Quantum Mechanics – II.

Feb. 22, 2010

☆ 公布了評分標準，課本，上課內容計畫，考試若非有正當理由及證明缺考者零分並不得補考，學習上有問題的同學，必須在開學第二週內找我談。

☆ **2-body problem remind**

One of the most simple problems in QM.

Interact via a central potential $V(|\vec{r}_1-\vec{r}_2|)$

$$-\frac{1}{2m_1}\nabla_1^2\psi(\vec{r}_1,\vec{r}_2)-\frac{1}{2m_2}\nabla_2^2\psi(\vec{r}_1,\vec{r}_2)+V(r)\psi(\vec{r}_1,\vec{r}_2)=E\psi(\vec{r}_1,\vec{r}_2)$$

$$r=|\vec{r}_1-\vec{r}_2|\ ,\quad \vec{r}\equiv\vec{r}_1-\vec{r}_2=x\hat{i}+y\hat{j}+z\hat{k}$$

$$\&\quad \vec{R}\equiv\frac{m_1\vec{r}_1+m_2\vec{r}_2}{m_1+m_2}=X\hat{i}+Y\hat{j}+Z\hat{k}$$

In terms of $\vec{r}$ & $\vec{R}$, the Schrodinger Eq becomes:

$$-\frac{1}{2M}\nabla_R^2\psi-\frac{1}{2\mu}\nabla_r^2\psi+V(r)\psi=E\psi.$$

where $M=m_1+m_2$

$$\nabla_R^2\equiv\frac{\partial^2}{\partial X^2}+\frac{\partial^2}{\partial Y^2}+\frac{\partial^2}{\partial Z^2}$$

$$\nabla_r^2\equiv\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}+\frac{\partial^2}{\partial z^2}$$

$$\mu=\frac{m_1m_2}{m_1+m_2}$$

is the <u>reduced mass</u>.

$$\Rightarrow\quad \psi=\Phi(R)\varphi(r)\qquad \&\quad E=E_{CM}+E_0$$

$$-\frac{1}{2M}\nabla_R^2\Phi=E_{CM}\Phi$$

while

$$-\frac{1}{2\mu}\nabla_r^2\varphi+V(r)\varphi=E_0\varphi$$

In spherical polar coordinates,

$$\nabla_r^2=\frac{\partial^2}{\partial r^2}+\frac{2}{r}\frac{\partial}{\partial r}-\frac{1}{r^2}L^2$$

then the Schrödinger Eq becomes

$$\frac{\partial^2}{\partial r^2}\varphi+\frac{2}{r}\frac{\partial}{\partial r}\varphi-\frac{1}{r^2}L^2\varphi+\frac{2\mu}{\hbar}\left[E-V(r)\right]\varphi=0$$

let $\psi = R_{nl}(r)\, Y_l^m(\theta, \phi)$.

since $L^2 Y_l^m(\theta,\phi) = l(l+1)\, Y_l^m$

$$\Rightarrow \quad R'' + \frac{2}{r} R' + \frac{2M}{\hbar^2}\left[E - \left(V(r) + \frac{\hbar^2 l(l+1)}{2M r^2}\right)\right] R = 0$$

It's convenient to make the substitution $\chi = rR$

$$\Rightarrow \quad \chi'' + \frac{2M}{\hbar^2}\left[E - V_{eff}\right]\chi = 0$$

This is a <u>1-D</u> radial equation with effective potential:

$$V_{eff} = V(r) + \underbrace{\frac{\hbar^2 l(l+1)}{2M r^2}}$$

is called the "centrifugal potential".

In the limit $r \to 0$, if V goes to ∞ more slowly than $\frac{1}{r^2}$,

$$\Rightarrow \quad \chi'' \simeq \frac{l(l+1)}{r^2}\chi \qquad \text{for} \quad r \ll 1$$

$$\Rightarrow \quad \chi \simeq a_l\, r^{l+1} \qquad \text{or} \qquad R \to a_l\, r^l \quad \text{for small } r.$$

$l = 0, 1, 2, \cdots$ so R must be finite at the origin $\Rightarrow \chi(0) = 0$

☆ $\boxed{\text{The Virial theorem}}$

In C.M. say $V(r) = -\frac{a}{r^p}$

$$m r \omega^2 = \left|\frac{pa}{r^{p+1}}\right| \qquad \text{centrifugal force.}$$

$$\Rightarrow \quad T = \frac{1}{2} m r^2 \omega^2 = -\frac{p}{2} V$$

$$\Rightarrow \quad E = T + V \quad \Rightarrow \quad \begin{cases} T = -\frac{p}{2-p} E \\ V = \frac{2}{2-p} E \end{cases}$$

How about in QM?

Consider a bound state ψ with $E \leq 0$ in a central potential $V(r)$

Let A be any observable.

Since $H\psi = E\psi$, we have

$$\langle \psi | AH - HA | \psi \rangle = (E - E) \langle \psi | A | \psi \rangle = 0$$

Pick $A = \vec{r} \cdot \vec{p}$ & $H = \frac{p^2}{2m} + V(r)$ as usual

Then $[A, H] = [A, \frac{p^2}{2m}] + [A, V(r)]$

$$[\vec{r}\cdot\vec{p}, \frac{p^2}{2m}] = \frac{1}{2m}[x_i p_i, p_j p_j]$$

$$= \frac{1}{2m}(x_i p_i p_j p_j - p_j p_j x_i p_i)$$

$$= \frac{1}{2m}(x_i p_j p_j p_i - p_j p_j x_i p_i) = \frac{i\hbar}{m} p^2 = 2i\hbar T$$

$$\{-p_j x_i p_j p_i + p_j x_i p_j p_i\}$$

and $[\vec{r}\cdot\vec{p}, V(r)] = -i\hbar r \frac{\partial V}{\partial r}$

Therefore, we have

$$\langle 2T \rangle = \langle r \frac{\partial V}{\partial r} \rangle$$

If $V = \frac{-a}{r^p}$, $r\frac{\partial V}{\partial r} = -pV$

$\Rightarrow \quad \langle T \rangle + \frac{p}{2}\langle V \rangle = 0$ same as the CM case.

$$\Rightarrow \begin{cases} \langle T \rangle = -\frac{p}{2-p} E \\ \langle V \rangle = \frac{2}{2-p} E \end{cases}$$

for Coulomb potential $p = 1$

$\Rightarrow \langle T \rangle = -E$

& $\langle V \rangle = 2E$

Free particle

For a free particle, $V=0$ and $E>0$.
The corresponding Schrödinger Eq is

$$R'' + \frac{2}{r}R' + \frac{2\mu}{\hbar^2}\left[E - \frac{\hbar^2 \ell(\ell+1)}{2\mu r^2}\right]R = 0$$

$m_1 = m$, $m_2 = \infty$, $\Rightarrow \mu = m_1 = m$

With change of variable $\rho = \underbrace{\sqrt{\frac{2mE}{\hbar^2}}}_{\equiv k}\, r$, the above Eq becomes

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

This second order differential eq has two independent solutions.

The one which is regular at $\rho=0$ is

$$R_\ell(\rho) = \sqrt{\frac{\pi}{2\rho}}\, \underbrace{J_{\ell+\frac{1}{2}}}(\rho) \equiv j_\ell(\rho)$$

Bessel Function of order $(\ell+\frac{1}{2})$.

& $j_\ell(\rho) = j_\ell(kr)$ is the corresponding spherical Bessel function.

The first few spherical Bessel functions are.

$\ell=0$: $\quad j_0(kr) = \frac{\sin kr}{kr}$

$\ell=1$: $\quad j_1(kr) = \frac{\sin kr}{(kr)^2} - \frac{\cos kr}{kr}$

$\ell=2$: $\quad j_2(kr) = \left[\frac{3}{(kr)^3} - \frac{1}{(kr)}\right]\sin kr - \frac{3}{(kr)^2}\cos kr$

Useful properties:

$$\lim_{\rho\to 0} j_\ell(\rho) \simeq \frac{\rho^\ell}{(2\ell+1)!}$$

$$\lim_{\rho\to\infty} j_\ell(\rho) \simeq \frac{\sin(\rho - \frac{\ell\pi}{2})}{\rho}$$

~~A~~ A beautiful trick to solve the spherical Bessel function.

again, let $\chi_\ell = \rho R_\ell$

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

$$\Rightarrow \left(\frac{\chi}{\rho}\right)'' + \frac{2}{\rho}\left(\frac{\chi}{\rho}\right)' + \left[1 - \frac{\ell(\ell+1)}{\rho^2}\right]\frac{\chi}{\rho} = 0$$

$$+\left(\cancel{2\frac{\chi}{\rho^3}} - \cancel{\frac{2\chi'}{\rho^2}} + \frac{\chi''}{\rho}\right) + \frac{2}{\rho}\left(-\cancel{\frac{\chi}{\rho^2}} + \cancel{\frac{\chi'}{\rho}}\right) + \left[1 - \frac{\ell(\ell+1)}{\rho^2}\right]\frac{\chi}{\rho} = 0$$

$$\Rightarrow \qquad \left(-\frac{d^2}{d\rho^2} + \frac{\ell(\ell+1)}{\rho^2}\right]\chi_\ell(\rho) = \chi_\ell(\rho)$$

The LHS operator can be casted into a "SUSY" products

$$d_\ell = \frac{d}{d\rho} + \frac{\ell}{\rho}, \qquad d_\ell^+ = -\frac{d}{d\rho} + \frac{\ell}{\rho}$$

(lowering/annihilation) (raising/creation)

$$d_\ell^+ d_\ell = -\frac{d^2}{d\rho^2} + \frac{\ell}{\rho^2} + \frac{\ell^2}{\rho^2} = -\frac{d^2}{d\rho^2} + \frac{\ell(\ell+1)}{\rho^2}$$

$$d_\ell d_\ell^+ = -\frac{d^2}{d\rho^2} - \frac{\ell}{\rho^2} + \frac{\ell^2}{\rho^2} = -\frac{d^2}{d\rho^2} + \frac{\ell(\ell-1)}{\rho^2} = d_{\ell-1}^+ d_{\ell-1}$$

The original diff Eq can be expressed as

$$\Rightarrow \quad d_\ell^+ d_\ell \chi_\ell(\rho) = \chi_\ell(\rho)$$

$$\Rightarrow \quad d_\ell(d_\ell^+ d_\ell)\chi_\ell(\rho) = d_\ell \chi_\ell(\rho) \quad \text{(apply } d_\ell \text{ on both side)}$$

$$\Rightarrow \quad (d_{\ell-1}^+ d_{\ell-1})\, \underline{d_\ell \chi_\ell(\rho)} = \underline{d_\ell \chi_\ell(\rho)}$$

Which means that $\chi_{\ell-1}(\rho) \sim d_\ell \chi_\ell(\rho)$

and similarly you can get $\chi_\ell(\rho) \sim d_\ell^+ \chi_{\ell-1}(\rho)$

$\left(\text{from } \quad d_\ell d_\ell^+ \chi_{\ell-1}(\rho) = \chi_{\ell-1}(\rho)\right)$

so $\quad d_\ell^+ \rho j_{\ell-1}(\rho) = \rho j_\ell(\rho)$

Starting from $\ell = 0$,

$$-\frac{d^2}{d\rho^2}\chi_0(\rho) = \chi_0(\rho).$$

also, $\chi_0(0) = 0 \Rightarrow \chi_0 = \rho j_0(\rho) = \sin\rho$

and rewrite the creation/raising operator as

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

Then we have

$$\rho j_\ell(\rho) = \left(d_\ell^+ \cdot d_{\ell-1}^+ \cdots d_2^+ d_1^+\right)\sin\rho$$

$$= (-1)^\ell \left[\rho^\ell \frac{d}{d\rho}\left(\frac{1}{\rho^\ell}\right)\right]\left[\rho^{\ell-1}\frac{d}{d\rho}\left(\frac{1}{\rho^{\ell-1}}\right)\right]\cdots \underbrace{\left[\rho^2\frac{d}{d\rho}\left(\frac{1}{\rho^2}\right)\right]\left[\rho\frac{d}{d\rho}\left(\frac{1}{\rho}\right)\right]\sin\rho}$$

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

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

or

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

let's check.

$$j_1(\rho) = (-\rho)\left(\frac{1}{\rho}\frac{d}{d\rho}\right)\left(\frac{\sin\rho}{\rho}\right) = -\frac{d}{d\rho}\frac{\sin\rho}{\rho}$$

$$= \frac{\sin\rho}{\rho^2} - \frac{\cos\rho}{\rho}$$

&

$$j_2(\rho) = (-\rho)^2\left(\frac{1}{\rho}\frac{d}{d\rho}\right)\left(-\frac{\sin\rho}{\rho^3} + \frac{\cos\rho}{\rho^2}\right) = +\rho\frac{d}{d\rho}\left(-\frac{\sin\rho}{\rho^3} + \frac{\cos\rho}{\rho^2}\right)$$

$$= \rho\left[\frac{3\sin\rho}{\rho^4} - \frac{\cos\rho}{\rho^3} - \frac{2\cos\rho}{\rho^3} - \frac{\sin\rho}{\rho^2}\right]$$

$$= \left(\frac{3}{\rho^3} - \frac{1}{\rho}\right)\sin\rho - \frac{3\cos\rho}{\rho^2}$$

\#

You should get the following relation by yourself.

$$j_\ell' + \frac{\ell+1}{\rho} j_\ell = j_{\ell-1}$$

$$-j_\ell' + \frac{\ell}{\rho} j_\ell = j_{\ell+1}$$

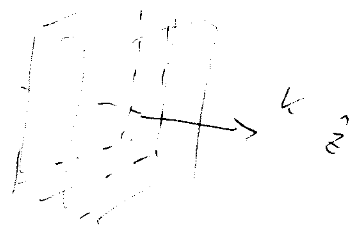
and

$$j_\ell' = \frac{\ell}{2\ell+1} j_{\ell-1} - \frac{\ell+1}{2\ell+1} j_{\ell+1}$$

HW 1

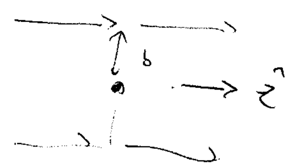
☆ $\boxed{\text{Plane wave decomposition}}$

pick the $\vec{k} = k\hat{z}$. then the plane wave should be decomposed into



$$e^{i\vec{k}\cdot\vec{r}} = e^{ikr\cos\theta}$$

$$= \sum_{\ell=0}^{\infty} a_\ell\, j_\ell(kr) \underbrace{P_\ell(\cos\theta)}_{\langle \ell, m=0\rangle}$$



in CM.
$|\vec{L}| = mvb$
no z-comp

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

Our task is to determine the unknown coefficient a_ℓ

lets look at the small ρ behavior of the spherical bessel function

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

$$\sin\rho = \frac{\rho}{1!} - \frac{\rho^3}{3!} + \frac{\rho^5}{5!} + \cdots = \sum_{n=0}^{\infty} \frac{(-)^n \rho^{2n+1}}{(2n+1)!}$$

$$= (-\rho)^\ell \left(\frac{1}{\rho}\frac{d}{d\rho}\right)^\ell \sum_{n=0}^{\infty} \frac{\rho^{2n}(-)^n}{(2n+1)!}$$

$$x = \rho^2 \qquad dx = 2\rho\, d\rho \qquad \frac{d}{dx} = \frac{d\rho}{dx}\frac{d}{d\rho} = \frac{1}{2\rho}\frac{d}{d\rho}$$

$$= (-\rho)^\ell \left(\frac{2d}{dx}\right)^\ell \sum_{n=0}^{\infty} \frac{(-x)^n}{(2n+1)!}$$

$$\rho \to 0 \quad \sim (+2\rho)^\ell \frac{\ell!}{(2\ell+1)!} + O(\rho^{\ell+1}) \simeq \frac{2^\ell \ell!\, \rho^\ell}{(2\ell+1)!} + \cdots$$

Also, we know the Legendre polynomial

$$P_\ell(x) = \frac{1}{2^\ell \ell!}\frac{d^\ell}{dx^\ell}(x^2-1)^\ell \sim \frac{1}{2^\ell \ell!}\frac{(2\ell)!}{\ell!}\underbrace{x^\ell + \cdots}_{\left[x^\ell - \frac{\ell(\ell+1)}{2(2\ell+1)!}x^{\ell-2} + \cdots\right]}$$

Therefore $\sum_{\ell=0}^{\infty} a_\ell j_\ell(kr) P_\ell(\cos\theta)$

$$\sim \sum_{\ell=0}^{\infty} \frac{a_\ell}{\ell!(2\ell+1)}(kr\cos\theta)^\ell \quad \Leftarrow \text{collect both the } \rho^\ell \text{ and } x^\ell$$

This is to match $e^{ikr\cos\theta} \sim 1 + ikr\cos\theta + \frac{(i)^2}{2!}(kr\cos\theta)^2 + \cdots$

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

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

☆ or take $\theta = 0$, $\quad e^{i\rho} = \sum_\ell a_\ell j_\ell(\rho)$

$$\sum_{\ell=0}^{\infty} a_\ell \left(\frac{2^\ell \ell! \rho^\ell}{(2\ell+1)!} + O(\rho^{\ell+1})\right)\left[\frac{(2\ell)!}{2^\ell(\ell!)^2}\left(x^\ell - \frac{\ell(\ell+1)}{2(2\ell+1)!}x^{\ell-2} + \cdots\right)\right]$$

for a given ℓ, $(\ell<n)$, the highest power of x is $\ell(<n)$,

ℓ, $(\ell>n)$, the lowest power of ρ is $\ell(>n)$

Therefore in the power series of $e^{i\rho x}$, only $\ell = n$ contributes.

☆ Also, by applying $P_\ell(\cos\theta) = \frac{4\pi}{2\ell+1}\sum_{m=-\ell}^{\ell} Y_\ell^{m*}(\hat{k}) Y_\ell^m(\hat{r})$, where θ is the angle between $\hat{k}$ & $\hat{r}$

$$\Rightarrow \boxed{e^{i\vec{k}\cdot\vec{r}} = 4\pi \sum_{\ell=0}^{\infty} i^\ell j_\ell(\vec{k}\cdot\vec{r}) Y_\ell^{m*}(\hat{k}) Y_\ell^m(\hat{r})}$$