

Quantum Physics III (8.06) Spring 2006 Solution Set 3

February 27, 2006

1. Classical motion in a Magnetic Field (10 points)

(a) **(5 points)** The Hamiltonian of the particle in the magnetic field is given by

$$\mathcal{H}(\vec{x}, \vec{p}) = \frac{1}{2m} \left(\vec{p} - \frac{q}{c} \vec{A} \right)^2 + q\phi.$$

The first Hamilton's equation is

$$\dot{\vec{x}} = \frac{\partial \mathcal{H}}{\partial \vec{p}} = \frac{1}{m} \left(\vec{p} - \frac{q}{c} \vec{A} \right)$$

and therefore

$$\vec{p} = m\vec{v} + \frac{q}{c} \vec{A} \tag{1}$$

where $v \equiv \dot{x}$. The second Hamilton's equation is

$$\begin{aligned} \dot{\vec{p}} &= -\frac{\partial \mathcal{H}}{\partial \vec{x}} \\ &= -\vec{\nabla} \left(\frac{1}{2m} \left(\vec{p} - \frac{q}{c} \vec{A} \right)^2 + q\phi \right). \end{aligned} \tag{2}$$

Using (1) we compute

$$\begin{aligned} \frac{1}{2m} \nabla_i \left(\vec{p} - \frac{q}{c} \vec{A} \right)^2 &= -\frac{q}{c} \frac{1}{m} \left(p_j - \frac{q}{c} A_j \right) \nabla_i A_j \\ &= -\frac{q}{c} v_j \nabla_i A_j. \end{aligned} \tag{3}$$

Taking the time derivative of (1) we have

$$\begin{aligned} \dot{\vec{p}} &= \frac{\partial}{\partial t} \left(m\dot{\vec{x}} + \frac{q}{c} \vec{A}(x(t), t) \right) \\ &= m\ddot{\vec{x}} + \frac{q}{c} \frac{\partial \vec{A}}{\partial t} + \frac{q}{c} (\vec{v} \cdot \vec{\nabla}) \vec{A} \end{aligned} \tag{4}$$

Plugging (4), (3) into (2) we have

$$\begin{aligned} m\ddot{\vec{x}} &= \frac{q}{c} \vec{v} \times \vec{B} - q\vec{\nabla}\phi - \frac{q}{c} \frac{\partial \vec{A}}{\partial t} \\ &= \frac{q}{c} \vec{v} \times \vec{B} + q\vec{E}. \end{aligned}$$

(b) **(5 points)**

Consider a particle moving on a circle with constant speed v and angular velocity ω_L . We will assume that $q > 0, B > 0$. The radius of the circle, called cyclotron radius, is

$$R = v/\omega_L.$$

The vector $\vec{R}$ pointing from the center of the circle to the particle is perpendicular to $\vec{v}$ and has length v/ω_L and therefore

$$\vec{R} = \left(-\frac{v_y}{\omega_L}, \frac{v_x}{\omega_L}\right)$$

where the correct choice of sign is determined by the right hand rule. Therefore

$$x_0 = x + \frac{v_y}{\omega_L}, \quad y_0 = y - \frac{v_x}{\omega_L}.$$

2. Gauge invariance and the Schrodinger equation (14 points)

(a) **(4 points)** In the unprimed gauge, we have the Schrodinger equation

$$\left[\frac{1}{2m} \left(\vec{p} - \frac{q}{c} \vec{A} \right)^2 + q\phi \right] \psi = i\hbar \frac{\partial \psi}{\partial t}. \quad (5)$$

The Schrodinger equation in the primed gauge, written in terms of the unprimed quantities, is

$$\left[\frac{1}{2m} \left(\vec{p} - \frac{q}{c} \vec{A} + \frac{q}{c} \vec{\nabla} f \right)^2 + q\phi + \frac{q}{c} \frac{\partial f}{\partial t} \right] \psi' = i\hbar \frac{\partial \psi'}{\partial t}. \quad (6)$$

Let us substitute $\psi \equiv \exp(iqf(\vec{x}, t)/\hbar c) \psi'$ into eqn. (5). The right hand side becomes,

$$i\hbar \frac{\partial}{\partial t} \left(e^{\frac{iq}{\hbar c} f(\vec{x}, t)} \psi' \right) = e^{\frac{iq}{\hbar c} f(\vec{x}, t)} \left(i\hbar \frac{\partial \psi'}{\partial t} - \frac{q}{c} \frac{\partial f}{\partial t} \psi' \right). \quad (7)$$

The action of $(\vec{p} - q\vec{A}/c)$ on $\exp(iqf(\vec{x}, t)/\hbar c) \psi'$ gives

$$\left(\vec{p} - \frac{q}{c} \vec{A} \right) e^{\frac{iq}{\hbar c} f(\vec{x}, t)} \psi' = e^{\frac{iq}{\hbar c} f(\vec{x}, t)} \left(\vec{p} - \frac{q}{c} \vec{A} + \frac{q}{c} \vec{\nabla} f \right) \psi',$$

hence for left hand side we get,

$$\left[\frac{1}{2m} \left(\vec{p} - \frac{q}{c} \vec{A} \right)^2 + q\phi \right] e^{\frac{iq}{\hbar c} f} \psi' = e^{\frac{iq}{\hbar c} f} \left[\frac{1}{2m} \left(\vec{p} - \frac{q}{c} \vec{A} + \frac{q}{c} \vec{\nabla} f \right)^2 + q\phi \right] \psi'. \quad (8)$$

Comparing the right hand sides of the equations (7) and (8) we precisely get the Schrodinger equation in the primed gauge, eqn. (6) above. Therefore ψ' given by eqn. (2) in the problem set must be the solution of eqn. (6).

(b) **(2 points)** The inner product of ψ with itself is $\langle \psi | \psi \rangle = \int dx \psi^* \psi = \int dx (\psi')^* \psi' = \langle \psi' | \psi' \rangle$. The position dependent phase factor $e^{-iqf/\hbar c}$ does not change the norm of ψ . Similarly, the expectation value of x is $\langle \psi | x | \psi \rangle = \int dx x \psi^* \psi = \int dx x (\psi')^* \psi' = \langle \psi' | x | \psi' \rangle$.

(c) **(5 points)** The expectation value of p_x is $\langle \psi | p_x | \psi \rangle = -i\hbar \int dx \psi^* \frac{\partial \psi}{\partial x}$ in the unprimed gauge, but in the primed gauge we find

$$\begin{aligned} \langle \psi' | p_x | \psi' \rangle &= -i\hbar \int dx (\psi')^* \left(\frac{-iq}{\hbar c} \frac{\partial f}{\partial x} \psi + e^{-iqf/\hbar c} \frac{\partial \psi}{\partial x} \right) \\ &= -i\hbar \int dx \psi^* \left(\frac{-iq}{\hbar c} \frac{\partial f}{\partial x} + \frac{\partial}{\partial x} \right) \psi \\ &\neq \langle \psi | p_x | \psi \rangle. \end{aligned}$$

In order to construct a gauge invariant quantity, we need to add something whose gauge variation will cancel off the gauge variation of p_x that we found above. This “something” is, of course, the vector potential:

$$\begin{aligned}\langle\psi|(p_x - \frac{q}{c}A_x)|\psi\rangle &= -i\hbar \int dx \psi^* (\frac{\partial}{\partial x} - \frac{iq}{\hbar c}A_x)\psi \\ &= -i\hbar \int dx \psi^* (\frac{\partial}{\partial x} - \frac{iq}{\hbar c}A_x + \frac{iq}{\hbar c}\frac{\partial f}{\partial x} - \frac{iq}{\hbar c}\frac{\partial f}{\partial x})\psi \\ &= \langle\psi'|(p_x - \frac{q}{c}A'_x)|\psi'\rangle.\end{aligned}$$

Thus the kinetic momentum $p_x - qA_x/c$ is a gauge invariant operator, while p_x is not. The above discussion applies without change to other components.

Let us take the gauge variation $f(\vec{x}, t) = f(\vec{x})$ to be time independent. In this case, the scalar potential ϕ is now gauge invariant, as (by assumption) $\frac{\partial f}{\partial t} = 0$. Moreover, $q\phi$ contains no differential operators, so it is easy to conclude $\langle\psi|q\phi|\psi\rangle = \langle\psi'|q\phi|\psi'\rangle$. Since $\vec{p} - q\vec{A}/c$ is a gauge invariant operator, and therefore $H = \frac{1}{2m}(\vec{p} - q\vec{A}/c)^2 + q\phi$ is also gauge invariant.

[**Note:** Now suppose $\frac{\partial f}{\partial t} \neq 0$. In this case it is *not* true that $\langle\psi|H|\psi\rangle = \langle\psi'|H'|\psi'\rangle$, as we can easily demonstrate. Suppose, for simplicity, ψ is an energy eigenstate of H with eigenvalue E . Then

$$H'\psi' = i\hbar \frac{\partial \psi'}{\partial t} = E\psi' - \frac{q}{c} \frac{\partial f}{\partial t} \psi'.$$

Thus H is not gauge invariant. When we make a time-dependent gauge transformation, we are changing the zero of our energy scale, and therefore the energies that we measure do indeed change. However, only energy differences are observable, and these are indeed gauge invariant quantities: suppose we wish to measure the matrix element $\langle\phi|x|\phi\rangle$, where $|\phi\rangle = \alpha|\psi_1\rangle + \beta|\psi_2\rangle$, and $|\psi_{1,2}\rangle$ are eigenstates with eigenenergies $E_{1,2}$. We know that this matrix element is gauge invariant. Let's see what it works out to:

$$\langle\phi(t)|x|\phi(t)\rangle = |\alpha|^2 \langle\psi_1(0)|x|\psi_1(0)\rangle + |\beta|^2 \langle\psi_2(0)|x|\psi_2(0)\rangle + (\alpha\beta^* e^{i(E_2-E_1)t/\hbar} \langle\psi_2(0)|x|\psi_1(0)\rangle + c.c.).$$

All quantities on the right hand side of the above equation are known to be gauge invariant except for $e^{i(E_2-E_1)t/\hbar}$. But since the left hand side must be gauge invariant, this tells us that $E_2 - E_1$ must be a gauge invariant quantity.]

(d) **(3 points)** Since ψ_n is eigenstate of Hamiltonian in unprimed gauge with eigenvalue E_n , therefore ψ_n satisfies,

$$\left[\frac{1}{2m} \left(\vec{p} - \frac{q}{c} \vec{A} \right)^2 + q\phi \right] \psi_n = E_n \psi_n.$$

Substitute $\psi_n = \exp(iqf(\vec{x})/\hbar c) \psi'_n$ in the above equation to get,

$$\begin{aligned}e^{\frac{iq}{\hbar c}f(\vec{x})} E_n \psi'_n(\vec{x}) &= \left[\frac{1}{2m} \left(\vec{p} - \frac{q}{c} \vec{A} \right)^2 + q\phi \right] e^{\frac{iq}{\hbar c}f(\vec{x})} \psi'_n(\vec{x}) \\ &= e^{\frac{iq}{\hbar c}f(\vec{x})} \left[\frac{1}{2m} \left(\vec{p} - \frac{q}{c} \vec{A} + \frac{q}{c} \vec{\nabla} f \right)^2 + q\phi \right] \psi'_n \\ &= e^{\frac{iq}{\hbar c}f(\vec{x})} \left[\frac{1}{2m} \left(\vec{p} - \frac{q}{c} \vec{A}' \right)^2 + q\phi' \right] \psi'_n,\end{aligned}$$

where in the last step we have used $\phi' = \phi$, since f is time-independent. Canceling the phase on both sides of the previous equation we see that ψ'_n is an eigenstate of the Hamiltonian in the primed gauge, with the same eigenvalue E_n .

3. General aspects of quantum motion in a magnetic Field (15 points)

(a) (4 points) The commutator is easy to compute, since

$$[\hat{p}_i, \hat{p}_j] = [A_i, A_j] = 0 \quad \text{and} \quad [\hat{p}_i, A_j] = -i\hbar \frac{\partial A_j}{\partial x_i}$$

we have

$$\begin{aligned} [\hat{v}_i, \hat{v}_j] &= -\frac{q}{m^2 c} ([\hat{p}_i, A_j] + [A_i, \hat{p}_j]) \\ &= \frac{i\hbar q}{m^2 c} \left(\frac{\partial A_j}{\partial x_i} - \frac{\partial A_i}{\partial x_j} \right) \\ &= \frac{i\hbar q}{m^2 c} \epsilon_{ijk} B_k. \end{aligned}$$

We see that when $\vec{B} \neq 0$ the commutator $[\hat{v}_i, \hat{v}_j]$ is proportional to the component of $\vec{B}$ perpendicular to the ij -plane.

The non-vanishing of the above commutators implies that the motions in different directions are not commutative.

(b) (4 points) The commutator is

$$\begin{aligned} [\hat{x}_0, \hat{y}_0] &= -\frac{1}{\omega_L} ([\hat{x}, \hat{v}_x] + [\hat{y}, \hat{v}_y]) + \frac{1}{\omega_L^2} [\hat{v}_x, \hat{v}_y] \\ &= -\frac{2i\hbar}{m\omega_L} + \frac{i\hbar q}{m^2 \omega_L^2 c} B_z \\ &= -\frac{i\hbar c}{qB} \end{aligned}$$

where we used $\omega_L = qB/mc$.

We see, that the coordinates of the center of the particle's rotation in magnetic field do not commute. Therefore, although the coordinates of the particle itself may be observed simultaneously the coordinates of the center of the orbit cannot be observed at the same time. This is similar to the fact that angular momentum components do not commute and thus the particle's wave function may only be the eigenstate of one of angular momentum components.

(c) (4 points) We have

$$\begin{aligned} [\hat{x}_0, \hat{v}_x] &= [\hat{x}, \hat{v}_x] + \frac{1}{\omega_L} [\hat{v}_y, \hat{v}_x] = \frac{i\hbar}{m} - \frac{i\hbar q B}{m^2 \omega_L c} = 0, \\ [\hat{x}_0, \hat{v}_y] &= [\hat{x}, \hat{v}_y] + \frac{1}{\omega_L} [\hat{v}_y, \hat{v}_y] = 0, \\ [\hat{y}_0, \hat{v}_x] &= [\hat{y}, \hat{v}_x] - \frac{1}{\omega_L} [\hat{v}_x, \hat{v}_x] = 0, \\ [\hat{y}_0, \hat{v}_y] &= [\hat{y}, \hat{v}_y] - \frac{1}{\omega_L} [\hat{v}_x, \hat{v}_y] = \frac{i\hbar}{m} - \frac{i\hbar q B}{m^2 \omega_L c} = 0. \end{aligned} \tag{9}$$

(d) **(3 points)** Recall that the Hamiltonian for the motion in $x - y$ plane is given by

$$H = \frac{1}{2}m(\hat{v}_x^2 + \hat{v}_y^2) \quad (10)$$

Since all the commutators in (9) vanish

$$[\hat{x}_0, H] = 0,$$

$$[\hat{y}_0, H] = 0.$$

Since $\hat{x}_0$ and $\hat{y}_0$ commute with the Hamiltonian but not with each other, we can eigenstates of $\hat{x}_0$ and H or of $\hat{y}_0$ and H but not of all three.

Note: if we include an electric potential term $q\phi$ in (10) then the commutators $[x_0, H]$ and $[y_0, H]$ may not vanish. The center of orbital rotation could drift due to electric force and x_0 and y_0 may not be conserved any more.

4. Electromagnetic current density in quantum mechanics (12 points)

(a) **(6 points)** From the Schrodinger equation, we have

$$i\hbar\psi^*\frac{\partial\psi}{\partial t} = \frac{1}{2m}\psi^*\left(-i\hbar\vec{\nabla} - \frac{q}{c}\vec{A}\right)^2\psi + q\phi\psi^*\psi.$$

Subtracting the complex conjugate of the above equation from the equation itself, we have

$$i\hbar\left(\psi^*\frac{\partial\psi}{\partial t} + \psi\frac{\partial\psi^*}{\partial t}\right) = \frac{1}{2m}\left[\psi^*\left(-i\hbar\vec{\nabla} - \frac{q}{c}\vec{A}\right)^2\psi - \psi\left(i\hbar\vec{\nabla} - \frac{q}{c}\vec{A}\right)^2\psi^*\right],$$

which can be further simplified to

$$i\hbar\frac{\partial(\psi^*\psi)}{\partial t} = \frac{1}{2m}\left[-\hbar^2(\psi^*\nabla^2\psi - \psi\nabla^2\psi^*) + \frac{2i\hbar q}{c}\vec{A}(\psi^*\vec{\nabla}\psi + \psi\vec{\nabla}\psi^*)\right],$$

where we have used the gauge condition $\vec{\nabla} \cdot \vec{A} = 0$. Thus,

$$\begin{aligned} \frac{\partial(\psi^*\psi)}{\partial t} &= \frac{i\hbar}{2m}(\psi^*\vec{\nabla}^2\psi - \psi\vec{\nabla}^2\psi^*) + \frac{q}{mc}\vec{A}(\psi^*\vec{\nabla}\psi + \psi\vec{\nabla}\psi^*) \\ &= -\vec{\nabla} \cdot \vec{S}. \end{aligned}$$

We have just derived the charge conservation equation starting from the Schrodinger equation.

(b) **(2 points)** It suffices to show that $[S] = [1/(At)]$. Now

$$[S] = \left[\frac{\hbar}{m} \frac{1}{l} \frac{1}{l^3}\right] = \left[\frac{t m l^2}{m l^4 t^2}\right] = \left[\frac{1}{t l^2}\right]$$

which is indeed units of inverse area times inverse time.

(c) **(4 points)** We now want to show that S is gauge invariant. In the primed gauge,

$$\begin{aligned} \vec{S}' &= \frac{\hbar}{m} \text{Im} \left(\psi^* \vec{\nabla} \psi - \frac{iq}{\hbar c} \psi^* (\vec{\nabla} f) \psi \right) - \frac{q}{mc} \psi^* \psi (A - \vec{\nabla} f) \\ &= \vec{S} - \frac{q}{mc} \psi^* \psi \vec{\nabla} f + \frac{q}{mc} \psi^* \psi \vec{\nabla} f \\ &= \vec{S}. \end{aligned}$$

5. Translation invariance in a uniform magnetic field (14 points)

(a) **(2 points)** Using the definition of $\vec{v}$ from problem 3 and plugging the explicit expression for $\vec{A}$ we have

$$\begin{aligned} Q_x &= -\frac{qB}{c}\hat{y}_0 \\ &= -\frac{qB}{c}\left(\hat{y} - \frac{1}{m\omega_L}\left(\hat{p}_x - \frac{q}{c}A_x\right)\right) \\ &= -\frac{qB}{c}\left(\hat{y}\left(1 - \frac{qB}{mc\omega_L}\right) - \frac{1}{m\omega_L}\hat{p}_x\right) \\ &= \hat{p}_x \end{aligned}$$

where in the last step we used $\omega_L = qB/mc$. Similarly

$$\begin{aligned} Q_y &= \frac{qB}{c}\hat{x}_0 \\ &= \frac{qB}{c}\left(\hat{x} + \frac{1}{m\omega_L}\hat{p}_y\right) \\ &= \hat{p}_y + \frac{qB}{c}\hat{x}. \end{aligned}$$

(b) **(4 points)** We take $\psi(x, y)$ to be an eigenfunction of H with eigenvalue E . We define $\tilde{\psi}(x, y) = e^{iqB_0bx/\hbar c}\psi(x, y + b)$. Now

$$\begin{aligned} H\tilde{\psi}(x, y) &= -\frac{\hbar^2}{2m}\left[\frac{\partial^2}{\partial y^2} + \left(\frac{\partial}{\partial x} + \frac{iqB_0}{\hbar c}y\right)^2\right]e^{iqB_0bx/\hbar c}\psi(x, y + b) \\ &= e^{iqB_0bx/\hbar c}\frac{-\hbar^2}{2m}\left[\frac{\partial^2}{\partial(y+b)^2} + \left(\frac{\partial}{\partial x} - \frac{iqB_0}{\hbar c}(y+b)\right)^2\right]\psi(x, y + b) \\ &= e^{iqB_0bx/\hbar c}E\psi(x, y + b) \\ &= E\tilde{\psi}(x, y). \end{aligned}$$

Therefore, $\tilde{\psi}$ is also an eigenfunction of H with eigenvalue E .

(c) **(3 points)** $U_a = e^{\frac{i}{\hbar}a\hat{p}_x}$ is the usual translation operator and we have

$$U_a\psi(x, y) = e^{a\frac{\partial}{\partial x}}\psi(x, y) = \psi(x + a, y). \quad (11)$$

Note: The definition of translation operator used here, $U_af(x) = f(x + a)$, differs by a sign from what one obtains considering geometric translation $x \rightarrow x + a$, which transforms $f(x)$ to $f(x - a)$.

Since $[\hat{p}_y, \hat{x}] = 0$ we have

$$\begin{aligned} V_b\psi(x, y) &= e^{\frac{i}{\hbar}Q_yb}\psi(x, y) \\ &= e^{\frac{i}{\hbar}(\hat{p}_y + \frac{qB}{c}\hat{x})b}\psi(x, y) \\ &= e^{\frac{i}{\hbar}\hat{p}_yb}e^{\frac{iqBb}{\hbar c}\hat{x}}\psi(x, y) \\ &= e^{\frac{iqBbx}{\hbar c}}\psi(x, y + b) = \tilde{\psi}(x, y). \end{aligned}$$

(d) (**5 points**) The commutator is

$$\begin{aligned}[U_a, V_b] &= (U_a V_b U_a^{-1} - V_b) U_a \\ &= V_b U_a \left(e^{\frac{iqBab}{\hbar c}} - 1 \right).\end{aligned}$$

where we have used that

$$U_a V_b U_a^{-1} = e^{\frac{i}{\hbar}(\hat{p}_y + \frac{qB}{c}(\hat{x}+a))b} = e^{\frac{iqBab}{\hbar c}} V_b$$

since $[\hat{p}_x, \hat{p}_y] = 0$ and

$$e^{\frac{i}{\hbar}a\hat{p}_x} g(\hat{x}) e^{-\frac{i}{\hbar}a\hat{p}_x} = g(\hat{x} + a)$$

for any function g .

The commutator vanishes if

$$\frac{qBab}{\hbar c} = 2\pi n, \quad n \in \mathbb{Z}$$

or, equivalently

$$\Phi = n\Phi_0, \quad n \in \mathbb{Z}$$

where $\Phi = abB$ is the flux through the area ab and $\Phi_0 = hc/q$ is the quantum of flux.