L81-Partial Waves

Friday, April 15, 2016 09:23

* goal: Solve Schrödinger equation with boundary conditions $\psi_{inc} = Ae^{ikz}$ [incident wave] and project asymptotic outgoing wave into the form $\psi_{scat} = A f(\theta) \frac{e^{ikr}}{r}$.

problem: e^{ikz} and e^{ikr}/r are different basis functions - must solve the complete problem in one basis.

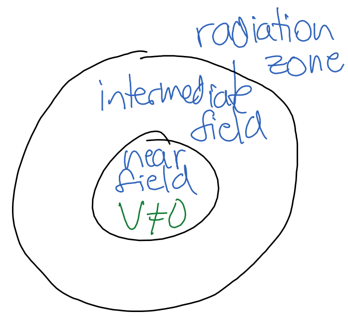
solution: let's write everything in spherical waves

* Central potential asymptotic solutions:

a) $\Big[\underbrace{\frac{-\hbar^2}{2m}\frac{d^2}{dr^2}}_{\text{kinetic}} + V(r) \underbrace{- \frac{\hbar^2}{2m}\frac{\ell(\ell+1)}{r^2}}_{\text{centrifugal}}\Big]u(r) = Eu(r)$ where $\psi(r,\theta,\phi) = \frac{u(r)}{r} Y_{\ell m}(\theta,\phi)$

let $V(r)\to 0$ as $u'' \gg \frac{\ell(\ell+1)}{r^2}u$ as $r \to 0$, $[\ell = 0]$

then $\left(\frac{d^2}{dr^2} - k^2\right)u = 0$ $\quad u = \underbrace{Ce^{ikr}}_{\text{outgoing}} + \underbrace{De^{-ikr}}_{\text{incoming}}$ [radiation field]



b) let $V(r) = 0$ but consider $\ell \neq 0$

$$\left[\frac{d^2}{dr^2} - \frac{\ell(\ell+1)}{r^2}\right]u = -k^2 u \quad \text{[spherical Bessel equation]}$$

$$u = A r j_\ell(kr) + B r n_\ell(kr) \qquad \text{like } A\sin(kr) + B\cos(kr)$$

$$= \underbrace{C r h_\ell^{(1)}(kr)}_{\text{outgoing}} + \underbrace{D r h_\ell^{(2)}(kr)}_{\text{incoming}} \qquad \text{like } Ce^{ikr} + De^{-ikr}$$

where $h_\ell^{(1,2)}(kr) \equiv j_\ell(kr) \pm i n_\ell(kr)$ $\quad$ like $e^{\pm ikr} = \cos(kr) \pm i\sin(kr)$

* the exact solution outside the scattering region is

$$\psi(r) = A\left\{e^{ikz} + \sum_{\ell,m} C_{\ell m} h_\ell^{(1)}(kr) Y_{\ell m}(\theta,\phi)\right\}$$

$m=0$ [spherically symmetric] $\quad Y_{\ell 0} = \sqrt{\frac{2\ell+1}{4\pi}}\, P_\ell(\cos\theta) \quad$ let $C_{\ell 0} \equiv i^{\ell+1} k \sqrt{4\pi(2\ell+1)}\, \underbrace{a_\ell}_{\text{partial wave amplitude}}$

$$\psi(\vec{r}) = A\left\{ e^{ikz} + k\sum_{\ell=0}^{\infty} i^{\ell+1}(2\ell+1)\, a_\ell\, h_\ell^{(1)}(kr)\, P_\ell(\cos\theta)\right\}$$

$$\xrightarrow{r\to\infty} A\left\{ e^{ikz} + \underbrace{\sum_{\ell=0}^{\infty}(2\ell+1)\, a_\ell\, P_\ell(\cos\theta)}_{f(\theta)}\, \frac{e^{ikr}}{r}\right\} \qquad \left[h_\ell^{(1)}(x) \to (-i)^{\ell+1}\frac{e^{ikx}}{x}\right]$$

$$f(\theta) = \sum_{\ell=0}^{\infty}(2\ell+1)\, a_\ell\, P_\ell(\cos\theta) \qquad a_\ell = \left\{\begin{array}{l}\text{components of } f(\theta)\\ \text{in the } P_\ell(\cos\theta) \text{ basis}\end{array}\right.$$

thus $\frac{d\sigma}{d\Omega} = |f(\theta)|^2 = \sum_{\ell,\ell'}(2\ell+1)(2\ell'+1)\, a_\ell^* a_{\ell'}\, P_\ell(\cos\theta)\, P_{\ell'}(\cos\theta)$

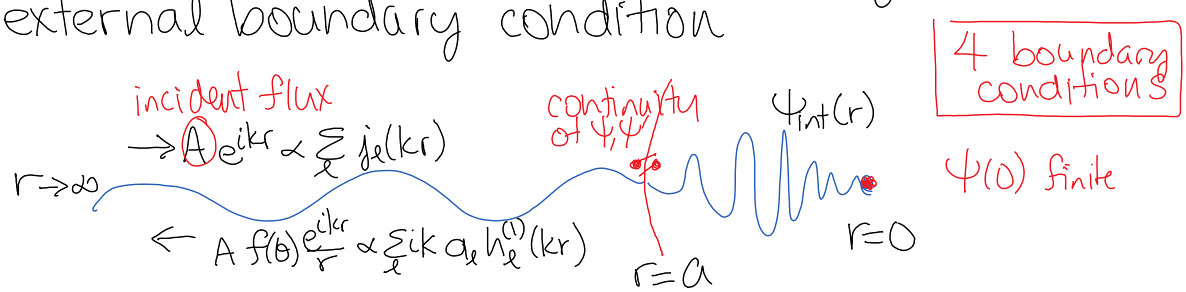
$$\sigma = \int \frac{d\sigma}{d\Omega}\, d\Omega = \sum_{\ell,\ell'} a_\ell^* a_{\ell'} \cdot 2\pi \underbrace{\int_{x=-1}^{1} P_\ell(x) P_{\ell'}(x)\, dx}_{\frac{2}{\ell+1}\delta_{\ell\ell'}} = 4\pi\sum_{\ell=0}^{\infty}(2\ell+1)|a_\ell|^2$$

* convert incoming wave to spherical basis:

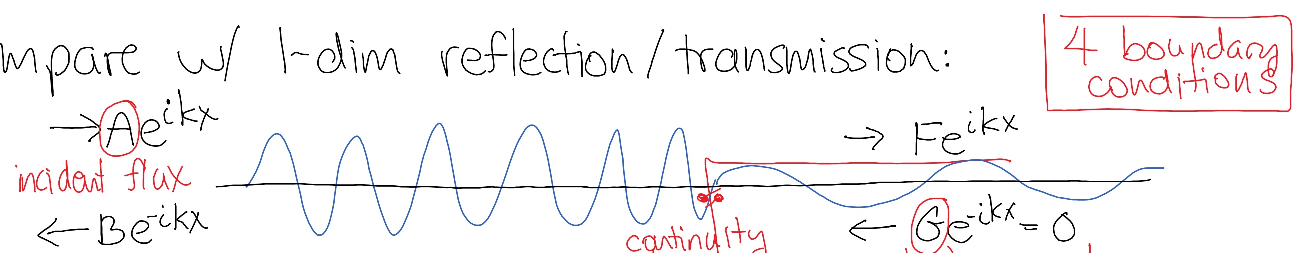
$$e^{ikz} = \sum_{\ell=0}^{\infty} i^\ell(2\ell+1)\, j_\ell(kr)\, P_\ell(\cos\theta) \qquad \text{[Rayleigh's formula]}$$

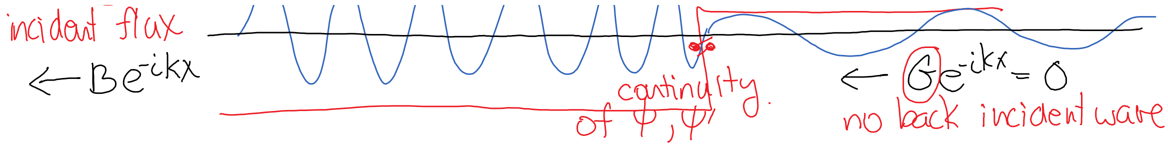
$$\psi_{ext}(\vec{r}) = A\sum_{\ell=0}^{\infty} i^\ell(2\ell+1)\left[j_\ell(kr) + ik\, a_\ell\, h_\ell^{(1)}(kr)\right] P_\ell(\cos\theta)$$

* now we can solve a simple 1-dim scattering problem for $a_\ell(k)$ for each k,ℓ by solving the Schrödinger equation in 2 regions $\psi_{ext}(\vec{r})$ in $r>a$ where $V(r)=0$ and $\psi_{int}(\vec{r})$ in $r<a$ where $V(r)\neq 0$, using Ae^{ikz} as the external boundary condition



* compare w/ 1-dim reflection/transmission:




incident flux
← Be^{-ikx}
continuity of ψ, ψ'
← $Ge^{-ikx} = 0$
no back incident wave