

ELECTROMAGNETISM IN QUANTUM MECHANICS: EXAMPLE

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Reference: Griffiths, David J. (2005), Introduction to Quantum Mechanics, 2nd Edition; Pearson Education - Problem 4.60.

Following on from the post on the quantum treatment of electromagnetic force, suppose we have a system described by the vector potential

$$(0.1) \quad \mathbf{A} = \frac{B_0}{2} (x\hat{\mathbf{j}} - y\hat{\mathbf{i}})$$

and the scalar potential

$$(0.2) \quad \phi = Kz^2$$

This question is easier if we use cylindrical coordinates. First, we convert the vector potential into cylindrical coordinates using the transformation

$$(0.3) \quad \hat{\mathbf{i}} = \hat{\mathbf{r}} \cos \theta - \hat{\boldsymbol{\theta}} \sin \theta$$

$$(0.4) \quad \hat{\mathbf{j}} = \hat{\mathbf{r}} \sin \theta + \hat{\boldsymbol{\theta}} \cos \theta$$

$$(0.5) \quad \hat{\mathbf{k}} = \hat{\mathbf{z}}$$

Applying this we get

$$(0.6) \quad \mathbf{A} = \frac{B_0}{2} r \hat{\boldsymbol{\theta}}$$

Thus the vector potential depends only on r . Applying the formula for the curl in cylindrical coords we get

$$(0.7) \quad \mathbf{B} = \nabla \times \mathbf{A}$$

$$(0.8) \quad = B_0 \hat{\mathbf{z}}$$

Thus the magnetic field is constant and directed along the z axis.

The electric field is

$$(0.9) \quad \mathbf{E} = -\nabla\phi - \frac{\partial\mathbf{A}}{\partial t}$$

$$(0.10) \quad = -2Kz\hat{\mathbf{z}}$$

since \mathbf{A} does not depend on time.

Since we are looking for stationary states, we wish to solve the Schrödinger equation in the form $H\Psi = E\Psi$. The Hamiltonian is given in the previous post, so the equation to be solved is

$$(0.11) \quad \frac{1}{2m} \left(-\hbar^2 \nabla^2 \Psi + \frac{\hbar q}{-i} (2\mathbf{A} \cdot \nabla \Psi + \Psi \nabla \cdot \mathbf{A}) + q^2 |\mathbf{A}|^2 \Psi \right) + q\phi \Psi = E\Psi$$

From above, staying in cylindrical coordinates, we have

$$(0.12) \quad \nabla^2 \Psi = \frac{1}{r} \frac{\partial}{\partial r} \left(r \frac{\partial \Psi}{\partial r} \right) + \frac{1}{r^2} \frac{\partial^2 \Psi}{\partial \theta^2} + \frac{\partial^2 \Psi}{\partial z^2}$$

$$(0.13) \quad = \frac{\partial^2 \Psi}{\partial r^2} + \frac{1}{r} \frac{\partial \Psi}{\partial r} + \frac{1}{r^2} \frac{\partial^2 \Psi}{\partial \theta^2} + \frac{\partial^2 \Psi}{\partial z^2}$$

$$(0.14) \quad \mathbf{A} \cdot \nabla \Psi = \frac{B_0 r}{2} \frac{1}{r} \frac{\partial \Psi}{\partial \theta}$$

$$(0.15) \quad = \frac{B_0}{2} \frac{\partial \Psi}{\partial \theta}$$

$$(0.16) \quad \nabla \cdot \mathbf{A} = 0$$

$$(0.17) \quad |\mathbf{A}|^2 = \frac{B_0^2}{4} r^2$$

We therefore have the equation

$$(0.18) \quad -\frac{\hbar^2}{2m} \left[\frac{\partial^2 \Psi}{\partial r^2} + \frac{1}{r} \frac{\partial \Psi}{\partial r} + \frac{1}{r^2} \frac{\partial^2 \Psi}{\partial \theta^2} + \frac{\partial^2 \Psi}{\partial z^2} \right] +$$

$$(0.19) \quad \frac{i\hbar q B_0}{2m} \frac{\partial \Psi}{\partial \theta} + \frac{q^2 B_0^2}{8m} r^2 \Psi + qKz^2 \Psi = E\Psi$$

To get the angular momentum operator L_z in cylindrical coordinates, we need to write the cylindrical unit vectors in terms of rectangular coordinates

$$(0.20) \quad \hat{\mathbf{r}} = \cos \theta \hat{\mathbf{x}} + \sin \theta \hat{\mathbf{y}}$$

$$(0.21) \quad \hat{\theta} = -\sin \theta \hat{\mathbf{x}} + \cos \theta \hat{\mathbf{y}}$$

$$(0.22) \quad \hat{\mathbf{z}} = \hat{\mathbf{z}}$$

The angular momentum operator $\mathbf{L} = -i\hbar\mathbf{R} \times \nabla$ (where I've used an uppercase \mathbf{R} to represent the vector from the origin to the observation point, to distinguish it from the \mathbf{r} in cylindrical coordinates). We have

$$(0.23) \quad \mathbf{R} = r\hat{\mathbf{r}} + z\hat{\mathbf{z}}$$

and the gradient is

$$(0.24) \quad \nabla = \hat{\mathbf{r}} \frac{\partial}{\partial r} + \hat{\theta} \frac{1}{r} \frac{\partial}{\partial \theta} + \hat{\mathbf{z}} \frac{\partial}{\partial z}$$

Therefore

$$(0.25) \quad L_z = [-i\hbar\mathbf{R} \times \nabla]_z$$

$$(0.26) \quad = -i\hbar \frac{\partial}{\partial \theta}$$

We can therefore write 0.19 as

$$(0.27) \quad -\frac{\hbar^2}{2m} \left[\frac{\partial^2 \Psi}{\partial r^2} + \frac{1}{r} \frac{\partial \Psi}{\partial r} + \frac{\partial^2 \Psi}{\partial z^2} \right] + \frac{L_z^2}{2mr^2} \Psi -$$

$$(0.28) \quad \frac{qB_0}{2m} L_z \Psi + \frac{q^2 B_0^2}{8m} r^2 \Psi + qKz^2 \Psi = E\Psi$$

Since L_z commutes with H , we can choose Ψ to be an eigenfunction of both L_z and H . The eigenvalues of L_z are $\hbar m_z$ where m_z is an integer, so we can write 0.28 as

$$(0.29) \quad -\frac{\hbar^2}{2m} \left[\frac{\partial^2 \Psi}{\partial r^2} + \frac{1}{r} \frac{\partial \Psi}{\partial r} + \frac{\partial^2 \Psi}{\partial z^2} \right] + \frac{\hbar^2 m_z^2}{2mr^2} \Psi -$$

$$(0.30) \quad \frac{\hbar q B_0}{2m} m_z \Psi + \frac{q^2 B_0^2}{8m} r^2 \Psi + qKz^2 \Psi = E\Psi$$

Rearranging to put the constant coefficients on the RHS we get

$$(0.31) \quad -\frac{\hbar^2}{2m} \left[\frac{\partial^2 \Psi}{\partial r^2} + \frac{1}{r} \frac{\partial \Psi}{\partial r} + \frac{\partial^2 \Psi}{\partial z^2} \right] + \frac{\hbar^2 m_z^2}{2mr^2} \Psi$$

$$(0.32) \quad + \frac{q^2 B_0^2}{8m} r^2 \Psi + qKz^2 \Psi = \left(E + \frac{\hbar q B_0}{2m} m_z \right) \Psi$$

To solve this, we use separation of variables so that

$$(0.33) \quad \Psi(r, \theta, z) \equiv R(r)\Theta(\theta)Z(z)$$

We then get, after dividing through by $R(r)\Theta(\theta)Z(z)$ and separating into two equations, one for r and one for z :

$$(0.34) \quad -\frac{\hbar^2}{2m} \left[R'' + \frac{1}{r} R' - \frac{m_z^2}{r^2} R \right] + \frac{q^2 B_0^2}{8m} r^2 R = E_r R$$

$$(0.35) \quad -\frac{\hbar^2}{2m} Z'' + qKz^2 Z = E_z Z$$

where

$$(0.36) \quad E_r + E_z = E + \frac{\hbar q B_0}{2m} m_z$$

Equation 0.35 has the same form as a harmonic oscillator, so we know that the energy levels are

$$(0.37) \quad E_z = \left(n_z + \frac{1}{2} \right) \hbar \omega_z$$

where the angular frequency is

$$(0.38) \quad \omega_z \equiv \sqrt{\frac{2qK}{m}}$$

To solve 0.34, we can resort to a series solution in the same way as we solved the harmonic oscillator originally. Multiplying through by $-2m/\hbar^2$ we have

$$(0.39) \quad R'' + \frac{1}{r} R' - \frac{m_z^2}{r^2} R - \frac{q^2 B_0^2}{4\hbar^2} r^2 R = -\frac{2mE_r}{\hbar^2} R$$

First, we define the variable $\rho \equiv r\sqrt{qB_0/2\hbar} \equiv rx$. Making this substitution converts the equation to

$$(0.40) \quad x^2 R'' + \frac{x^2}{\rho} R' - x^2 \frac{m_z^2}{\rho^2} R - x^2 \rho^2 R = -\frac{2mE_r}{\hbar^2} R$$

$$(0.41) \quad R'' + \frac{1}{\rho} R' - \frac{m_z^2}{\rho^2} R - \rho^2 R = -\frac{4mE_r}{qB_0\hbar} R$$

Using the same analysis as in the harmonic oscillator case, we look at the behaviour of this equation for large ρ and observe that

$$(0.42) \quad R'' \approx \rho^2 R$$

so we can try factoring out a term $e^{-\rho^2/2}$ to get $R(\rho) = s(\rho)e^{-\rho^2/2}$ for some function $s(\rho)$ to be determined. We then get for the derivatives

$$(0.43) \quad R' = s' e^{-\rho^2/2} - \rho s e^{-\rho^2/2}$$

$$(0.44) \quad R'' = s'' e^{-\rho^2/2} - 2\rho s' e^{-\rho^2/2} + (\rho^2 - 1) s e^{-\rho^2/2}$$

Substituting these back into the original equation gives us an equation in the function $s(r)$.

$$(0.45) \quad s'' - \left(2\rho + \frac{1}{\rho}\right) s' - 2s - \frac{m_z^2}{\rho^2} s = -\frac{4m}{qB_0\hbar} E_r s$$

We now propose a series solution:

$$(0.46) \quad s(\rho) = \sum_{j=0}^{\infty} c_j \rho^j$$

$$(0.47) \quad s'(\rho) = \sum_{j=0}^{\infty} j c_j \rho^{j-1}$$

$$(0.48) \quad s''(\rho) = \sum_{j=0}^{\infty} j(j-1) c_j \rho^{j-2}$$

Inserting these into 0.45 and equating terms for each power of ρ gives

$$(0.49) \quad [(j+2)(j+1) + (j+2) - m_z^2] c_{j+2} - 2(j+1) c_j = -\frac{4m}{qB_0\hbar} E_r c_j$$

$$(0.50) \quad [(j+2)^2 - m_z^2] c_{j+2} - 2(j+1) c_j = -\frac{4m}{qB_0\hbar} E_r c_j$$

This gives the recursion relation

$$(0.51) \quad c_{j+2} = \frac{2(j+1) - \frac{4m}{qB_0\hbar} E_r}{(j+2)^2 - m_z^2} c_j$$

For large j this has the asymptotic form $c_{j+2} \sim 2c_j/j$ so to keep the solution finite, the series must terminate, so for some value of j we must have

$$(0.52) \quad E_r = \frac{qB_0\hbar}{m} \frac{(j+1)}{2}$$

Since 0.51 is a recursion relation for every second coefficient, the only way the series can terminate is if either $c_0 = 0$ or $c_1 = 0$. If $c_1 = 0$ then all the j s are even and from 0.36 and 0.37 the total energy is

The total energy is therefore

$$(0.53) \quad E = E_z + E_r - \frac{\hbar q B_0}{2m} m_z$$

$$(0.54) \quad = \left(n_z + \frac{1}{2} \right) \hbar \omega_z + \hbar \omega_r \left(n_r + \frac{1}{2} \right)$$

$$(0.55) \quad n_r = \frac{j - m_z}{2}$$

$$(0.56) \quad \omega_z = \sqrt{2qK/m}$$

$$(0.57) \quad \omega_r = qB_0/m$$

I'm not entirely satisfied with this solution, since there's no obvious reason why we should exclude the odd j series. Also, it appears that n_r is restricted only to *half*-integer values, since m_z is an integer and even if j is even, $j - m_z$ can be either even or odd.