QM1 Problem Set 5 solutions — Mike Saelim

If you find any errors with these solutions, please email me at mjs496@cornell.edu.

1 Recall from the last problem set that the Hamiltonian is given by

$$H = \frac{\vec{\Pi}^2}{2m} + e\phi(\vec{x}) = \frac{1}{2m}\left(\vec{p} - \frac{e}{c}\vec{A}(\vec{x})\right)^2 + e\phi(\vec{x})$$
$$= \frac{\vec{p}^2}{2m} - \frac{e}{2mc}[\vec{p}\cdot\vec{A}(\vec{x}) + \vec{A}(\vec{x})\cdot\vec{p}] + \frac{e^2}{2mc^2}\vec{A}^2(\vec{x}) + e\phi(\vec{x})$$

Let's solve for the probability flux first. With the Schrödinger equation, we don't have to deal with bras and kets - just the wavefunction.

$$\frac{\partial\rho}{\partial t} = \frac{\partial}{\partial t}|\psi(\vec{x}')|^2$$
$$= \left(\frac{\partial\psi(\vec{x}')^*}{\partial t}\right)\psi(\vec{x}') + \psi(\vec{x}')^*\left(\frac{\partial\psi(\vec{x}')}{\partial t}\right)$$
$$= \left(\frac{\partial\psi(\vec{x}')}{\partial t}\right)^*\psi(\vec{x}') + \psi(\vec{x}')^*\left(\frac{\partial\psi(\vec{x}')}{\partial t}\right)$$

The time derivatives of the wavefunctions are given by the Schrödinger equation:

$$\frac{\partial\psi}{\partial t} = \frac{1}{i\hbar}H\psi(\vec{x}')$$
$$= \frac{1}{i\hbar}\left[\frac{-\hbar^2}{2m}\nabla^2\psi - \frac{e}{2mc}\left(\frac{\hbar}{i}\nabla\cdot(\vec{A}\psi) + \vec{A}\cdot\frac{\hbar}{i}\nabla\psi\right) + \frac{e^2}{2mc^2}\vec{A}^2\psi + e\phi\psi\right]$$
$$= \frac{i\hbar}{2m}\nabla^2\psi + \frac{e}{2mc}\left[\nabla\cdot(\vec{A}\psi) + \vec{A}\cdot\nabla\psi\right] + \frac{1}{i\hbar}\left[\frac{e^2}{2mc^2}\vec{A}^2\psi + e\phi\psi\right]$$
$$\left(\frac{\partial\psi}{\partial t}\right)^* = \frac{-i\hbar}{2m}\nabla^2\psi^* + \frac{e}{2mc}\left[\nabla\cdot(\vec{A}\psi^*) + \vec{A}\cdot\nabla\psi^*\right] + \frac{1}{-i\hbar}\left[\frac{e^2}{2mc^2}\vec{A}^2\psi^* + e\phi\psi^*\right],$$

where ψ, ψ^*, A, ϕ, and H are all c-number (non-operator) functions of $\vec{x}'$. Plugging these in,

$$\frac{\partial\rho}{\partial t} = \frac{-i\hbar}{2m}(\nabla^2\psi^*)\psi + \frac{e}{2mc}\left[(\nabla\cdot(\vec{A}\psi^*))\psi + \vec{A}\cdot(\nabla\psi^*)\psi\right] + \frac{1}{-i\hbar}\left[\frac{e^2}{2mc^2}\vec{A}^2|\psi|^2 + e\phi|\psi|^2\right]$$
$$+ \frac{i\hbar}{2m}\psi^*\nabla^2\psi + \frac{e}{2mc}\left[\psi^*\nabla\cdot(\vec{A}\psi) + \psi^*\vec{A}\cdot\nabla\psi\right] + \frac{1}{i\hbar}\left[\frac{e^2}{2mc^2}\vec{A}^2|\psi|^2 + e\phi|\psi|^2\right].$$

Notice that the $\frac{1}{-i\hbar}$ terms on the right easily cancel, and the $\frac{e}{2mc}$ terms in the middle add up to two total derivatives which are the same. We can make the second derivative terms on the left into total derivatives if we add

$$\frac{-i\hbar}{2m}(\nabla\psi^*)\cdot(\nabla\psi) + \frac{i\hbar}{2m}(\nabla\psi^*)\cdot(\nabla\psi).$$

So now we have

$$\frac{\partial\rho}{\partial t} = \frac{-\hbar}{m}\nabla\cdot\mathrm{Im}(\psi^*\nabla\psi) + \frac{e}{mc}\nabla\cdot(\vec{A}|\psi|^2)$$

and thus

$$\frac{\partial\rho}{\partial t} + \nabla\cdot\vec{j} = 0 \qquad \text{where} \qquad \vec{j} = \frac{\hbar}{m}\mathrm{Im}(\psi^*\nabla\psi) - \frac{e}{mc}\vec{A}|\psi|^2.$$

We get the continuity equation for our probability density, with an extra term in the probability current proportional to the probability that the particle is at a spot and the EM field strength at that spot. The coupling to the EM field changes how the wavefunction evolves with time.

For the second part of this problem, we'll be working solely with operators. From the Heisenberg equation of motion,

$$\frac{d\vec{\Pi}}{dt} = \frac{1}{i\hbar}[\vec{\Pi}, H] = \frac{1}{i\hbar}\left(\frac{1}{2m}[\vec{\Pi}, \vec{\Pi}^2] + e[\vec{\Pi}, \phi]\right).$$

Let's work with the individual components here. I'll work in Einstein notation, which is a common convention for equations in physics: any repeated index in a term is understood to be summed over. In effect, I'm just dropping the summation signs in front of the expressions. Any index that you only see one copy of in a term is not summed over.

The second commutator is pretty simple:

$$[\Pi_i, \phi] = [p_i, \phi] = -i\hbar\partial_i\phi$$

where $\partial_i = \frac{\partial}{\partial x_i}$. The first commutator, however, is not as simple as it looks. The canonical commutation relations involve x_i and p_i, and Π_i contains both of them. While $[\Pi_i, \Pi_i] = 0$, $[\Pi_i, \Pi_j]$ is not necessarily 0.

$$\begin{aligned}
[\Pi_i, \Pi_j] &= -\frac{e}{c}\left([p_i, A_j] + [A_i, p_j]\right) = \frac{ie\hbar}{c}(\partial_i A_j - \partial_j A_i) \\
&= \frac{ie\hbar}{c}(\delta_{ki}\delta_{lj} - \delta_{kj}\delta_{li})\partial_k A_l \\
&= \frac{ie\hbar}{c}\epsilon_{mkl}\epsilon_{mij}\partial_k A_l \\
&= \frac{ie\hbar}{c}\epsilon_{ijm}(\nabla \times \vec{A})_m \\
&= \frac{ie\hbar}{c}\epsilon_{ijm}B_m
\end{aligned}$$

where ϵ_{ijk} is the Levi-Civita tensor and I've used the contracted epsilon identity and the definition of the cross product. If you are not familiar with Einstein notation, this is a good opportunity to learn: i and j are not contracted anywhere in any of this stuff (how can they be, since they are not summed over in the commutator?) but the rest of the indices are contracted and summed over.

With the foresight we have by looking at what the final answer is, let's try to compute what $\frac{dx_i}{dt}$ is for this Hamiltonian:

$$\begin{aligned}
\frac{dx_i}{dt} &= \frac{1}{i\hbar}[x_i, H] = \frac{1}{i\hbar}\left[x_i, \frac{p_j p_j}{2m} - \frac{e}{2mc}(p_k A_k + A_k p_k)\right] \\
&= \frac{p_i}{m} - \frac{e}{mc}A_i = \frac{\Pi_i}{m},
\end{aligned}$$

so, as some may have expected, the position operator evolves with time according to the kinematic momentum $\vec{\Pi}$, just like it did for the free particle Hamiltonian.

Finally, we can put this all together:

$$\begin{aligned}
\frac{d\Pi_i}{dt} &= \frac{1}{i\hbar}\left(\frac{1}{2m}(\Pi_j[\Pi_i,\Pi_j] + [\Pi_i,\Pi_j]\Pi_j) + e[\Pi_i,\phi]\right) \\
&= \frac{e}{2mc}\left(\epsilon_{ijm}\Pi_j B_m + \epsilon_{ijm}B_m\Pi_j\right) - e\partial_i\phi \\
&= \frac{e}{2c}\left(\epsilon_{ijm}\frac{\Pi_j}{m}B_m - \epsilon_{imj}B_m\frac{\Pi_j}{m}\right) - e\partial_i\phi \\
&= \frac{e}{2c}\left[\left(\frac{d\vec{x}}{dt}\times\vec{B}\right)_i - \left(\vec{B}\times\frac{d\vec{x}}{dt}\right)_i\right] - e\partial_i\phi \\
\Longrightarrow \frac{d\vec{\Pi}}{dt} &= \frac{e}{2c}\left[\frac{d\vec{x}}{dt}\times\vec{B} - \vec{B}\times\frac{d\vec{x}}{dt}\right] - e\nabla\phi.
\end{aligned}$$

2 Sakurai p.150, #37

We want to compute the phase shift produced by the time evolution of the neutron's wavefunction in the magnetic field. For simplicity, we'll only consider the component of the magnetic field perpendicular to the neutron's motion (since that's the only part of the field that affects the neutron anyway), and we have the freedom to let that field be in the x-direction, while the neutron travels in the z-direction.

Our time-evolution operator is

$$\begin{aligned}
\exp\left[-\frac{i}{\hbar}HT\right] &= \exp\left[-\frac{i}{\hbar}\left(\frac{p_z^2}{2m} - \vec{\mu}\cdot\vec{B}\right)T\right] \\
&= \exp\left[-\frac{i}{\hbar}\left(\frac{p_z^2}{2m} - g_n\frac{eB}{m_n c}S_x\right)T\right].
\end{aligned}$$

The first term in the exponent will be the same for both arms, but the second term will be different because it depends on the magnetic field. Because the S_x operator returns an eigenvalue of $\hbar/2$ regardless of whether the neutron is spin-up or spin-down,

$$-\frac{i}{\hbar}(-\vec{\mu}\cdot\vec{B})T = \frac{i}{\hbar}g_n\frac{e\hbar B}{2m_n c}T.$$

But, we also have

$$T = \frac{l}{v_z} = \frac{l}{p_z/m_n} = \frac{lm_n}{h/\lambda} = \frac{\lambda l m_n}{2\pi\hbar}$$

where the neutrons travel through a magnetic field region of length l with de Broglie wavelength λ. Thus, the neutron picks up a phase shift

$$\phi = \frac{g_n eB}{2m_n c}\frac{\lambda l m_n}{2\pi\hbar} = \frac{g_n e\lambda l}{4\pi\hbar c}B$$

from the interaction with the magnetic field. The difference in the phase shifts between neutrons in magnetic fields that correspond to successive maxima in the counting rates must equal 2π, so

$$\Delta\phi = \frac{g_n|e|\lambda l}{4\pi\hbar c}\Delta B = 2\pi \qquad \Longrightarrow \qquad \Delta B = \frac{8\pi^2\hbar c}{g_n|e|\lambda l}.$$

3 SHO Partiton Function

(a) I hope you like Gaussian integrals. They are awesome because $\int_{-\infty}^{\infty} dx\, e^{-x^2} = \sqrt{\pi}$. Also note that $\sin(ix) = i\,\sinh(x)$ and $\cos(ix) = \cosh(x)$.

$$\begin{aligned} Z &= \int_{-\infty}^{\infty} dx \sqrt{\frac{m\omega}{2\pi i \sin\omega t}} \exp\left\{ i\frac{m\omega}{2\sin\omega t}\, 2[\cos\omega t - 1]\, x^2 \right\}\Bigg|_{t=-i\hbar\beta} \\ &= \int_{-\infty}^{\infty} dx \sqrt{\frac{m\omega}{2\pi i \sin(-i\beta\hbar\omega)}} \exp\left\{ i\frac{m\omega}{2\sin(-i\beta\hbar\omega)}\, 2[\cos(-i\beta\hbar\omega) - 1]\, x^2 \right\} \\ &= \sqrt{\frac{m\omega}{2\pi \sinh(\beta\hbar\omega)}} \int_{-\infty}^{\infty} dx\, \exp\left\{ -\frac{m\omega}{\sinh(\beta\hbar\omega)} [\cosh(\beta\hbar\omega) - 1]\, x^2 \right\} \end{aligned}$$

To get this into Gaussian integral form, make the transformation

$$u = \sqrt{\frac{m\omega}{\sinh(\beta\hbar\omega)}} \sqrt{\cosh(\beta\hbar\omega) - 1}\; x.$$

$$\begin{aligned} Z &= \sqrt{\frac{m\omega}{2\pi\sinh(\beta\hbar\omega)}} \sqrt{\frac{\sinh(\beta\hbar\omega)}{m\omega}} \sqrt{\frac{1}{\cosh(\beta\hbar\omega) - 1}} \int_{-\infty}^{\infty} du\, e^{-u^2} \\ &= \frac{1}{\sqrt{2}} \sqrt{\frac{1}{\cosh(\beta\hbar\omega) - 1}} \\ &= \sqrt{\frac{1}{e^{\beta\hbar\omega} + e^{-\beta\hbar\omega} + 2}} \\ &= \sqrt{\frac{e^{-\beta\hbar\omega}}{(1 - e^{-\beta\hbar\omega})^2}} \\ &= \frac{e^{-\beta\hbar\omega/2}}{1 - e^{-\beta\hbar\omega}} = \sum_{j=0}^{\infty} e^{-\beta(j+1/2)\hbar\omega}. \end{aligned}$$

(b) It is pretty simple to show that $-\frac{\partial}{\partial\beta}\ln Z = \sum_i E_i P_i$:

$$\begin{aligned} -\frac{\partial}{\partial\beta}\ln Z &= -\frac{1}{Z}\frac{\partial}{\partial\beta}\sum_i e^{-\beta E_i} \\ &= \sum_i E_i \frac{e^{-\beta E_i}}{Z} = \sum_i E_i P_i = \bar{E}. \end{aligned}$$

Then, we can show that $-\frac{\partial}{\partial\beta}\ln Z$ equals the listed value:

$$\begin{aligned} \bar{E} &= -\frac{\partial}{\partial\beta}\ln\left(\frac{e^{-\beta\hbar\omega/2}}{1 - e^{-\beta\hbar\omega}}\right) \\ &= -\frac{\partial}{\partial\beta}\left[-\frac{\beta\hbar\omega}{2} - \ln\left(1 - e^{-\beta\hbar\omega}\right)\right] \\ &= \hbar\omega\left(\frac{1}{2} + \frac{e^{-\beta\hbar\omega}}{1 - e^{-\beta\hbar\omega}}\right) \\ &= \hbar\omega\left(\frac{1}{2} + \frac{1}{e^{\beta\hbar\omega} - 1}\right). \end{aligned}$$

Alternatively, we can also show that the definition of $\bar{E}$ also equals the listed value, though this takes a bit more work:

$$\begin{aligned}
\bar{E} = \sum_n E_n \frac{e^{-\beta E_n}}{Z} &= \sum_{n=0}^{\infty}\left(n+\frac{1}{2}\right)\hbar\omega\; e^{-\beta(n+1/2)\hbar\omega}\;\frac{1-e^{-\beta\hbar\omega}}{e^{-\beta\hbar\omega/2}} \\
&= \hbar\omega(1-e^{-\beta\hbar\omega})\left\{\frac{1}{2}\sum_{n=0}^{\infty}\left(e^{-\beta\hbar\omega}\right)^n + \sum_{n=0}^{\infty} n\left(e^{-\beta\hbar\omega}\right)^n\right\} \\
&= \hbar\omega(1-e^{-\beta\hbar\omega})\left\{\frac{1}{2}\frac{1}{1-e^{-\beta\hbar\omega}} + e^{-\beta\hbar\omega}\sum_{n=0}^{\infty} n\left(e^{-\beta\hbar\omega}\right)^{n-1}\right\} \\
&= \frac{\hbar\omega}{2} + \hbar\omega(1-e^{-\beta\hbar\omega})e^{-\beta\hbar\omega}\frac{d}{de^{-\beta\hbar\omega}}\sum_{n=0}^{\infty}\left(e^{-\beta\hbar\omega}\right)^n \\
&= \frac{\hbar\omega}{2} + \hbar\omega(1-e^{-\beta\hbar\omega})e^{-\beta\hbar\omega}\frac{d}{de^{-\beta\hbar\omega}}\frac{1}{1-e^{-\beta\hbar\omega}} \\
&= \frac{\hbar\omega}{2} + \hbar\omega(1-e^{-\beta\hbar\omega})e^{-\beta\hbar\omega}\frac{1}{(1-e^{-\beta\hbar\omega})^2} \\
&= \hbar\omega\left(\frac{1}{2}+\frac{1}{e^{\beta\hbar\omega}-1}\right).
\end{aligned}$$

(c) For this part, it helps to know that $\frac{\partial\beta}{\partial T} = \frac{-1}{k_B T^2}$ and $\frac{\theta_E}{T} = \beta\hbar\omega$.

$$\begin{aligned}
C = \frac{1}{N_0}\frac{\partial \bar{E}_{\text{crystal}}}{\partial T} &= \frac{3N_0}{N_0}\frac{\partial\bar{E}}{\partial\beta}\frac{\partial\beta}{\partial T} \\
&= 3\hbar\omega\,\frac{-\hbar\omega e^{\beta\hbar\omega}}{(e^{\beta\hbar\omega}-1)^2}\,\frac{-1}{k_B T^2} \\
&= 3k_B\left(\frac{\hbar\omega}{k_B T}\right)^2\frac{e^{\beta\hbar\omega}}{(e^{\beta\hbar\omega}-1)^2} \\
&= 3k_B\left(\frac{\theta_E}{T}\right)^2\frac{e^{\theta_E/T}}{(e^{\theta_E/T}-1)^2}.
\end{aligned}$$

For high temperatures, $\frac{\theta_E}{T} \ll 1$, so we can expand the exponentials and cut off higher-order terms:

$$C \longrightarrow 3k_B\left(\frac{\theta_E}{T}\right)^2\frac{1+\ldots}{(1+\frac{\theta_E}{T}+\ldots-1)^2} \longrightarrow 3k_B.$$

For low temperatures, $\frac{\theta_E}{T} \gg 1$, so we can rewrite the fraction in terms of $\exp(-\theta_E/T)$ and argue that the exponential in the denominator is much, much smaller than 1:

$$C = 3k_B\left(\frac{\theta_E}{T}\right)^2\frac{e^{-\theta_E/T}}{(1-e^{-\theta_E/T})^2} \longrightarrow 3k_B\left(\frac{\theta_E}{T}\right)^2 e^{-\theta_E/T}.$$

4 Sakurai, p148, #25

(a) Alright. Let's solve the Schrödinger equation for this wavefunction, pursuant to the boundary conditions:

$$-\frac{\hbar^2}{2m_e}\nabla^2\psi(\rho,\phi,z) = E\psi(\rho,\phi,z) \qquad \begin{cases} \psi(\rho_a,\phi,z) = \psi(\rho_b,\phi,z) = 0 \\ \psi(\rho,\phi,0) = \psi(\rho,\phi,L) = 0 \\ \psi(\rho,\phi+2\pi,z) = \psi(\rho,\phi,z) \end{cases}$$

Since we'll be naturally operating in cylindrical coordinates, we'll need the Laplacian in cylindrical coordinates:

$$\nabla^2 = \frac{1}{\rho}\frac{\partial}{\partial\rho}\left(\rho\frac{\partial}{\partial\rho}\right)+\frac{1}{\rho^2}\frac{\partial^2}{\partial\phi^2}+\frac{\partial^2}{\partial z^2}.$$

As with most of the tractable partial differential equations given to physics students, this one is solvable by separation of variables, so let's let

$$\psi(\rho,\phi,z) = R(\rho)Y(\phi)Z(z).$$

This allows us to rewrite our differential equation by introducing this definition of ϕ and dividing both sides by ϕ. In the end, we get

$$\frac{1}{R(\rho)}\frac{1}{\rho}\frac{\partial}{\partial\rho}\left(\rho\frac{\partial R(\rho)}{\partial\rho}\right)+\frac{1}{Y(\phi)}\frac{1}{\rho^2}\frac{\partial^2 Y(\phi)}{\partial\phi^2}+\frac{1}{Z(z)}\frac{\partial^2 Z(z)}{\partial z^2}+\frac{2m_eE}{\hbar^2}=0$$

with boundary conditions

$$\begin{cases} R(\rho_a) = R(\rho_b) = 0 \\ Z(0) = Z(L) = 0 \\ Y(\phi+2\pi) = Y(\phi) \end{cases}$$

Note that, in this form, the $Z(z)$ term is the only one dependent on z and it is not dependent on any other variables. So, the term must be a constant. With a little foresight and the knowledge that whatever we get will have to satisfy the boundary conditions at $z = 0$ and $z = L$, we'll let this constant be $-C_z^2$.

$$\frac{\partial^2 Z(z)}{\partial z^2} = -C_z^2 Z(z)$$

This admits solutions $Z(z) = A\cos(C_z z)+B\sin(C_z z)$. Applying the boundary conditions on $Z(z)$, we find that

$$Z(z) = A_z \sin\left(\frac{l\pi}{L}z\right) \qquad\qquad C_z = \frac{l\pi}{L}, \quad l = 1, 2, 3, \ldots$$

where our restrictions on the possible values of l ensure that our solutions satisfy the boundary conditions, are nontrivial, and are unique.

We return to our original equation and note that, if we multiply both sides by ρ^2, we again get a term that only depends on one variable, ϕ, and is the only term dependent on ϕ:

$$\frac{\rho}{R(\rho)}\frac{\partial}{\partial\rho}\left(\rho\frac{\partial R(\rho)}{\partial\rho}\right)+\frac{1}{Y(\phi)}\frac{\partial^2 Y(\phi)}{\partial\phi^2}+\rho^2\left[-\left(\frac{l\pi}{L}\right)^2+\frac{2m_eE}{\hbar^2}\right]=0$$

The differential equation for $Y(\phi)$ is the same, and we'll let it be $Y(\phi) = A_\phi e^{im\phi}$. Because of the periodic boundary condition, m is constrained to be an integer.

Let's go back to our original equation, expand the first term, and multiply both sides by $R(\rho)$.

$$\rho^2\frac{\partial^2 R(\rho)}{\partial\rho^2}+\rho\frac{\partial R(\rho)}{\partial\rho}+\left\{\rho^2\left[-\left(\frac{l\pi}{L}\right)^2+\frac{2m_eE}{\hbar^2}\right]-m^2\right\}R(\rho)=0; \qquad l = 1,2,3,\ldots; m \in Z$$

This is almost in the form we need to realize $R(\rho)$ as a solution to Bessel's differential equation, but we need to get rid of the coefficient of $\rho^2 R(\rho)$. Let

$$\xi = \sqrt{\frac{2m_eE}{\hbar^2}-\left(\frac{l\pi}{L}\right)^2}$$

and note that solving the differential equation in terms of $\xi\rho$ instead of ρ will leave the form of the first two terms untouched. Now we have

$$(\xi\rho)^2\frac{\partial^2 R(\xi\rho)}{\partial(\xi\rho)^2} + (\xi\rho)\frac{\partial R(\xi\rho)}{\partial(\xi\rho)} + [(\xi\rho)^2 - m^2]R(\xi\rho) = 0$$

which admits solutions $R(\xi\rho) = AJ_m(\xi\rho) + BN_m(\xi\rho)$ where J_m and N_m are Bessel functions of the first and second kind, respectively, with order m. Applying our boundary conditions gives us a system of equations

$$AJ_m(\xi\rho_a) + BN_m(\xi\rho_b) = 0$$
$$AJ_m(\xi\rho_b) + BN_m(\xi\rho_b) = 0.$$

with which we can solve for the allowed values of ξ that make the radial wavefunction become zero at both the inner and outer cylinder walls:

$$J_m(\xi\rho_b)N_m(\xi\rho_a) - J_m(\xi\rho_a)N_m(\xi\rho_b) = 0.$$

Let us designate the nth value of ξ that solves this mth-order equation k_{mn}. We can now write out the full non-normalized wavefunction:

$$\psi_{lmn}(\rho,\phi,z) = A[N_m(k_{mn}\rho_*)J_m(k_{mn}\rho) - J_m(k_{mn}\rho_*)N_m(k_{mn}\rho)]\; e^{im\phi}\; \sin\left(\frac{l\pi}{L}z\right)$$

where $\rho_* = \rho_a$ or ρ_b, $l = 1, 2, 3, \ldots$, $m \in Z$, and k_{mn} is the nth root of the equation

$$J_m(k_{mn}\rho_b)N_m(k_{mn}\rho_a) - J_m(k_{mn}\rho_a)N_m(k_{mn}\rho_b) = 0.$$

Finally, we can get the energy levels from the definition of $\xi = k_{mn}$:

$$k_{mn} = \sqrt{\frac{2m_e E_{lmn}}{\hbar^2} - \left(\frac{l\pi}{L}\right)^2} \qquad \Longrightarrow \qquad E_{lmn} = \frac{\hbar^2}{2m_e}\left[k_{mn}^2 + \left(\frac{l\pi}{L}\right)^2\right].$$

(b) Our Hamiltonian changes to the form

$$H = \frac{\vec{p}^2}{2m_e} - \frac{e}{2m_e c}(\vec{p}\cdot\vec{A} + \vec{A}\cdot\vec{p}) + \frac{e^2}{2m_e c^2}\vec{A}^2.$$

So what is $\vec{A}$, if all we know is $\vec{B} = B\hat{z}$ for $\rho < \rho_a$ and zero elsewhere?

The easiest way I know to get $\vec{A}$ involves applying Stokes' theorem to a flat, 2D circular disk in the $\rho - \phi$ plane and centered at $\rho = 0$. In the region $\rho < \rho_a$, we let the disk have radius $\rho < \rho_a$:

$$\int_S (\nabla\times\vec{A})\cdot d\vec{S} = \oint_{\partial S} \vec{A}\cdot d\vec{l}$$
$$\int_S \vec{B}\cdot d\vec{S} = \oint_{\partial S} \vec{A}\cdot d\vec{l}$$
$$B\,(\pi\rho^2) = A_\phi\,(2\pi\rho)$$
$$A_\phi = \frac{B}{2}\rho; \qquad\qquad \rho < \rho_a.$$

If we let the other components of $\vec{A}$ be zero, we find that we get the correct magnetic field inside $\rho < \rho_a$. Of course, this is gauge-dependent, and you can pick any gauge you want. Outside of ρ_a, the magnetic field drops to zero, so

$$B\,(\pi\rho_a^2) = A_\phi\,(2\pi\rho)$$
$$A_\phi = \frac{B\rho_a^2}{2}\frac{1}{\rho}; \qquad\qquad \rho \geq \rho_a.$$

Again letting the other components of $\vec{A}$ be zero, we recover zero magnetic field outside ρ_a and a continuous vector potential.

Let's put our answer for $\vec{A}$ into the Hamiltonian. With this choice of $\vec{A}$, it turns out that $\vec{A}$ and the gradient operator commute.

$$\begin{aligned} H &= \frac{\vec{p}^2}{2m_e} - \frac{e}{m_e c}\vec{A}\cdot\vec{p} + \frac{e^2}{2m_e c^2}\vec{A}^2 \\ &= -\frac{\hbar^2}{2m_e}\nabla^2 + i\frac{e\hbar B\rho_a^2}{2m_e c}\frac{1}{\rho^2}\frac{\partial}{\partial\phi} + \frac{eB^2\rho_a^4}{8m_e c^2}\frac{1}{\rho^2} \end{aligned}$$

With the benefit of foresight, let

$$\zeta = \frac{eB\rho_a^2}{2\hbar c},$$

which is dimensionless. Then, our Hamiltonian becomes

$$H = -\frac{\hbar^2}{2m_e}\left[\nabla^2 - i\frac{2\zeta}{\rho^2}\frac{\partial}{\partial\phi} - \frac{\zeta^2}{\rho^2}\right].$$

Redoing the same steps with this new Hamiltonian,

$$\frac{1}{R(\rho)}\frac{1}{\rho}\frac{\partial}{\partial\rho}\left(\rho\frac{\partial R(\rho)}{\partial\rho}\right) + \frac{1}{Y(\phi)}\frac{1}{\rho^2}\left[\frac{\partial^2 Y(\phi)}{\partial\phi^2} - i2\zeta\frac{\partial Y(\phi)}{\partial\phi}\right] + \frac{1}{Z(z)}\frac{\partial^2 Z(z)}{\partial z^2} + \frac{2m_e E}{\hbar^2} - \frac{\zeta^2}{\rho^2} = 0$$

with the same boundary conditions as before. The solution in the $Z(z)$ sector is the same, but we end up with a different differential equation for $Y(\phi)$:

$$\frac{\partial^2 Y(\phi)}{\partial\phi^2} - i2\zeta\frac{\partial Y(\phi)}{\partial\phi} + C_\phi^2 Y(\phi) = 0.$$

Knowing that we still need a sinusoidal solution in ϕ that obeys the periodic boundary condition, we can try a trial solution $Y(\phi) = A_\phi e^{iM\phi}$ where $M \in Z$. This gives us the equation

$$-M^2 + 2\zeta M + C_\phi^2 = 0 \qquad \Longrightarrow \qquad -C_\phi^2 = -M^2 + 2\zeta M.$$

Putting this back in,

$$\begin{aligned} \frac{1}{R(\rho)}\frac{1}{\rho}\frac{\partial}{\partial\rho}\left(\rho\frac{\partial R(\rho)}{\partial\rho}\right) + \frac{1}{\rho^2}(-M^2 + 2\zeta M) - \left(\frac{l\pi}{L}\right)^2 + \frac{2m_e E}{\hbar^2} - \frac{\zeta^2}{\rho^2} = 0 \\ \rho^2\frac{\partial^2 R(\rho)}{\partial\rho^2} + \rho\frac{\partial R(\rho)}{\partial\rho} + \left\{\left[-\left(\frac{l\pi}{L}\right)^2 + \frac{2m_e E}{\hbar^2}\right]\rho^2 - (M-\zeta)^2\right\}R(\rho) = 0 \end{aligned}$$

We get the same equation we had before, with the same formulas for the wavefunction and energy spectrum, except that $m \longrightarrow M - \zeta = \frac{eB\rho_a^2}{2\hbar c}$! This shifts the orders of the Bessel functions to different values, which are not necessarily integers. The spacing between the orders is still 1, however.

(c) If switching on the magnetic field doesn't result in an energy change in the ground state, then the Bessel orders $M - \zeta$ must still be integers. But since M is an integer, this means that ζ must be an integer:

$$\begin{aligned} \zeta &= \frac{eB\rho_a^2}{2\hbar c} = N \\ \Phi &= B\pi\rho_a^2 = \frac{2\pi\hbar c}{e}N = \frac{hc}{e}N; \qquad N \in Z \end{aligned}$$

$\boxed{5}$ Charged particle in a magnetic field

(a) Classically, the charged particle will obey the Lorentz force law: $\vec{F} = \frac{e}{c}\vec{v} \times \vec{B}$. $\vec{B} = \nabla \times \vec{A} = B\hat{z}$, so

$$\begin{aligned} m\ddot{x} &= \frac{eB}{c}\dot{y} \\ m\ddot{y} &= -\frac{eB}{c}\dot{x} \\ m\ddot{z} &= 0. \end{aligned}$$

Identifying $\omega_0 = \frac{eB}{mc}$, we can solve the first two equations by taking another derivative:

$$\begin{aligned} \ddot{x} &= \omega_0 \dot{y} \\ \ddot{y} &= -\omega_0 \dot{x} \end{aligned} \qquad \Longrightarrow \qquad \begin{aligned} \dddot{x} &= \omega_0 \ddot{y} = -\omega_0^2 \dot{x} \\ \dddot{y} &= -\omega_0 \ddot{x} = -\omega_0^2 \dot{y} \end{aligned}$$

With some foresight, let's choose the solutions

$$\begin{aligned} \dot{x}(t) &= -\omega_0 A \sin(\omega_0 t + \delta) \\ \dot{y}(t) &= -\omega_0 A \cos(\omega_0 t + \delta) \end{aligned}$$

so that our final answer ends up being

$$\begin{aligned} x(t) &= A\cos(\omega_0 t + \delta) + x_0 \\ y(t) &= -A\sin(\omega_0 t + \delta) + y_0 \\ z(t) &= v_{0z} t + z_0. \end{aligned}$$

(b) We make the canonical transformation to

$$\begin{aligned} Q &= \frac{c}{eB}\Pi_x = \frac{c}{eB}\left(p_x + \frac{eB}{2c}y\right) \\ P &= \Pi_y = p_y - \frac{eB}{2c}x. \end{aligned}$$

We can show that this transformation is indeed canonical by computing the commutator:

$$[Q, P] = \frac{c}{eB}[\Pi_x, \Pi_y] = \frac{c}{eB}\frac{ie\hbar}{c}B = i\hbar$$

where I have used $[\Pi_i, \Pi_j] = \frac{ie\hbar}{c}\epsilon_{ijm}B_m$ from problem (1).

Writing the Hamiltonian in terms of P and Q,

$$H = \frac{1}{2m}\left(\frac{e^2B^2}{c^2}Q^2 + P^2 + p_z^2\right) = \frac{P^2}{2m} + \frac{1}{2}m\left(\frac{eB}{mc}\right)^2 Q^2 + \frac{p_z^2}{2m}.$$

The first two terms represent a 1D simple harmonic oscillator with $\omega_0 = \frac{eB}{mc}$, while the last term represents a free particle in the z-direction. So, $E = (n + \frac{1}{2})\hbar\omega_0 + \frac{\hbar^2 k^2}{2m}$.

You might be wondering how what we did is kosher. How did we go from a 2D simple harmonic oscillator to a 1D simple harmonic oscillator, just by redefining our variables? We seem to have lost two degrees of freedom. Well, fear not: we can define a second set of canonical variables that are conjugate to Q and P,

$$\begin{aligned} \bar{Q} &= \frac{c}{eB}\left(p_y + \frac{eB}{2c}x\right) \\ \bar{P} &= p_x - \frac{eB}{2c}y, \end{aligned}$$

which satisfy $[\bar{Q}, \bar{P}] = i\hbar$, $[Q, \bar{Q}] = 0$, and $[P, \bar{P}] = 0$. These canonical variables do not appear in the Hamiltonian because they represent helical motion opposing the direction preferred by the magnetic field.

(c) Expand!

$$\begin{aligned}
H &= \frac{1}{2m}\left[\left(p_x + \frac{eB}{2c}y\right)^2 + \left(p_y - \frac{eB}{2c}x\right)^2 + p_z^2\right] \\
&= \frac{p_x^2}{2m} + \frac{1}{2}m\left(\frac{eB}{2mc}\right)^2 x^2 + \frac{p_y^2}{2m} + \frac{1}{2}m\left(\frac{eB}{2mc}\right)^2 y^2 + \frac{p_z^2}{2m} - \frac{eB}{2mc}(xp_y - yp_x) \\
&= \frac{p_x^2}{2m} + \frac{1}{2}m\left(\frac{\omega_0}{2}\right)^2 x^2 + \frac{p_y^2}{2m} + \frac{1}{2}m\left(\frac{\omega_0}{2}\right)^2 y^2 + \frac{p_z^2}{2m} - \frac{\omega_0}{2}L_z \\
&= H\left(\frac{\omega_0}{2}, m\right) - \frac{\omega_0}{2}L_z
\end{aligned}$$

The basis for diagonalizing $H(\frac{\omega_0}{2}, m)$ will also diagonalize H if $[H(\frac{\omega_0}{2}, m), H] = 0$:

$$\begin{aligned}
\left[H\left(\frac{\omega_0}{2}, m\right), H\right] &= \left[H\left(\frac{\omega_0}{2}, m\right), -\frac{\omega_0}{2}L_z\right] \\
&= -\frac{\omega_0}{2}\left\{\frac{1}{2m}[p_x^2 + p_y^2, xp_y - yp_x] + \frac{1}{2}m\left(\frac{\omega_0}{2}\right)^2 [x^2 + y^2, xp_y - yp_x]\right\} \\
&= -\frac{\omega_0}{2}\left\{\frac{1}{2m}\left([p_x^2, x]p_y - [p_y^2, y]p_x\right) + \frac{1}{2}m\left(\frac{\omega_0}{2}\right)^2\left(-y[x^2, p_x] + x[y^2, p_y]\right)\right\} \\
&= -\frac{\omega_0}{2}\left\{\frac{1}{2m}\left(-2i\hbar p_x p_y + 2i\hbar p_y p_x\right) + \frac{1}{2}m\left(\frac{\omega_0}{2}\right)^2\left(-2i\hbar yx + 2i\hbar xy\right)\right\} \\
&= 0
\end{aligned}$$

So, this is indeed the case. The full Hamiltonian not only shares the same states as the Hamiltonian of a 2D SHO with angular frequency $\Omega = \frac{\omega_0}{2}$, but also the same energy levels and creation and annihilation operators:

$$a_x = \sqrt{\frac{m\Omega}{2\hbar}}\left(x + \frac{ip_x}{m\Omega}\right) \qquad a_x^\dagger = \sqrt{\frac{m\Omega}{2\hbar}}\left(x - \frac{ip_x}{m\Omega}\right)$$
$$a_y = \sqrt{\frac{m\Omega}{2\hbar}}\left(y + \frac{ip_y}{m\Omega}\right) \qquad a_y^\dagger = \sqrt{\frac{m\Omega}{2\hbar}}\left(y - \frac{ip_y}{m\Omega}\right)$$

with commutation relations $[a_x, a_x^\dagger] = [a_y, a_y^\dagger] = 1$ and 0 otherwise. The states are $\{\,|n_x', n_y', \hbar k_z\rangle\,\}$. We can also rewrite the angular momentum operator in terms of these ladder operators,

$$\begin{aligned}
L_z &= xp_y - yp_x \\
&= \left(\sqrt{\frac{\hbar}{2m\Omega}}(a_x + a_x^\dagger)\right)\left(-i\sqrt{\frac{m\Omega\hbar}{2}}(a_y - a_y^\dagger)\right) - \left(-i\sqrt{\frac{m\Omega\hbar}{2}}(a_y + a_y^\dagger)\right)\left(\sqrt{\frac{\hbar}{2m\Omega}}(a_x - a_x^\dagger)\right) \\
&= i\hbar(a_x a_y^\dagger - a_y a_x^\dagger)
\end{aligned}$$

and we get the Hamiltonian

$$H = \hbar\Omega(1 + a_x^\dagger a_x + a_y^\dagger a_y) - i\hbar\Omega(a_x a_y^\dagger - a_y a_x^\dagger) + \frac{p_z^2}{2m}.$$

However, since the classical motion is circular and our eigenstates of the Hamiltonian are also definite states of angular momentum L_z, let's rewrite the entire system in terms of clockwise and counterclockwise creation and annihilation operators

$$a_+ = \frac{1}{\sqrt{2}}(a_x - ia_y) \qquad a_+^\dagger = \frac{1}{\sqrt{2}}(a_x^\dagger + ia_y^\dagger)$$
$$a_- = \frac{1}{\sqrt{2}}(a_x + ia_y) \qquad a_-^\dagger = \frac{1}{\sqrt{2}}(a_x^\dagger - ia_y^\dagger).$$

These creation and annihilation operators also satisfy the normal commutation relations: $[a_+, a_+^\dagger] = [a_-, a_-^\dagger] = 1$ and 0 otherwise. Just as the previous set of ladder operators created and annihilated oscillations in the x- and y-directions, this set of ladder operators creates and annihilates oscillations in the clockwise and counterclockwise directions. To put the Hamiltonian in this form, we'll need the reverse conversion:

$$a_x = \frac{1}{\sqrt{2}}(a_+ + a_-) \qquad a_x^\dagger = \frac{1}{\sqrt{2}}(a_+^\dagger + a_-^\dagger)$$
$$a_y = \frac{i}{\sqrt{2}}(a_+ - a_-) \qquad a_y^\dagger = \frac{-i}{\sqrt{2}}(a_+^\dagger - a_-^\dagger)$$

so that

$$a_x^\dagger a_x + a_y^\dagger a_y = a_+^\dagger a_+ + a_-^\dagger a_- = n_+ + n_- \qquad a_x a_y^\dagger - a_y a_x^\dagger = -i(a_+^\dagger a_+ - a_-^\dagger a_-) = -i(n_+ - n_-),$$
$$L_z = \hbar(n_+ - n_-)$$

and

$$\begin{aligned} H &= \hbar\Omega(1 + n_+ + n_-) - \hbar\Omega(n_+ - n_-) + \frac{p_z^2}{2m} \\ &= \hbar\omega_0\left(\frac{1}{2} + n_-\right) + \frac{p_z^2}{2m}. \end{aligned}$$

Thus, we obtain the energy spectrum

$$E(n_-, k_z) = \hbar\omega_0\left(\frac{1}{2} + n_-\right) + \frac{\hbar^2 k_z^2}{2m_e}$$

with angular momenta $m = n_+ - n_-$. Note that the number of quanta for the + oscillator doesn't figure into this equation! This means that every energy level has infinite degeneracy.

To write it in the form indicated in the prompt, note that

$$n_+ + n_- = \begin{cases} 2n_- + |m| & m > 0 \\ 2n_+ + |m| & m < 0 \end{cases}$$

so that

$$\begin{aligned} H &= \hbar\Omega(1 + n_+ + n_-) - \hbar\Omega L_z + \frac{p_z^2}{2m_e} \\ E &= \hbar\Omega(1 + 2k + |m|) - \hbar\Omega m + \frac{\hbar k_z^2}{2m_e} \\ &= \hbar\omega_0\left(\frac{1}{2} + k + \frac{1}{2}(|m| - m)\right) + \frac{\hbar^2 k_z^2}{2m_e} \end{aligned}$$

where $k =\geq 0$. In this form, we see that for each state of definite angular momentum, there is a tower of possible energy levels. For states with angular momentum $m > 0$, the m-dependence disappears and you get the normal tower of levels starting with energy $\frac{1}{2}\hbar\omega_0$, but for states with $m < 0$, the tower effectively starts at $(\frac{1}{2} + |m|)\hbar\omega_0$. This is because setting m constrains the difference in numbers of quanta $n_+ - n_-$, and n_+ and n_- must both be ≥ 0.

You might be having a lot of trouble trying to visualize what this all conceptually means. There's a reason for this! L_z is the canonical angular momentum, not the physical angular momentum, analogous with how $\vec{p}$ is no longer the physical momentum upon the introduction of a vector potential. The physical angular momentum is

$$\begin{aligned} K_z &= x\Pi_y - y\Pi_x; \qquad\qquad \vec{\Pi} = \vec{p} - \frac{e}{c}\vec{A} \\ &= L_z - \frac{eB}{2c}(x^2 + y^2) \\ &= -\hbar(1 + 2a_-^\dagger a_- + a_+ a_- + a_+^\dagger a_-^\dagger). \end{aligned}$$

Calculating the expectation value of this for a given state $|n_+, n_-, k_z\rangle$, we get the relation

$$E = \frac{\omega_0}{2}(-\langle K_z\rangle) + \frac{\hbar^2 k_z^2}{2m_e}$$

which is what we would expect classically, given that $\langle K_z\rangle$ will be negative for $B > 0$.