Problem Set # 7, Due: Wednesday Mar 8 by 11:00am

PHY 362K - Quantum Mechanics II, UT Austin, Spring 2017
(Dated: March 8, 2017)

Quantum mechanics of charged particles in a magnetic field

I. PARTICLE ON A RING THREADED BY A SOLENOID

Consider an electron (charge $q = -e$, mass m_e) that is constrained to move on a 1D ring of radius R in the xy-plane. Let's parameterize the position of the particle on the ring by the angle φ that it makes relative to the x-axis. Since the particle is stuck on the ring, its momentum can only have components tangential to the ring (in the φ direction only), so we can write the momentum operator in the position basis as: $\hat{\vec{p}} = \vec{e}_\varphi \left(\frac{-i\hbar}{R}\frac{\partial}{\partial\varphi}\right)$ (where $\vec{e}_\varphi$ is the unit vector in the φ direction).

Suppose we insert a thin solenoid into the center of the ring, with magnetic field in the z-direction (perpendicular to the ring) $B^z = \Phi_B \delta(\vec{r})$, which we can represent by a vector potential: $\vec{A} = \frac{\Phi_B}{2\pi r}\vec{e}_\varphi$ that is constant along the ring ($r = R$). (You can easily check that $\nabla \times \vec{A} = B^z \vec{e}_z$, by integrating this equation around the ring, and using Stoke's theorem to relate this to the magnetic flux through the ring).

1. Write down the Schrodinger equation for this system by making the "minimal substitution", of taking the usual zero-field ($\Phi_B = 0$) Schrodinger equation for a massive particle on a ring, and replacing: $\vec{p} \to \vec{p} - \frac{q}{c}\vec{A}$. Solve for the energy levels and corresponding wave-functions as a function of Φ_B.

   Solution: For a massive particle on a ring, the momentum operator can be written in the position basis as $\hat{\vec{p}} = \vec{e}_\varphi \left(\frac{-i\hbar}{R}\frac{\partial}{\partial\varphi}\right)$. With this, the zero-field Hamiltonian equation for a massive particle on a ring is

$$\hat{H}_0 = \frac{\hat{p}^2}{2m} = \frac{-\hbar^2}{2mR^2}\frac{\partial^2}{\partial\phi^2}$$

   If we make the substitution $\vec{p} \to \vec{p} - \frac{q}{c}\vec{A}$, where in this case $\vec{A} = \frac{\Phi_B}{2\pi R}\vec{e}_\phi$, then we obtain the Hamiltonian

$$\begin{aligned}\hat{H} = \frac{\left(\vec{p} - \frac{q}{c}\vec{A}\right)^2}{2m} &= \frac{1}{2m}\left(-\frac{i\hbar}{R}\frac{\partial}{\partial\phi}\vec{e}_\phi - \frac{q\Phi_B}{2\pi c R}\vec{e}_\phi\right)^2 \\ &= \frac{1}{2mR^2}\left(-\hbar^2\frac{\partial^2}{\partial\phi^2} + \frac{i\hbar q\Phi_B}{\pi c}\frac{\partial}{\partial\phi} + \frac{q^2\Phi_B^2}{4\pi^2c^2}\right)\end{aligned}$$

   Using this Hamiltonian, we find the Schrodinger equation to be

$$\boxed{\frac{1}{2mR^2}\left(-\hbar^2\frac{\partial^2\psi}{\partial\phi^2} + \frac{i\hbar q\Phi_B}{\pi c}\frac{\partial\psi}{\partial\phi} + \frac{q^2\Phi_B^2}{4\pi^2c^2}\psi\right) = E\psi} \tag{1}$$

   If we denote $\frac{\partial\psi}{\partial\phi}$ as ψ', define $\nu = \frac{q\Phi_B}{\pi c}$, and rearrange equation 1, we obtain

$$-\hbar^2\psi'' + i\hbar\nu\psi' + \left(\frac{1}{4}\nu^2 - 2mR^2E\right)\psi = 0$$

To solve this differential equation, we will make the guess that the solution has the form $\psi(\phi) = Be^{i\alpha\phi}$. Plugging in this trial solution gives

$$Be^{ir\phi}\left(\hbar\alpha^2 - \hbar\nu\alpha + \left(\frac{1}{4}\nu^2 - 2mR^2E\right)\right) = 0$$

The exponential factor can never be zero, therefore the quadratic polynomial in α must be zero. Using the quadratic formula, we find the values of α to be

$$\begin{aligned}\alpha_\pm &= \frac{\hbar\nu \pm \sqrt{\hbar^2\nu^2 - 4\hbar^2\left(\frac{1}{4}\nu^2 - 2mR^2E\right)}}{2\hbar^2} \\ &= \frac{\nu \pm \sqrt{8mR^2E}}{2\hbar}\end{aligned}$$

Therefore, for a given value of E, the Schrodinger equation has the two solutions

$$\psi_\pm(\phi) = Be^{i\alpha_\pm\phi}$$

We will now enforce the periodic boundary conditions $\psi_\pm(\phi) = \psi_\pm(\phi + 2\pi)$. Enforcing these conditions gives

$$Be^{i\alpha_\pm\phi} = Be^{i\alpha_\pm(\phi+2\pi)} \implies e^{2\pi i\alpha_\pm} = 1 \implies \alpha_\pm \in \mathbb{Z}$$

Since $\alpha_\pm$ must be integers, we will rename the $\alpha_\pm$ to $k, k \in \mathbb{Z}$ for ease of notation. Using this notation along with the solution of the quadratic obtained from the differential equation, we find

$$k = \frac{\nu \pm \sqrt{8mR^2E}}{2\hbar}$$

Solving for E and letting $q = -e$, we find the allowed energies to be

$$\boxed{E_k = \frac{\left(2\hbar k + \frac{e\Phi_B}{\pi c}\right)^2}{8mR^2}} \tag{2}$$

If we now enforce the normalization condition $\int_0^{2\pi}\psi_\pm^*(\phi)\psi_\pm(\phi)d\phi = 1$, then we find

$$\int_0^{2\pi} B^2 e^{-i\alpha_\pm\phi}e^{i\alpha_\pm\phi}d\phi = B^2\int_0^{2\pi} = 1 \implies B = \frac{1}{\sqrt{2\pi}}$$

Therefore, the energies have the corresponding wave functions

$$\boxed{\psi_\pm(\phi) = \frac{1}{\sqrt{2\pi}}\exp\left[i\left(\frac{-\frac{e\Phi_B}{\pi c} \pm \sqrt{8mR^2E}}{2\hbar}\right)\phi\right]} \tag{3}$$

2. Show that we can make a gauge transformation to make $A_\varphi = 0$, but that this changes the boundary conditions from periodic ones: $\psi(\varphi = 0) = \psi(\varphi = 2\pi)$, to "twisted" ones: $\psi(\varphi \to 2\pi) = e^{2\pi i \Phi_B/\Phi_0}\psi(\varphi = 0)$, where $\Phi_0 = \frac{2\pi\hbar c}{e}$ is the elementary flux quantum. Verify that the energy levels are the same in this new gauge with $A_\varphi = 0$ and twisted boundary conditions.

   Solution: We know that the vector potential is gauge invariant, meaning that we can add the gradient of any scalar function to A and this will not change the physics of the problem. Therefore, we can replace $\vec{A}$ by $\vec{A} + \nabla\lambda$ where λ is a scalar function. We want our gauge transformation to satisfy $\vec{A}_\phi + (\nabla\lambda)_\phi = 0 \implies (\nabla\lambda)_\phi = -\frac{\Phi_B}{2\pi r}$. The ϕ component of the gradient of a scalar function in cylindrical coordinates is given by $(\nabla\lambda)_\phi = \frac{1}{r}\frac{\partial\lambda}{\partial\phi}$. Therefore, in this case we must have

$$\frac{1}{r}\frac{\partial\lambda}{\partial\phi} = -\frac{\Phi_B}{2\pi r} \implies \lambda = -\frac{\Phi_B}{2\pi}\phi$$

   Now, although the physics of the problem is invariant under gauge transformations, the Schrodinger equation, $\frac{\left(\vec{p}-\frac{q}{c}\vec{A}\right)^2}{2m}\psi(\phi) = E\psi(\phi)$ is not. In order to compensate for this gauge transformation, we must transform our wavefunctions from ψ to $\psi' = e^{i\frac{q\lambda}{\hbar c}}\psi$ so that they satisfy the gauge transformed Schrodinger equation. Making this transformation and letting $q = -e$, we find

$$\psi'_\pm(\phi) = \frac{1}{\sqrt{2\pi}} e^{i\frac{e}{\hbar c}\frac{\Phi_B}{2\pi}\phi} \exp\left[i\left(\frac{-\frac{e\Phi_B}{\pi c} \pm \sqrt{8mR^2E}}{2\hbar}\right)\phi\right]$$

   So now,

$$\psi'_\pm(2\pi) = \frac{1}{\sqrt{2\pi}} e^{i\frac{e\Phi_B}{\hbar c}} = \frac{1}{\sqrt{2\pi}} e^{2\pi i\frac{\Phi_B}{\Phi_0}} \neq \frac{1}{\sqrt{2\pi}} = \psi'_\pm(0)$$

   So under this gauge transformation we must change from periodic boundary conditions, $\psi'(2\pi) = \psi'(0)$, to twisted boundary conditions, $\psi'(2\pi) = e^{2\pi i\frac{\Phi_B}{\Phi_0}}\psi'(0)$.

   In this new gauge, the Schrodinger equation reduces to that of the free particle on a ring (because $A_\phi = 0$).

$$-\frac{\hbar^2}{2mR^2}\frac{\partial^2\psi}{\partial\phi^2} = E\psi$$

   This equation can be rewritten as

$$\frac{\partial^2\psi}{\partial\phi^2} = -\frac{2mR^2E}{\hbar^2}\psi$$

   which has the well known solution $\psi(\phi) = Ce^{\pm i\frac{R\sqrt{2mE}}{\hbar}\phi}$. If we now enforce the twisted boundary conditions, we find

$$\psi'(2\pi) = e^{2\pi i\frac{\Phi_B}{\Phi_0}}\psi(0) \implies Ce^{\pm 2\pi i\frac{R\sqrt{2mE}}{\hbar}} = Ce^{2\pi i\frac{\Phi_B}{\Phi_0}} \implies e^{2\pi i\left(\pm\frac{R\sqrt{2mE}}{\hbar} - \frac{\Phi_B}{\Phi_0}\right)} = 1$$

and therefore $\pm\frac{R\sqrt{2mE}}{\hbar} - \frac{\Phi_B}{\Phi_0}$, must be an integer. Therefore we have,

$$\pm\frac{R\sqrt{2mE}}{\hbar} - \frac{\Phi_B}{\Phi_0} = k \qquad k \in \mathbb{Z}$$

Solving for E, we find

$$\boxed{E = \frac{\left(\hbar k + \hbar\frac{\Phi_B}{\Phi_0}\right)^2}{2mR^2} = \frac{\left(2\hbar k + \frac{e\Phi_B}{\pi c}\right)^2}{8mR^2}} \tag{4}$$

Therefore the allowed energies are the same in the new gauge.

II. LANDAU LEVELS FOR A 2D DIRAC PARTICLE

Massless relativistic spin-1/2 fermions are described by the Dirac equation rather than the Schrodinger equation. A 2-Dimensional (2D) version of the Dirac equation also describes electrons in certain solids like graphene (an atomically thin layer of carbon) or the surface of "topological insulators". In this context the Hamiltonianb for this massless 2D Dirac (for no electric or magnetic fields) is:

$$\hat{H}_D = v\hat{\vec{p}} \cdot \vec{\sigma} \tag{5}$$

where $\vec{\sigma}$ are the spin-1/2 Pauli matrices in the spin-basis, and $\vec{p}$ contains only x and y components (since the particle is confined to the 2D plane), and v is the velocity of the Dirac electron. For a massless relativistic particle, setting we would have $v = c$ (the speed of light) but in graphene and topological insulators the velocity is determined by the periodic potential of the crystal and is about $100\times$ smaller than c.

1. What are the eigen-energies of $\hat{H}_D$?

Solution: We will begin by squaring the Hamiltonian and finding the eigen-energies of $\hat{H}_D^2$ which we can call E^2. Then the eigen-energies of $\hat{H}_D^2$ are $E = \pm\sqrt{E^2}$. Squaring the Hamiltonian, we obtain,

$$\hat{H}_D^2 = (v\hat{p} \cdot \vec{\sigma})^2 = v^2 \left(\hat{p}_x\sigma_x + \hat{p}_y\sigma_y\right)^2$$

Where the last equality follows from the fact that $\hat{p} = \hat{p}_x\vec{e}_x + \hat{p}_y\vec{e}_y$. Expanding further,

$$\hat{H}_D^2 = v^2 \left(\hat{p}_x^2\sigma_x^2 + \hat{p}_y^2\sigma_y^2 + \hat{p}_x\hat{p}_y\sigma_x\sigma_y + \hat{p}_y\hat{p}_x\sigma_y\sigma_x\right)$$

Now, we know that $\sigma_{x,y,z}^2 = I$, and $\sigma_x\sigma_y = i\sigma_z = -\sigma_y\sigma_x$, so we can write

$$\begin{aligned}
\hat{H}_D^2 &= v^2 \left(\hat{p}_x^2\sigma_x^2 + \hat{p}_y^2\sigma_y^2\right) \\
&= v^2 \left(\left(-i\hbar\frac{\partial}{\partial x}\right)^2 + \left(-i\hbar\frac{\partial}{\partial y}\right)^2\right) \\
&= -v^2\hbar^2 \left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2}\right) \\
&= 2mv^2\hat{H}_f
\end{aligned}$$

Where $\hat{H}_f$ is the free particle Hamiltonian for a particle of mass m. We know that the eigenenergies of $\hat{H}_f$ are $E_k = \frac{\hbar^2 k^2}{2m}$, where $k \in \mathbb{R}$. Therefore the eigenenergies of $\hat{H}_D^2$ are $E^2 = 2mv^2 E_k = \hbar^2 v^2 k^2$, and so the eigen-energies of $\hat{H}_D$ are

$$\boxed{E = \hbar v k \qquad k \in \mathbb{R}} \tag{6}$$

2. Find the energy levels if we add a "mass" term so that the Hamiltonian is: $\hat{H}_m = \hat{H}_D + mv^2\sigma^z$? Show that these energies reproduce the non-relativistic limit of a massive particle when momentum is much less than $p \ll mv$.

   Solution: If we follow a similar procedure as in part 1, we find that

$$\begin{aligned}\hat{H}_m^2 &= \left(\hat{H}_D + mv^2\sigma_z\right)^2 = \hat{H}_D^2 + mv^2\hat{H}_D\sigma_z + mv^2\sigma_z\hat{H}_D + m^2v^4\sigma_z^2 \\ &= \hat{H}_D^2 + mv^2\left(\hat{p}_x\sigma_x\sigma_z + \hat{p}_y\sigma_y\sigma_z + \hat{p}_x\sigma_z\sigma_x + \hat{p}_y\sigma_z\sigma_y\right) + m^2v^4\end{aligned}$$

   However, $\sigma_x\sigma_z = -\sigma_z\sigma_x$ and $\sigma_y\sigma_z = -\sigma_z\sigma_y$. Therefore,

$$\hat{H}_m^2 = \hat{H}_D^2 + m^2v^4$$

   If we denote the eigenenergies of $\hat{H}_m^2$ as E_m^2 and the eigenenergies of $\hat{H}_D^2$ as E^2, then we can clearly see from the above expression for $\hat{H}_m^2$ that $E_m^2 = E^2 + m^2v^4$. Therefore, the eigenenergies of $\hat{H}_m$ are $E_m = \pm\sqrt{E_m^2} = \pm\sqrt{E^2 + m^2v^4}$ and so

$$\boxed{E_m = \pm\sqrt{\hbar^2v^2k^2 + m^2v^4} \qquad k \in \mathbb{R}} \tag{7}$$

   Now, $\hbar k = p$, so we can write the energies in the form

$$E_m = \pm mv^2\sqrt{1 + \frac{p^2}{m^2v^2}}$$

   In the limit when $p \ll mv$, we can perform a binomial expansion on the radical to obtain

$$E_m = \pm mv^2\left(1 + \frac{p^2}{2m^2v^2} + O\left(\left(\frac{p^2}{m^2v^2}\right)^2\right)\right)$$

   Neglecting terms of order ≥ 2 in $\frac{p^2}{m^2v^2}$, we find

$$E_m = \pm\left(mv^2 + \frac{p^2}{2m}\right)$$

   which agrees with the nonrelativistic energy of a massive particle with potential energy mv^2.

3. Find the Hamiltonian and energy levels of a massless 2D Dirac electron in a magnetic field: $\vec{B} = B\vec{e}_z$ in the z direction (i.e. perpendicular to the plane of motion for the electron).

   Solution: We begin by defining a vector potential that corresponds to this magnetic field. We will use the vector potential $\vec{A} = Bx\vec{e}_y$. It can easily be shown that $\nabla \times \vec{A} = B\vec{e}_z$.

   Using this vector potential and making the substitution $\vec{p} \to \vec{p} - \frac{q}{c}\vec{A}$, our Hamiltonian becomes

$$\begin{aligned}\hat{H}_B &= v\left(\vec{p} - \frac{q}{c}B\hat{x}\vec{e}_y\right)\cdot\vec{\sigma} \\ &= \hat{H}_D - \frac{q}{c}Bv\hat{x}\sigma_y\end{aligned}$$

If we square this Hamiltonian, we obtain

$$\begin{aligned}\hat{H}_B^2 &= \hat{H}_D^2 - \frac{q}{c}Bv\hat{H}_D\hat{x}\sigma_y - \frac{q}{c}Bv\hat{x}\sigma_y\hat{H}_D + \frac{q^2}{c^2}B^2v^2\hat{x}^2\sigma_y^2 \\ &= \hat{H}_D^2 - \frac{q}{c}Bv\left(\hat{H}_D\hat{x}\sigma_y + \hat{x}\sigma_y\hat{H}_D\right) + \frac{q^2}{c^2}B^2v^2\hat{x}^2\sigma_y^2\end{aligned}$$

However, we have

$$\hat{H}_D\hat{x}\sigma_y = v\left(\hat{p}_x\sigma_x\hat{x}\sigma_y + \hat{p}_y\sigma_y\hat{x}\sigma_y\right) = v\left(i\sigma_z\hat{p}_x\hat{x} + \hat{p}_y\hat{x}\right)$$

where the last equality follows from the fact that $\sigma_x\sigma_y = i\sigma_z$ and $\sigma_y^2 = I$.
And also,

$$\hat{x}\sigma_y\hat{H}_D = v\left(\hat{x}\hat{p}_x\sigma_y\sigma_x + \hat{x}\hat{p}_y\sigma_y\sigma_y\right) = v\left(-i\sigma_z\hat{x}\hat{p}_x + \hat{x}\hat{p}_y\right)$$

Plugging these into the expression for our squared Hamiltonian, we find

$$\begin{aligned}\hat{H}_B^2 &= \hat{H}_D^2 - \frac{q}{c}Bv^2\left(i\sigma_z\hat{p}_x\hat{x} + \hat{p}_y\hat{x} - i\sigma_z\hat{x}\hat{p}_x + \hat{x}\hat{p}_y\right) + \frac{q^2}{c^2}B^2v^2\hat{x}^2\sigma_y^2 \\ &= \hat{H}_D^2 - \frac{q}{c}Bv^2\left(i\sigma_z[\hat{p}_x, \hat{x}] + 2\hat{p}_y\hat{x}\right) + \frac{q^2}{c^2}B^2v^2\hat{x}^2\sigma_y^2\end{aligned}$$

However, we know that $[\hat{p}_x, \hat{x}] = i\hbar$. Therefore,

$$\begin{aligned}\hat{H}_B^2 &= \hat{H}_D^2 - \frac{q}{c}Bv^2\left(-\hbar\sigma_z + 2\hat{p}_y\hat{x}\right) + \frac{q^2}{c^2}B^2v^2\hat{x}^2 \\ &= \hat{H}_D^2 + \frac{q^2}{c^2}B^2v^2\left(\hat{x}^2 - 2\frac{c}{qB}\hat{x}\hat{p}_y + \frac{c^2}{q^2B^2}\hat{p}_y^2 - \frac{c^2}{q^2B^2}\hat{p}_y^2\right) + \frac{q}{c}\hbar v^2B\sigma_z \\ &= \hat{H}_D^2 + \frac{q^2}{c^2}B^2v^2\left(\hat{x} - \frac{c}{qB}\hat{p}_y\right)^2 - v^2\hat{p}_y^2 + \frac{q}{c}\hbar v^2B\sigma_z\end{aligned}$$

Note that this hamiltonian does not depend on $\hat{y}$, therefore $\hat{p}_y$ commutes with this Hamiltonian and so we can replace the operator $\hat{p}_y$ with its eigenvalue p_y. In addition, we showed in part 1 that $\hat{H}_D = v^2\left(\hat{p}_x^2 + \hat{p}_y^2\right)$, and so,

$$\begin{aligned}\hat{H}_B^2 &= v^2\hat{p}_x^2 + \frac{q^2}{c^2}B^2v^2\left(\hat{x} - \frac{c}{qB}p_y\right)^2 + \frac{q}{c}\hbar v^2B\sigma_z \\ &= 2mv^2\left(\frac{\hat{p}_x^2}{2m} + \frac{1}{2m}\frac{q^2}{c^2}B^2\left(\hat{x} - \frac{c}{qB}p_y\right)^2\right) + \frac{q}{c}\hbar v^2B\sigma_z \\ &= 2mv^2\left(\frac{\hat{p}_x^2}{2m} + \frac{1}{2}m\left(\frac{qB}{mc}\right)^2\left(\hat{x} - \frac{c}{qB}p_y\right)^2\right) + \frac{q}{c}\hbar v^2B\sigma_z \\ &= 2mv^2\hat{H}_{HO} + \frac{q}{c}\hbar v^2B\sigma_z\end{aligned}$$

where $\hat{H}_{HO}$ is the Hamiltonian for a particle of mass m in a harmonic oscillator potential centered at $x = \frac{c}{qB}p_y$, with $\omega = \frac{qB}{mc}$. We know that the eigen-energies of the harmonic oscilator are $E_{HO} = \hbar\omega(n+1/2) = \hbar\frac{qB}{mc}(n+1/2), \quad n \in \mathbb{Z}$. In addition, the electron is a spin-1/2 particle, so the second term contributes an energy $E_s = \pm\frac{e}{c}\hbar v^2 B$, where we have let $q = -e$. Therefore the eigenenergies of $\hat{H}_B^2$ are $E_B^2 = 2mv^2 E_{HO} + E_s = \frac{\hbar q B v^2}{c}(2n+1) \pm \frac{e}{c}\hbar v^2 B$. Therefore the eigen-energies of $\hat{H}_B$ are

$$\boxed{E_B = \pm\sqrt{\frac{\hbar q B v^2}{c}(2n+1) \pm \frac{e}{c}\hbar v^2 B}, \quad n \in \mathbb{Z}} \tag{8}$$