Adwait Naravane QM-2 Endsem
19MS151 PH3102

Q1)

a) Observables are represented by Hermitian operators as Hermiltian operators have real eigenvalues. Any observable measurement which represents a physical measurement is naturally represented by real numbers.

b). 1-D free particle

$\hat{H} = \frac{\hat{p}^2}{2m}$.

Schrodinger's equation.

$-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\psi(x) = E\psi(x)$.

take $\psi_p(x) = e^{ip\cdot x/\hbar}$. , ($e^{-ip\cdot x/\hbar}$ is same)

$\Rightarrow -\frac{\hbar^2}{2m}\left(-\frac{p^2}{\hbar^2}\right)e^{ip\cdot x/\hbar} = E_p e^{ip\cdot x/\hbar}$.

$\Rightarrow E_p = \frac{p^2}{2m}$ is eigenvalue.

$\psi(x) \to \psi(-x)$. does not change the equation.

$\frac{\partial}{\partial x^2}e^{ip\cdot x/\hbar} = -\frac{p^2}{\hbar^2}e^{ip\cdot x/\hbar}$, $\frac{\partial}{\partial x^2}e^{-ip\cdot x/\hbar} = -\frac{p^2}{\hbar^2}e^{-ip\cdot x/\hbar}$.

where $e^{\mp ip\cdot x/\hbar}$ get cancelled.

$\therefore$ ~~as~~ $\therefore$ Π is parity.

$\Rightarrow \Pi\psi(x) = \psi(-x)$.

$\Rightarrow \Pi(c\psi(x) + c\psi(-x)) = c(\psi(x) + \psi(-x).)$

& $\Pi(c\psi(x) - c\psi(-x)) = -c(\psi(x) - \psi(-x))$

has 2 ~~eigenvalues with~~ eigenstates with eigenvalue 1 & -1.

$\Pi^2 = \mathbb{1}$

$\therefore$ has symmetric & antisymmetric eigenstates.,

$$\psi(x) + \psi(-x) = e^{ip\cdot x/\hbar} + e^{-ip\cdot x/\hbar} \propto \cos\left(\frac{px}{\hbar}\right)$$

$$\psi(x) - \psi(-x) = e^{-ip\cdot x/\hbar} - e^{-ip\cdot x/\hbar} \propto \sin\left(\frac{px}{\hbar}\right)$$

are eigenstates

c) Mixed state.

$\rho_1 = |\uparrow\rangle\langle\uparrow|$, $\rho_2 = |\downarrow\rangle\langle\downarrow|$.

$\Rightarrow \rho_{total} = \frac{3}{5}\rho_1 + \frac{2}{5}\rho_2$.

$$= \begin{pmatrix} 3/5 & 0 \\ 0 & 0 \end{pmatrix} + \begin{pmatrix} 0 & 0 \\ 0 & 2/5 \end{pmatrix}$$

$$\rho_{total} = \begin{pmatrix} 3/5 & 0 \\ 0 & 2/5 \end{pmatrix}.$$

Cannot be represented by wavefunction

$$tr(\rho^2) = \frac{13}{25} \neq 1$$

$$S_x = \frac{\hbar}{2}\sigma_x = \frac{\hbar}{2}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$

$$\langle S_x \rangle = tr(\rho S_x) = tr\left(\begin{pmatrix} 3/5 & 0 \\ 0 & 2/5 \end{pmatrix}\begin{pmatrix} 0 & \hbar/2 \\ \hbar/2 & 0 \end{pmatrix}\right)$$

$$= tr\left(\begin{pmatrix} 0 & 3\hbar/10 \\ 2\hbar/10 & 0 \end{pmatrix}\right) = \underline{\underline{0}}.$$

d) $\psi(x) = \sqrt{\frac{2}{L}} \sin\left(\frac{\pi x}{L}\right)$.

$\rho = |\psi\rangle\langle\psi| = \langle x|\rho|x'\rangle = \langle x|\psi\rangle\langle\psi|x'\rangle$

$\rho(x, x') = \frac{2}{L} \cdot \sin\left(\frac{\pi x}{L}\right) \sin\left(\frac{\pi x'}{L}\right)$.

$\langle x\rangle = tr(\rho x) = \cancel{\int_{-\infty}^{\infty} dx \cdot \frac{2}{L} \sin\left(\frac{\pi x}{L}\right) \sin\left(\frac{\pi x'}{L}\right) x\, dx}$

$= \int_{-\infty}^{\infty} dx \cdot \rho(x, x) \cdot x = \int_{-\infty}^{\infty} dx \, \frac{2}{L} \sin^2\left(\frac{\pi x}{L}\right) x$. (only diagonal terms)

$= \frac{2}{L} \int_{0}^{L} x \sin^2\left(\frac{\pi x}{L}\right) dx = \frac{L}{2}$.

-- integrate by parts.

$\langle p\rangle = tr(\rho p)$ $\quad \cancel{\rho p = |\psi\rangle\langle\psi| \hat{p}}$

$= \cancel{\int dx}$

$= \int dx \cdot \frac{\hbar}{i} \left.\frac{\partial}{\partial x'} \rho(x', x)\right|_{x=x'}$

$= \frac{\hbar}{i} \int_0^L dx \cdot \frac{2}{L} \cdot \frac{\pi}{L} \cdot \sin\left(\frac{\pi x}{L}\right) \cos\left(\frac{\pi x}{L}\right)$

$= \frac{2\pi\hbar}{L^2 i} \int_0^L dx \cdot \sin\left(\frac{\pi x}{L}\right) \cos\left(\frac{\pi x}{L}\right)$

$\langle p\rangle = 0$.

e). Translation operator

$$\psi(x) \longrightarrow \psi(x+a).$$

$$\psi(x+dx) = \cancel{\psi(x) + \frac{i x \cdot p}{\hbar} \psi(x)}$$

$$= \psi(x) + \left(\frac{d}{dx}\psi(x)\right) dx$$ — (assume small dx to first order)

$$\hat{p} = \frac{\hbar}{i}\frac{d}{dx} \Rightarrow \frac{d}{dx} \rightarrow \frac{ip}{\hbar}.$$

$$\psi(x+dx) = \psi(x) \cancel{+} - \frac{i\, dx \cdot p}{\hbar}\psi(x)$$

$$\Rightarrow \psi(x+dx) = \left(1 - \frac{i\,dx \cdot p}{\hbar}\right)\psi(x)$$

$$\Rightarrow T_{dx}(\psi(x)) = \left(1 - \frac{i\,dx\cdot p}{\hbar}\right)$$

let $dx = \frac{x'}{N}$

$$T(dx)^N \cancel{=} T(x') = \lim_{N\to\infty}\left[\left(1 - \frac{i x' p}{N\hbar}\right)^N\right]$$ (repeated products)

$$\Rightarrow T(x') = e^{-\frac{i x' \cdot p}{\hbar}}$$

is the translation operator.

$$\hat{p} = i\hbar \cdot \frac{\partial}{\partial x}\hat{T}(x')$$

Q3

$L^2|l,m\rangle = \hbar^2 l(l+1)|l,m\rangle$.

$L_z|l,m\rangle = \hbar m|l,m\rangle$.

$L_x^2+L_y^2+L_z^2 = L^2$

$L_+ = L_x + iL_y$. $L_- = L_x - iL_y$.

$L_+L_- = L_x^2+L_y^2 - i[L_x,L_y]$

$= L_x^2+L_y^2 + \hbar L_z$.

$L_-L_+ = L_x^2+L_y^2 - \hbar L_z = L^2 - \hbar L_z - L_z^2$

$L^2 = L_+L_- + L_z^2 - \hbar L_z$.

two identities

Now

$L_+|l,m\rangle = C_+\hbar|l,m+1\rangle$.

$L_-|l,m\rangle = C_-\hbar|l,m-1\rangle$

$\langle l,m|L_-L_+|l,m\rangle = \cancel{C_+}\, C_+^* C_+ \hbar^2 \langle l,m+1|l,m+1\rangle$.

$\langle l,m|L^2-L_z^2-\hbar L_z|l,m\rangle$

$= (l(l+1)-m(m+1))\hbar^2 \langle l,m|l,m\rangle$.

$\Rightarrow C_+ = \sqrt{l(l+1) - m(m+1)}$

Similarly with $\langle l,m|L_+L_-|l,m\rangle = |C_-|^2\langle l,m-1|l,m-1\rangle$

$\Rightarrow C_- = \sqrt{l(l+1)-m(m-1)}$ from second identity

a). $\cancel{L_+}$

$L_\pm|l,m\rangle = \sqrt{l(l+1)-m(m\pm1)}\,|l,m\pm1\rangle$.

$L_x = \frac{L_+ + L_-}{2}$

$L_x|l,m\rangle = \frac{1}{2}(L_+|l,m\rangle + L_-|l,m\rangle)$

$= \frac{1}{2}(\sqrt{l(l+1)-m(m+1)}\,|l,m+1\rangle + \sqrt{l(l+1)-m(m-1)}\,|l,m-1\rangle)$.

b) $\langle l,m|L_x|l,m\rangle = 0$.

$\cancel{L_x^2}$ $\cancel{L_+}$

$\langle l,m|L_x = \frac{1}{2}(\langle l,m|L_+ + \langle l,m|L_-)$

$= \frac{1}{2}(\langle l,m-1|\sqrt{l(l+1)-m(m-1)}$

$+ \langle l,m+1|\sqrt{l(l+1)-m(m+1)})$

-- [conjugate transpose $(L_+ = L_-^\dagger)$.]

$\langle lm | L_x^2 | l, m \rangle$

$= \frac{1}{4}\left(l(l+1) - m(m-1) + l(l+1) - m(m+1) \right)$

$= \frac{1}{4}\left(2l^2 + 2l - m^2 + \cancel{m} - m^2 - \cancel{m}\right)$

$= \frac{1}{4}\left(2l^2 + 2l - 2m^2\right)$

$= \frac{1}{2}\left(l^2 - m^2 + l\right)$

$L_x |l, m\rangle = \frac{1}{2}\left(\sqrt{l(l+1) - m(m+1)}\, |l, m+1\rangle + \sqrt{l(l+1) - m(m-1)}\, |l, m-1\rangle\right)$

c). $l = 1$, $m = -1, 0, 1$ ... $(m', m = \{-1, 0, 1\})$

$\Rightarrow$ ~~$\langle l, m$~~ $\langle 1, m' | L_x | 1, m\rangle$

$= \frac{1}{2}\sqrt{2 - m(m+1)}\,\langle 1, m' | 1, m+1\rangle + \frac{1}{2}\sqrt{2 - m(m-1)}\,\langle 1, m' | 1, m-1\rangle$

$m = -1$, $m' = 0$. ... (Matrix elements)

$\Rightarrow L_{0,-1} = \frac{1}{\sqrt{2}}$

$m = 0$, $\underline{m' = 1 \text{ or } -1}$

$L_{1,0} = \frac{1}{\sqrt{2}}$.

$\Rightarrow L_{-1,0} = \frac{1}{\sqrt{2}}$,

& $m = 1$, $m' = 0$ (L_x is Hermitian)

$\Rightarrow L_{0,1} = \frac{1}{\sqrt{2}}$

$$L_x = \frac{\hbar}{\sqrt{2}} \begin{array}{c|c} \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix} & \begin{array}{c} 1 \\ 0 \\ -1 \end{array} \\ \hline \begin{array}{ccc} -1 & 0 & 1 \end{array} & \end{array}$$

d) $\hat{H} = \frac{1}{I_1}(L_x^2 + L_y^2) + \frac{1}{I_2} L_z^2.$

$= \frac{1}{I_1}(L^2 - L_z^2) + \frac{1}{I_2} L_z^2$

$= \frac{L^2}{I_1} + \left(\frac{1}{I_2} - \frac{1}{I_1}\right) L_z^2$ $|l,m\rangle$ would be eigenstate.

$\hat{H}|l,m\rangle = \frac{L^2}{I_1}|l,m\rangle + L_z^2\left(\frac{1}{I_2} - \frac{1}{I_1}\right)|l,m\rangle$

$= \frac{\hbar^2 l(l+1)}{I_1}|l,m\rangle + \left(\frac{1}{I_2} - \frac{1}{I_1}\right)\hbar^2 m^2 |l,m\rangle.$

Eigenvalues $\Rightarrow \frac{\hbar^2 l(l+1)}{I_1} + \left(\frac{1}{I_2} - \frac{1}{I_1}\right)\hbar^2 m^2$

$= \frac{1}{I_1}\left(\hbar^2(l(l+1) - m^2)\right) + \frac{1}{I_2}(\hbar^2 m^2)$

Scanned with CamScanner

4) a). $\left(-\frac{\hbar^2}{2m}\nabla^2 + V\right)\psi = E\psi$,

In radial coordinates.

$$-\frac{\hbar^2}{2m}\left(\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial\psi}{\partial r}\right) + \frac{1}{r^2\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial\psi}{\partial\theta}\right) + \frac{1}{r^2\sin^2\theta}\frac{\partial^2\psi}{\partial\phi^2}\right) = E\psi - V\psi.$$

Sep. variables,

$\psi(r,\theta,\phi) = R(r)\,Y(\theta,\phi)$.

$$-\frac{\hbar^2}{2m}\left(\frac{Y}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial R}{\partial r}\right) + \frac{R}{r^2\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial Y}{\partial\theta}\right) + \frac{R}{r^2\sin^2\theta}\frac{\partial^2 Y}{\partial\phi^2}\right) + VRY = ERY.$$

Divide by ψ.

$$\Rightarrow \left(\frac{1}{R}\frac{\partial}{\partial r}\left(r^2\frac{\partial R}{\partial r}\right) - \frac{2mr^2}{\hbar^2}(V-E)\right) \rightarrow l(l+1)$$

$$+ \underbrace{\frac{1}{Y}\left(\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial Y}{\partial\theta}\right) + \frac{1}{\sin^2\theta}\frac{\partial^2 Y}{\partial\phi^2}\right)}_{-l(l+1)} = 0.$$

-- constants

radial part for $V = -\frac{e^2}{r}$.

$$\Rightarrow \cancel{\frac{1}{R}\frac{\partial}{\partial r}}$$

$$\frac{1}{R}\frac{d}{dr}\left(r^2\frac{dR}{dr}\right) + \frac{2mr^2}{\hbar^2}\left(\frac{e^2}{r^2} + E\right) = l(l+1).$$

effective potential

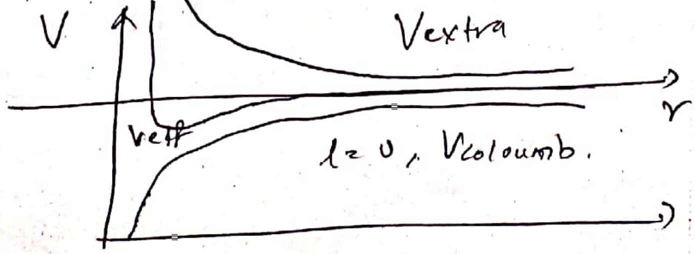
$$\boxed{V(r) = -\frac{e^2}{r^2} + \underbrace{\frac{\hbar^2}{2m}\frac{(l+1)l}{r^2}}_{\text{Centripetal term}}}$$

b) Feynman Hellmann lemma.

$$\frac{dE(\lambda)}{d\lambda} = \left\langle \frac{dH(\lambda)}{d\lambda} \right\rangle$$

$E_n = \frac{-2^2\hbar^2}{2ma_0^2 n^2}$, $H = \frac{p^2}{2m} - \frac{e^2}{r}$

$\lambda = e \Rightarrow \frac{1}{a_0^2} = \frac{m^2 e^4}{\hbar^4}$, $\frac{da_0^{-2}}{de} = \frac{4}{e}\frac{1}{a_0^2}$



$$\frac{dB}{de} = \frac{-Z\hbar^2}{mea_0 e n^2} \Rightarrow \left\langle \frac{dH}{de} \right\rangle = \left\langle -\frac{Ze}{r} \right\rangle$$

$$= -Ze\left\langle \frac{1}{r} \right\rangle.$$

$$\Rightarrow \left\langle \frac{1}{r} \right\rangle_{n,l} = \frac{\hbar^2}{me^2 a_0^2 n^2} = \frac{1}{a_0 n^2}$$

for $Z \neq 1$.

$$\left\langle \frac{1}{r} \right\rangle_{n,l} = \frac{Z}{a_0 n^2}$$

c). $\psi(r)$ for $r > a$, $\Rightarrow \psi(r) = 0$.

for $r \leq a$.

$$\frac{1}{R}\frac{d}{dr}\left(r^2 \frac{dR}{dr}\right) + \frac{2mr^2 E}{\hbar^2} = l(l+1).$$

$$V(r) = \begin{cases} 0 & r \leq a \\ \infty & r > a. \end{cases}$$

let $u = rR(r)$.

$$\Rightarrow \frac{r}{R}\frac{d^2u}{dr^2} + \frac{2mr^2E}{\hbar^2} = l(l+1).$$

$$\Rightarrow \frac{d^2u}{dr^2} = \left(\frac{l(l+1)}{r^2} - k^2\right)u(r).$$

where $k = \frac{\sqrt{2mE}}{\hbar}$.

$l = 0$ for ground state.

$$\Rightarrow u(r) = A\sin(kr) + B\cos(kr).$$

$$\Rightarrow R = A\frac{\sin(kr)}{r} + B\frac{\cos(kr)}{r} \to \infty \text{ at } r = 0.$$

$$\Rightarrow R = A\frac{\sin(kr)}{r}$$

$$R(a) = 0 \Rightarrow A\frac{\sin(ka)}{a} = 0$$

$$\Rightarrow ka = n\pi$$

or $E_{n,0} = \dfrac{n^2\pi^2\hbar^2}{2ma^2}$

for ground, $E_{10} = \dfrac{\pi^2\hbar^2}{2ma^2}$

Scanned with CamScanner

Q2

a). $\hat{H} = \frac{p^2}{2m} + V(x)$, $\hat{H}\psi = -\frac{\hbar}{i}\frac{\partial}{\partial t}\psi$.

$$\psi(x,t) = \int dp \frac{e^{ipx/\hbar}}{\sqrt{2\pi\hbar}} \cdot \phi(p,t).$$

$$i\hbar \cdot \frac{d}{dt}\left(\int dp \frac{e^{ipx/\hbar}}{\sqrt{2\pi\hbar}} \phi(p,t)\right)$$
$$= -\frac{\hbar^2}{2m} \cdot \frac{\partial^2}{\partial x^2}\int dp \frac{e^{\frac{ipx}{\hbar}}}{\sqrt{2\pi\hbar}} \phi(p,t)$$
$$+ V(x)\int \frac{dp}{\sqrt{2\pi\hbar}} e^{ipx/\hbar}\phi(p,t).$$

$$\phi(p,t) = \int \frac{dx}{\sqrt{2\pi\hbar}} e^{-ipx/\hbar}\psi(x,t).$$

$$V(x)\int dp \frac{e^{ipx/\hbar}}{\sqrt{2\pi\hbar}} \phi(p,t)$$
transform

$$\int dp \frac{e^{ipx/\hbar}}{\sqrt{2\pi\hbar}} \cdot \int dx' \frac{e^{-ipx/\hbar}}{\sqrt{2\pi\hbar}} \cdot V(x')\psi(x',t)$$

$$= \int dp \frac{e^{ipx/\hbar}}{\sqrt{2\pi\hbar}} V(p) * \phi(p,t).$$
convolution.

$$\Rightarrow \int \frac{dp\, e^{ipx/\hbar}}{\sqrt{2\pi\hbar}}\left(i\hbar\frac{\partial}{\partial t}\phi(p,t) = \frac{-\hbar^2}{2m}\left(-\frac{p^2}{\hbar^2}\phi(p,t)\right) + V(p) * \phi(p,t)\right)$$

$$\rightarrow i\hbar\frac{\partial}{\partial t}\phi(p,t) = \frac{p^2}{2m}\cdot\phi(p,t) + V(p) * \phi(p,t)$$

in momentum space.

Scanned with CamScanner

(b) $N(a^+)^n|0\rangle$ is eigenstate of $\hat{H}$ if,

$HN(a^+)^n|0\rangle = c\,N(a^+)^n|0\rangle$.

$HN(a^+)^n|0\rangle = N\hbar\omega(a^+a+\frac{1}{2})\,a^{+n}|0\rangle$.

$a^+a\,a^{+n}|0\rangle = (aa^+ - [a,a^+])\,a^{+n}|0\rangle$.

$\Rightarrow = a(a^+)^{n+1}|0\rangle - (a^+)^n|0\rangle$

$= aa^{+n}c|\phi\rangle - (a^+)^n|0\rangle$

as $[a,[a,a^+]] = 0$, $\Rightarrow [a,a^{+n}] = n(a^+)^{n-1}$

$\Rightarrow a^+a\,a^{+n}|0\rangle = (na^{+n-1} + a^{+n}a)c_1|\phi\rangle$.

$\cancel{+} - a^{+n}|0\rangle$.

$= \cancel{a}\,n\,a^{+n}a^+|0\rangle + (a^+)^n|0\rangle - a^{+n}\phi_0\rangle$

$= n\,a^+|0\rangle$.

$\Rightarrow NH(a^+)^n|0\rangle = N(\hbar\omega(n+\frac{1}{2}))\,a^{+n}|0\rangle$.

is an eigenstate

c) $a|0\rangle = 0$

$a = \sqrt{\frac{m\omega}{2\hbar}}\,x + i\frac{1}{\sqrt{2m\omega\hbar}}\,p$

$p = \frac{\hbar}{i}\frac{d}{dx}$

$a = \sqrt{\frac{m\omega}{2\hbar}}\,x + \sqrt{\frac{\hbar}{2m\omega}}\,\frac{d}{dx}$

let $x = \sqrt{\frac{\hbar}{m\omega}}\,y$.

$\Rightarrow a = \frac{1}{\sqrt{2}}(y + \frac{d}{dy})$.

$\frac{1}{\sqrt{2}}(y + \frac{d}{dy})\,\psi_0(y) = 0$

$\Rightarrow \frac{d\psi_0(y)}{\psi_0(y)} = -y\,dy$

Scanned with CamScanner

a) $\psi_0(y) = A_0 e^{-y^2/2}$

$\psi_0(x) = A_0 e^{-m\omega x^2/2\hbar}$

A_0 can be found from normalisation

$\psi_0(x) = \left(\frac{m\omega}{2\hbar}\right)^{1/4} e^{-m\omega x^2/2\hbar}$