

Problem 1

Problem Set 2

$$e^{iA} = \sum_{j=0}^{\infty} \frac{1}{j!} (iA)^j \quad \begin{array}{l} \text{+ For } A = VDV^T, \quad A^2 = \underbrace{VDV^TVDV^T}_{=I} = VD^2V^T \\ \text{+ then } A^j = VD^jV^T, \quad \text{so} \end{array}$$

$$= V \left[\sum_{j=0}^{\infty} \frac{1}{j!} (iD)^j \right] V^T = V e^{iD} V^T$$

$\begin{pmatrix} e^{ix_1} & & \\ & e^{ix_2} & \\ & & e^{ix_n} \end{pmatrix}$

Then for $U = e^{iA} = V e^{iD} V^T$, we have

$$U^T = (V e^{iD} V^T)^T = V e^{-iD} V^T = V \left[\sum_{j=0}^{\infty} \frac{1}{j!} (-iD)^j \right] V^T = e^{-iA}$$

$\begin{pmatrix} e^{-ix_1} & & \\ & e^{-ix_2} & \\ & & e^{-ix_n} \end{pmatrix}$

$$\text{and } U^T U = V e^{-iD} V^T V e^{iD} V^T = V \underbrace{e^{-iD} e^{iD}}_{=I} V^T = V V^T = I$$

Problem 2

The eigenvalue problem for L_2 : $L_2 V = V D$ has: $D = \begin{pmatrix} i & 0 & 0 \\ 0 & -i & 0 \\ 0 & 0 & 0 \end{pmatrix}$

so $V = \begin{pmatrix} i & -i & 0 \\ 1 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$, then $L_2 = V D V^{-1}$ and $V^{-1} = \begin{pmatrix} -i/2 & 1/2 & 0 \\ i/2 & 1/2 & 0 \\ 0 & 0 & 1 \end{pmatrix}$

As in the first problem, we have: $L_2^j = V D^j V^{-1}$, so that

$$e^{\theta L_2} = \sum_{j=0}^{\infty} \frac{(\theta L_2)^j}{j!} = V \left[\sum_{j=0}^{\infty} \frac{1}{j!} (\theta D)^j \right] V^{-1} = V e^{\theta D} V^{-1}$$

$$\text{so } e^{\theta D} = \begin{pmatrix} e^{i\theta} & 0 & 0 \\ 0 & e^{-i\theta} & 0 \\ 0 & 0 & 1 \end{pmatrix}, \quad \text{so } e^{\theta L_2} = V e^{\theta D} V^{-1} = \begin{pmatrix} \cos \theta & -\sin \theta & 0 \\ \sin \theta & \cos \theta & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

Problem 3

a.
$$-\frac{\hbar^2}{2m} \nabla^2 \psi + U\psi = i\hbar \frac{\partial \psi}{\partial t} \Rightarrow \frac{\partial \psi}{\partial t} = \frac{1}{i\hbar} \left[-\frac{\hbar^2}{2m} \nabla^2 \psi + U\psi \right] +$$

$$\frac{\partial \psi^*}{\partial t} = -\frac{1}{i\hbar} \left[-\frac{\hbar^2}{2m} \nabla^2 \psi^* + U\psi^* \right]$$

Now,
$$\frac{d}{dt} \int_{\Omega} \psi^* \psi d\tau = \int_{\Omega} \left[\frac{\partial \psi^*}{\partial t} \psi + \psi^* \frac{\partial \psi}{\partial t} \right] d\tau$$

$$= \int_{\Omega} \left\{ -\frac{1}{i\hbar} \left[-\frac{\hbar^2}{2m} \nabla^2 \psi^* \psi + U\psi^* \psi \right] + \frac{1}{i\hbar} \left[-\frac{\hbar^2}{2m} \nabla^2 \psi \psi^* + U\psi \psi^* \right] \right\} d\tau$$

$$= \frac{1}{i\hbar} \int_{\Omega} \left[\frac{\hbar^2}{2m} \nabla^2 \psi^* \psi - \frac{\hbar^2}{2m} \nabla^2 \psi \psi^* \right] d\tau \quad (*)$$

Note that $\int_{\Omega} \nabla \cdot (\nabla \psi^* \psi) d\tau = \oint_{\partial \Omega} (\nabla \psi^* \cdot \psi) \cdot d\vec{a}$ by the div. thm.
 (product rule)

$$\int_{\Omega} \left[\nabla^2 \psi^* \psi + \nabla \psi^* \cdot \nabla \psi \right] d\tau = \int_{\partial \Omega} [\nabla \psi^* \psi] \cdot d\vec{a}$$

then
$$\int_{\Omega} \nabla^2 \psi^* \psi d\tau = - \int_{\Omega} \nabla \psi^* \cdot \nabla \psi d\tau + \int_{\partial \Omega} [\nabla \psi^* \psi] \cdot d\vec{a}$$

o sm.
$$\int_{\Omega} \nabla^2 \psi \psi^* d\tau = - \int_{\Omega} \nabla \psi \cdot \nabla \psi^* d\tau + \int_{\partial \Omega} [\nabla \psi \psi^*] \cdot d\vec{a}$$

Using these back in (*),

$$\frac{d}{dt} \int_{\Omega} \psi^* \psi d\tau = \frac{\hbar}{i2m} \int_{\partial \Omega} [\psi \nabla \psi^* - \psi^* \nabla \psi] \cdot d\vec{a}$$

$$\text{so } \vec{J} = \frac{\hbar}{2mi} (\psi \nabla \psi^* - \psi^* \nabla \psi)$$

b. If Ω is all space, $-\int_{\partial \Omega} \vec{J} \cdot d\vec{a} = 0$ since $\psi \rightarrow 0$ as $r \rightarrow \infty$, where the integral is evaluated.

Problem 4

$$\text{For } \psi = R e^{iS}, \quad \frac{\partial \psi}{\partial t} = \dot{R} e^{iS} + iS \dot{R} e^{iS} = \left(\frac{\dot{R}}{R} + i\dot{S} \right) \psi$$

$$+ \nabla \psi = \nabla R e^{iS} + R e^{iS} i \nabla S \quad \nabla \psi^* = \nabla R e^{-iS} - R e^{-iS} i \nabla S$$

$$\begin{aligned} \nabla^2 \psi &= \nabla^2 R e^{iS} + i \nabla R \cdot \nabla S e^{iS} + i \nabla R \cdot \nabla S e^{iS} + i \nabla^2 S R e^{iS} - R \nabla S \cdot \nabla S e^{iS} \\ &= \left[\frac{\nabla^2 R}{R} + i \left(2 \frac{\nabla R \cdot \nabla S}{R} + \nabla^2 S \right) - \nabla S \cdot \nabla S \right] \psi \end{aligned}$$

then $-\frac{\hbar^2}{2m} \nabla^2 \psi + U \psi = i \hbar \frac{\partial \psi}{\partial t}$ becomes

$$-\frac{\hbar^2}{2m} \left[\frac{\nabla^2 R}{R} + i \left(2 \frac{\nabla R \cdot \nabla S}{R} + \nabla^2 S \right) - \nabla S \cdot \nabla S \right] \psi + U \psi = \left(\frac{i \hbar \dot{R}}{R} - \hbar \dot{S} \right) \psi$$

the real part of this eqn. is:

$$-\frac{\hbar^2}{2m} \left[\frac{\nabla^2 R}{R} - \nabla S \cdot \nabla S \right] + U = -\hbar \dot{S}$$

$$\text{w/ imaginary part: } -\frac{\hbar^2}{2m} \left[\frac{2 \nabla R \cdot \nabla S}{R} + \nabla^2 S \right] = \hbar \frac{\dot{R}}{R}$$

The probability density is: $\rho = \psi^* \psi = R^2$

$$\vec{J} = \hbar K [\psi \nabla \psi^* - \psi^* \nabla \psi]$$

$$= \hbar K [R e^{iS} (\nabla R e^{-iS} - R e^{-iS} i \nabla S) - R e^{-iS} (\nabla R e^{iS} + R e^{iS} i \nabla S)]$$

$$= \hbar K [R \nabla R - i R^2 \nabla S - R \nabla R - i R^2 \nabla S]$$

$$= -2i \hbar K R^2 \nabla S \quad \text{w/ } K = \frac{i \hbar}{2m}$$

$$\vec{J} = \frac{\hbar^2}{m} R^2 \nabla S$$

Problem 5

We have $\frac{dI}{dt} = \{I, H\}$ for functions I & H . The rule to get QM op. is

$$i\hbar \frac{d\hat{I}}{dt} = [\hat{I}, \hat{H}]$$

→ taking the expectation value of both sides,

$$\frac{d\langle \hat{I} \rangle}{dt} = \frac{1}{i\hbar} \langle [\hat{I}, \hat{H}] \rangle$$

Problem 6

Taking $\hat{I} = \vec{r}$, we need to compute: $[\vec{r}, \hat{H}]$ w/

$$\hat{H} = (\vec{p}^2 - q\vec{p} \cdot \vec{A} - q\vec{A} \cdot \vec{p} + q^2 A^2) \cdot \frac{1}{2m}$$

the first commutator is (take the x-component to get the pattern)

$$[x, \vec{p}^2 + p_y^2 + p_z^2] = [x, p_x^2] = x p_x A_x - p_x p_x x = (i\hbar + p_x x) p_x - p_x (x p_x - i\hbar) = 2i\hbar p_x$$

$$\text{o. sm. for } [y, p^2] = 2i\hbar p_y, [z, p^2] = 2i\hbar p_z$$

$$[x, p_x A_x + p_y A_y + p_z A_z] = [x, p_x A_x] = x p_x A_x - p_x A_x x = (p_x x + i\hbar) A_x - p_x x A_x = i\hbar A_x$$

$$\text{w/ } [y, \vec{p} \cdot \vec{A}] = i\hbar A_y + [z, \vec{p} \cdot \vec{A}] = i\hbar A_z$$

Then we have:

$$[x, A_x p_x + A_y p_y + A_z p_z] = [x, A_x p_x] = x A_x p_x - A_x p_x x = A_x x p_x - A_x (x p_x - i\hbar) = i\hbar A_x$$

$$\text{w/ } [y, \vec{A} \cdot \vec{p}] = i\hbar A_y, [z, \vec{A} \cdot \vec{p}] = i\hbar A_z$$

$$\begin{aligned} \text{Then: } [x, \hat{H}] &= \frac{1}{2m} ([x, p^2] - q[x, \vec{p} \cdot \vec{A}] - q[x, \vec{A} \cdot \vec{p}] + q^2 [x, A^2]) \\ &= \frac{1}{2m} (2i\hbar p_x - 2i\hbar q A_x) = i\hbar \frac{1}{m} (p_x - q A_x) \end{aligned}$$

$$\rightarrow [\vec{r}, \hat{H}] = i\hbar \frac{1}{m} (\vec{p} - q\vec{A})$$

$$\text{Ehrenfest's theorem says: } \frac{d\langle \vec{r} \rangle}{dt} = \frac{1}{i\hbar} \langle [\vec{r}, \hat{H}] \rangle$$

$$\frac{d\langle \vec{r} \rangle}{dt} = \frac{1}{m} \langle \vec{p} - q\vec{A} \rangle \checkmark$$