrace{\frac{e^{ikr}}{r}}_{\sim h_l^+(kr)}\left[1+2ikf_l(\theta)\right] + \underbrace{(-1)^{l+1}\frac{e^{-ikr}}{r}}_{\sim h_l^-(kr)}\right]$$

Compare to the partial wave asymptotic solution

$$A_l(r) \sim h_l^-(kr) + e^{2i\delta_l} h_l^+(kr)$$

$$\boxed{e^{2i\delta_l} = 1 + 2ik f_l(\theta)}$$

or $f_l(\theta) = \dfrac{e^{2i\delta_l}-1}{2ik} = e^{i\delta_l}\dfrac{\sin\delta_l}{k}$

Thus $f(\theta) = \dfrac{1}{k}\sum_{l=0}^{\infty}(2l+1)e^{i\delta_l}\sin\delta_l\, P_l(\cos\theta)$

$$\sigma = \int |f(\theta)|\, d\Omega = \frac{1}{k^2}\cdot 2\pi \sum_{l,l'}(2l+1)(2l'+1)e^{i\delta_l - i\delta_{l'}}\sin\delta_l \sin\delta_{l'}\underbrace{\int_0^\pi \sin\theta\, d\theta\, P_l(\cos\theta)P_{l'}(\cos\theta)}_{=\frac{2}{2l+1}\delta_{ll'}}$$

$$= \frac{4\pi}{k^2}\sum(2l+1)\sin^2\delta_l = \sum \sigma_l \qquad \sigma_l = \frac{4\pi}{k^2}(2l+1)\sin^2\delta_l$$

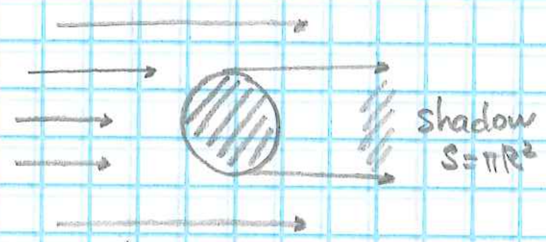
$$\beta_\ell\Big|_{r=R+} = kR\left[\frac{j_\ell'(kR)\cos\delta_\ell - n_\ell'(kR)\sin\delta_\ell}{j_\ell(kr)\cos\delta_\ell - n_\ell(kr)\sin\delta_\ell}\right] \Rightarrow$$

$$\Rightarrow \tan\delta_\ell = \frac{kR\, j_\ell'(kR) - \beta_\ell j_\ell(kR)}{kR\, n_\ell'(kR) - \beta_\ell n_\ell(kR)}$$

The values of β_ℓ are fixed from the solution of SE inside the potential region $(r<R)$, thus δ_ℓ values can be calculated.

Example: hard sphere

Consider $V(r) = \begin{cases} \infty & r \le R \\ 0 & r > R \end{cases}$



classical picture

$r \le R \quad A_\ell(r) = 0$

$$\cos\delta_\ell \cdot j_\ell(kR) - \sin\delta_\ell\, n_\ell(kR) = 0$$

$$\tan\delta_\ell = \frac{j_\ell(kR)}{n_\ell(kR)}$$

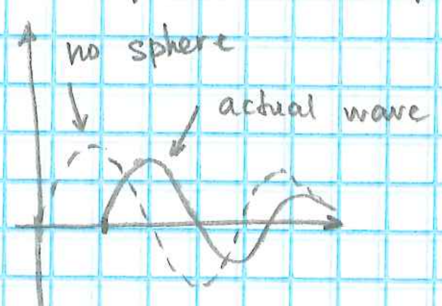
$$e^{2i\delta_\ell} = -\frac{h_\ell^-(kR)}{h_\ell^+(kR)}$$

S-wave scattering $\ell = 0$

$$\tan\delta_0 = \frac{j_0(kR)}{n_0(kR)} = \frac{\sin kR/kR}{-\cos kR/kR} = -\tan kR$$

$$\underline{\delta_0 = -kR}$$

$$\psi_0 \sim \frac{1}{r}\sin(kr+\delta_0) = \frac{1}{r}\sin k(r-R)$$



what about $\ell \geq 1$?

Low-energy limit $kR \ll 1$

$$\tan\delta_\ell = \frac{j_\ell(kR)}{n_\ell(kR)} \sim \frac{(kR)^\ell/(2\ell+1)!!}{-(2\ell-1)!!/(kR)^{\ell+1}} = -(kR)^{2\ell+1}\frac{(2\ell+1)}{[(2\ell+1)!!]^2}$$

negligeable effect
$\delta_\ell \approx 0$

Predominantly s-scattering amplitude

$$\frac{d\sigma}{d\Omega} = |f(\theta)|^2 \approx |f_0(\theta)|^2 = \frac{1}{k^2}\sin^2\delta_\ell = \frac{1}{k^2}\sin^2(kR) \approx R^2$$

$$\sigma_{tot} = \int d\sigma = 4\pi R^2$$

$4\times$ geometrical expectation