

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

$$\mathbf{A} = \frac{B_0}{2} (x\hat{\mathbf{j}} - y\hat{\mathbf{i}}) \quad (1)$$

and the scalar potential

$$\varphi = Kz^2 \quad (2)$$

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

$$\hat{\mathbf{i}} = \hat{\mathbf{r}} \cos \theta - \hat{\boldsymbol{\theta}} \sin \theta \quad (3)$$

$$\hat{\mathbf{j}} = \hat{\mathbf{r}} \sin \theta + \hat{\boldsymbol{\theta}} \cos \theta \quad (4)$$

$$\hat{\mathbf{k}} = \hat{\mathbf{z}} \quad (5)$$

Applying this we get

$$\mathbf{A} = \frac{B_0}{2} r \hat{\boldsymbol{\theta}} \quad (6)$$

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

$$\mathbf{B} = \nabla \times \mathbf{A} \quad (7)$$

$$= B_0 \hat{\mathbf{z}} \quad (8)$$

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

The electric field is

$$\mathbf{E} = -\nabla\varphi - \frac{\partial\mathbf{A}}{\partial t} \quad (9)$$

$$= -2Kz\hat{\mathbf{z}} \quad (10)$$

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

$$\frac{1}{2m} \left(-\hbar^2 \nabla^2 \Psi + \frac{\hbar q}{-i} (2\mathbf{A} \cdot \nabla \Psi + \Psi \nabla \cdot \mathbf{A}) + q^2 |\mathbf{A}|^2 \Psi \right) + q\phi \Psi = E\Psi \quad (11)$$

From above, staying in cylindrical coordinates, we have

$$\nabla^2 \Psi = \frac{1}{r} \frac{\partial}{\partial r} \left(r \frac{\partial \Psi}{\partial r} \right) + \frac{1}{r^2} \frac{\partial^2 \Psi}{\partial \theta^2} + \frac{\partial^2 \Psi}{\partial z^2} \quad (12)$$

$$= \frac{\partial^2 \Psi}{\partial r^2} + \frac{1}{r} \frac{\partial \Psi}{\partial r} + \frac{1}{r^2} \frac{\partial^2 \Psi}{\partial \theta^2} + \frac{\partial^2 \Psi}{\partial z^2} \quad (13)$$

$$\mathbf{A} \cdot \nabla \Psi = \frac{B_0 r}{2} \frac{1}{r} \frac{\partial \Psi}{\partial \theta} \quad (14)$$

$$= \frac{B_0}{2} \frac{\partial \Psi}{\partial \theta} \quad (15)$$

$$\nabla \cdot \mathbf{A} = 0 \quad (16)$$

$$|\mathbf{A}|^2 = \frac{B_0^2}{4} r^2 \quad (17)$$

We therefore have the equation

$$-\frac{\hbar^2}{2m} \left[\frac{\partial^2 \Psi}{\partial r^2} + \frac{1}{r} \frac{\partial \Psi}{\partial r} + \frac{1}{r^2} \frac{\partial^2 \Psi}{\partial \theta^2} + \frac{\partial^2 \Psi}{\partial z^2} \right] + \quad (18)$$

$$\frac{i\hbar q B_0}{2m} \frac{\partial \Psi}{\partial \theta} + \frac{q^2 B_0^2}{8m} r^2 \Psi + qKz^2 \Psi = E\Psi \quad (19)$$

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

$$\hat{\mathbf{r}} = \cos \theta \hat{\mathbf{x}} + \sin \theta \hat{\mathbf{y}} \quad (20)$$

$$\hat{\boldsymbol{\theta}} = -\sin \theta \hat{\mathbf{x}} + \cos \theta \hat{\mathbf{y}} \quad (21)$$

$$\hat{\mathbf{z}} = \hat{\mathbf{z}} \quad (22)$$

The angular momentum operator $\mathbf{L} = -i\hbar \mathbf{R} \times \nabla$ (where I've used an up-percase \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

$$\mathbf{R} = r\hat{\mathbf{r}} + z\hat{\mathbf{z}} \quad (23)$$

and the gradient is

$$\nabla = \hat{\mathbf{r}} \frac{\partial}{\partial r} + \hat{\boldsymbol{\theta}} \frac{1}{r} \frac{\partial}{\partial \theta} + \hat{\mathbf{z}} \frac{\partial}{\partial z} \quad (24)$$

Therefore

$$L_z = [-i\hbar \mathbf{R} \times \nabla]_z \quad (25)$$

$$= -i\hbar \frac{\partial}{\partial \theta} \quad (26)$$

We can therefore write 19 as

$$-\frac{\hbar^2}{2m} \left[\frac{\partial^2 \Psi}{\partial r^2} + \frac{1}{r} \frac{\partial \Psi}{\partial r} + \frac{\partial^2 \Psi}{\partial z^2} \right] + \frac{L_z^2}{2mr^2} \Psi - \quad (27)$$

$$\frac{qB_0}{2m} L_z \Psi + \frac{q^2 B_0^2}{8m} r^2 \Psi + qKz^2 \Psi = E\Psi \quad (28)$$

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 28 as

$$-\frac{\hbar^2}{2m} \left[\frac{\partial^2 \Psi}{\partial r^2} + \frac{1}{r} \frac{\partial \Psi}{\partial r} + \frac{\partial^2 \Psi}{\partial z^2} \right] + \frac{\hbar^2 m_z^2}{2mr^2} \Psi - \quad (29)$$

$$\frac{\hbar q B_0}{2m} m_z \Psi + \frac{q^2 B_0^2}{8m} r^2 \Psi + qKz^2 \Psi = E\Psi \quad (30)$$

Rearranging to put the constant coefficients on the RHS we get

$$-\frac{\hbar^2}{2m} \left[\frac{\partial^2 \Psi}{\partial r^2} + \frac{1}{r} \frac{\partial \Psi}{\partial r} + \frac{\partial^2 \Psi}{\partial z^2} \right] + \frac{\hbar^2 m_z^2}{2mr^2} \Psi \quad (31)$$

$$+ \frac{q^2 B_0^2}{8m} r^2 \Psi + qKz^2 \Psi = \left(E + \frac{\hbar q B_0}{2m} m_z \right) \Psi \quad (32)$$

To solve this, we use separation of variables so that

$$\Psi(r, \theta, z) \equiv R(r)\Theta(\theta)Z(z) \quad (33)$$

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 :

$$-\frac{\hbar^2}{2m} \left[R'' + \frac{1}{r} R' - \frac{m_z^2}{r^2} R \right] + \frac{q^2 B_0^2}{8m} r^2 R = E_r R \quad (34)$$

$$-\frac{\hbar^2}{2m} Z'' + qKz^2 Z = E_z Z \quad (35)$$

where

$$E_r + E_z = E + \frac{\hbar q B_0}{2m} m_z \quad (36)$$

Equation 35 has the same form as a harmonic oscillator, so we know that the energy levels are

$$E_z = \left(n_z + \frac{1}{2} \right) \hbar \omega_z \quad (37)$$

where the angular frequency is

$$\omega_z \equiv \sqrt{\frac{2qK}{m}} \quad (38)$$

To solve 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

$$R'' + \frac{1}{r} R' - \frac{m_z^2}{r^2} R - \frac{q^2 B_0^2}{4\hbar^2} r^2 R = -\frac{2mE_r}{\hbar^2} R \quad (39)$$

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

$$x^2 R'' + \frac{x^2}{\rho} R' - x^2 \frac{m_z^2}{\rho^2} R - x^2 \rho^2 R = -\frac{2mE_r}{\hbar^2} R \quad (40)$$

$$R'' + \frac{1}{\rho} R' - \frac{m_z^2}{\rho^2} R - \rho^2 R = -\frac{4mE_r}{qB_0\hbar} R \quad (41)$$

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

$$R'' \approx \rho^2 R \quad (42)$$

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

$$R' = s'e^{-\rho^2/2} - \rho se^{-\rho^2/2} \quad (43)$$

$$R'' = s''e^{-\rho^2/2} - 2\rho s'e^{-\rho^2/2} + (\rho^2 - 1)se^{-\rho^2/2} \quad (44)$$

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

$$s'' - \left(2\rho + \frac{1}{\rho}\right)s' - 2s - \frac{m_z^2}{\rho^2}s = -\frac{4m}{qB_0\hbar}E_r s \quad (45)$$

We now propose a series solution:

$$s(\rho) = \sum_{j=0}^{\infty} c_j \rho^j \quad (46)$$

$$s'(\rho) = \sum_{j=0}^{\infty} j c_j \rho^{j-1} \quad (47)$$

$$s''(\rho) = \sum_{j=0}^{\infty} j(j-1)c_j \rho^{j-2} \quad (48)$$

Inserting these into 45 and equating terms for each power of ρ gives

$$\left[(j+2)(j+1) + (j+2) - m_z^2\right] c_{j+2} - 2(j+1)c_j = -\frac{4m}{qB_0\hbar}E_r c_j \quad (49)$$

$$\left[(j+2)^2 - m_z^2\right] c_{j+2} - 2(j+1)c_j = -\frac{4m}{qB_0\hbar}E_r c_j \quad (50)$$

This gives the recursion relation

$$c_{j+2} = \frac{2(j+1) - \frac{4m}{qB_0\hbar}E_r}{(j+2)^2 - m_z^2} c_j \quad (51)$$

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

$$E_r = \frac{qB_0\hbar}{m} \frac{(j+1)}{2} \quad (52)$$

Since 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 36 and 37 the total energy is

The total energy is therefore

$$E = E_z + E_r - \frac{\hbar q B_0}{2m} m_z \quad (53)$$

$$= \left(n_z + \frac{1}{2} \right) \hbar \omega_z + \hbar \omega_r \left(n_r + \frac{1}{2} \right) \quad (54)$$

$$n_r = \frac{j - m_z}{2} \quad (55)$$

$$\omega_z = \sqrt{2qK/m} \quad (56)$$

$$\omega_r = qB_0/m \quad (57)$$

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.