Prob. 5

a) $\langle \vec{r} | \hat{p} | \vec{p} \rangle = \vec{p} \langle \vec{r} | \vec{p} \rangle$

$$= \vec{p}\, e^{i \vec{p}\cdot\vec{r}/\hbar}$$

$$= \frac{\hbar}{i} \vec{\nabla} \langle \vec{r} | \vec{p} \rangle$$

b)

$$\langle \vec{r} | \vec{p} | \psi \rangle = \int \frac{d^3p}{(2\pi\hbar)^3} \langle \vec{r} | \hat{p} | p \rangle \langle p | \psi \rangle$$

$$= \int \frac{d^3p}{(2\pi\hbar)^3} \frac{\hbar}{i} \vec{\nabla} \langle r | p \rangle \langle p | \psi \rangle$$

$$= \frac{\hbar}{i} \vec{\nabla} \langle r | \psi \rangle = \frac{\hbar}{i} \vec{\nabla} \psi(\vec{r})$$

c)

$$\langle \psi | T | \psi \rangle = \frac{1}{2m} \langle \psi | \hat{p}^2 | \psi \rangle$$

$$= \frac{1}{2m} \int d^3r \, \langle \psi | r \rangle \langle r | \hat{p}^2 | \psi \rangle$$

$$= \frac{1}{2m} \int d^3r \, \langle \psi | r \rangle \left(-\hbar^2 \nabla^2 \right) \langle r | \psi \rangle$$

$$= \frac{1}{2m} \int d^3r \, \psi^*(r) \left(-\hbar^2 \nabla^2 \right) \psi(r)$$

Charge particles in a magnetic field

$$m\frac{d^2\vec{r}}{dt^2} = \frac{q}{c}\vec{v}\times\vec{B}$$ can be derived from

$$L = \frac{1}{2}m\vec{v}^2 + \frac{q}{c}\vec{v}\cdot\vec{A} \qquad \vec{\nabla}\times\vec{A} = \vec{B}$$

The Hamiltonian: $H = \sum_i p_i \dot{q}_i - L(q_i, \dot{q}_i)$ $\qquad v_i = \dot{q}_i$

$$\vec{p} = \frac{\partial L}{\partial \dot{q}_i} = \frac{\partial L}{\partial v_i}$$

$$H = \vec{p}\cdot\vec{v} - \frac{1}{2}m\vec{v}^2 - \frac{q}{c}\vec{v}\cdot\vec{A}$$

$$= (\vec{p} - \frac{q}{c}\vec{A})\cdot\vec{v} - \frac{1}{2}m\vec{v}^2$$

$$\vec{p} = m\vec{v} + \frac{q}{c}\vec{A}$$

$$m\vec{v} = (\vec{p} - \frac{q}{c}\vec{A})$$

$$= \frac{(p - \frac{q}{c}\vec{A})^2}{m} - \frac{1}{2}\cancel{m}\frac{(p-\frac{q}{c})^2}{m^{\cancel{2}}}$$

$$\boxed{H = \frac{1}{2m}(\vec{p} - \frac{q}{c}\vec{A})^2} \rightarrow \hat{H} = \frac{1}{2m}(\hat{p} - \frac{q}{c}\vec{A})^2$$

$$\hat{H} = \frac{1}{2m}\left(\frac{\hbar\vec{\nabla}}{i} - \frac{q}{c}\vec{A}\right)^2 = \frac{1}{2m}\left(\hat{p}^2 - \frac{q}{c}(\hat{p}\cdot\vec{A} + \vec{A}\cdot\hat{p}) + \frac{q^2}{c^2}A^2\right)$$

A better form of $\hat{H}$

$$\hat{H} = \frac{1}{2m}\left(\frac{\hbar}{i}\vec{\nabla} - \frac{q}{c}\vec{A}\right)^2$$

$$= -\frac{\hbar^2}{2m}\left(\vec{\nabla} - \frac{iq}{\hbar c}\vec{A}\right)^2$$

$$\left(\vec{\nabla} - \frac{iq}{\hbar c}\vec{A}\right)\psi = \left(e^{i\frac{q}{\hbar c}f}\,\vec{\nabla}\,e^{-i\frac{q}{\hbar c}f}\right)\psi$$

$$\left(\vec{\nabla} - \frac{iq}{\hbar c}\vec{A}\right)^2 \qquad = \left[-i\frac{q}{\hbar c}\vec{\nabla}f\,\psi + \vec{\nabla}\psi\right]$$

$$= e^{i\frac{q}{\hbar c}f}\nabla^2 e^{-i\frac{q}{\hbar c}f} \qquad = \left(\vec{\nabla} - i\frac{q}{\hbar c}\vec{\nabla}f\right)\psi \quad \text{if } \vec{\nabla}f = \vec{A}$$

The wave function with $\vec{A} \neq 0$. $\quad f(\vec{r}) = \int^{r}\vec{A}\cdot d\vec{r}$

$$i\hbar\frac{\partial}{\partial t}\psi = \frac{-\hbar^2}{2m}\left(\vec{\nabla} - \frac{iq}{\hbar c}\vec{A}\right)^2\psi$$

$$= e^{i\frac{q}{\hbar c}f}\left(-\frac{1}{2}\frac{\hbar^2}{m}\nabla^2\right)\underbrace{e^{-i\frac{q}{\hbar c}f}\psi}_{\psi_0}$$

$$i\hbar\frac{\partial}{\partial t}\psi_0 = -\frac{1}{2}\frac{\hbar^2}{m}\nabla^2\psi_0$$

$$\Rightarrow \qquad \psi = e^{i\frac{q}{\hbar c}f}\psi_0$$

↖ without a magnetic field

Potential Problems

Hermitian operator: the Hermitian adjoint $B^\dagger$ of B is defined by $B^\dagger = (B^T)^*$

$$\Rightarrow \quad B^\dagger_{ij} = B^*_{ji}$$

$$\langle \Phi | B^\dagger | \Psi \rangle = \left(\langle \Psi | B | \Phi \rangle \right)^*$$

An operator is Hermitian if $B^\dagger = B$

Since $\langle \Phi | \Psi \rangle^* = \langle \Psi | \Phi \rangle$

any $\hat{r}$ or $\hat{p}$ operators (fct of them) are hermitian

$$\left(\langle \Phi | \hat{r} | \Psi \rangle \right)^* = \langle \Psi | \hat{r} | \Phi \rangle$$

$$\int d^3\vec{r} \left(\Phi^* \hat{r} \Psi \right)^* = \int d^3\vec{r} \; \Phi \hat{r} \Psi^*$$

$$\langle \Phi | \hat{p} | \Psi \rangle^* = \int \frac{d^3p}{(2\pi\hbar)^3} \langle \Phi | \hat{p} | p \rangle \langle p | \Psi \rangle$$

$$= \int \frac{d^3p}{(2\pi\hbar)^3} \langle \Phi | p \rangle^* \, p \, \langle p | \Psi \rangle^*$$

$$\langle p | \Phi \rangle \, p \, \langle \Psi | p \rangle$$

$$= \langle \Psi | p \rangle p \langle p | \Phi \rangle$$

$$= \langle \Psi | \hat{p} | \Phi \rangle$$

Let $\langle O\Phi | = \left(O | \Phi \rangle \right)^\dagger$

$$= \langle \Phi | O^*$$

$$\langle O\Phi | \Psi \rangle = \langle \Phi | O^* | \Psi \rangle = \langle \Psi | O | \Phi \rangle^* = \langle \Phi | O | \Psi \rangle$$

Since $\boxed{\langle O\psi|\phi\rangle = \langle\psi|O|\phi\rangle}$!

This shows that $\vec{r}$, $\vec{p}$ are Hermitian

but $r_i p_i \neq$ Hermitian

$$\langle\psi| r_i p_i |\phi\rangle = \langle r_i \psi | p_i |\phi\rangle$$
$$= \langle p_i r_i \psi | \phi\rangle$$

To make this hermitian take $\frac{1}{2}(r_i p_i + p_i r_i)$

Important results :

1) Eigenvalues of Hermitian operators are real.

$$B|b\rangle = b|b\rangle \qquad \langle b|b\rangle = 1$$

$$\langle b|B|b\rangle = b$$

$$\langle b|B|b\rangle^* = b^* \qquad b = b^*$$

$$\langle b|B^\dagger|b\rangle = b^*$$

2) Eigenvectors of an H O are orthonormal

$$\langle b_2|B|b_1\rangle = \langle b_2|b_1\rangle\, b_1$$

$$= \langle b_2|b_1\rangle\, b_2$$

$$0 = \langle b_2|b_1\rangle(b_1 - b_2) = 0$$

if $b_1 \neq b_2$ $\langle b_2|b_1\rangle = 0$

Let $\hat{H} = \frac{\hat{p}^2}{2m} + V(\vec{r})$ has explicit time-dependence

Let $|E\rangle$ = eigenvector of $\hat{H}$ with eigenvalue E

Since for any $|\psi(t)\rangle = e^{-i\frac{t}{\hbar}\hat{H}}|\psi(0)\rangle$

$$\langle E|\psi(t)\rangle = \langle E|e^{-i\frac{t}{\hbar}\hat{H}}|\psi(0)\rangle$$
$$= e^{-i\frac{tE}{\hbar}}\langle E|\psi(0)\rangle$$

Energy eigenstates are stationary states

$$|E,t\rangle = e^{-i\frac{t\hat{H}}{\hbar}}|E\rangle = e^{-i\frac{tE}{\hbar}}|E\rangle$$

$$\langle E,t|\hat{O}|E,t\rangle = \langle E|e^{i\frac{tE}{\hbar}}\hat{O}\,e^{-i\frac{tE}{\hbar}}|E\rangle$$
$$= \langle E|\hat{O}|E\rangle$$

The expectation of any $\hat{O}$ in an energy eigenstate is unchanged in time.

Moreover, for any $|\psi\rangle$, its time evolution is known in terms of $|E\rangle$

$$\langle\vec{r}|\psi(t)\rangle = \sum_E \langle\vec{r}|E\rangle\langle E|e^{-i\frac{t}{\hbar}\hat{H}}|\psi(0)\rangle$$
$$= \sum_E e^{-i\frac{t}{\hbar}E}\langle\vec{r}|E\rangle\underbrace{\langle E|\psi(0)\rangle}_{c_E}$$
$$\psi(r,t) = \sum_E c_E\, e^{-i\frac{tE}{\hbar}}\psi_E(r)$$

Let $ti = \tau$ imaginary time

$$\psi(r,\tau) = c_{E_0}e^{-\frac{\tau E}{\hbar}}\psi_{E_0}(r) + c_{E_1}e^{-\frac{\tau E_1}{\hbar}}\psi_{E_1}(r)$$

$\tau \to \infty$

imaginary time method of extracting $\psi_{E_0}(r)$.

$$e^{-i\frac{t\hat{H}}{\hbar}} \to e^{-\frac{\tau\hat{H}}{\hbar}}$$
$$\to e^{-\beta\hat{H}} = e^{-\frac{1}{kT}\hat{H}}$$