ELECTROMAGNETISM IN QUANTUM MECHANICS: EXAMPLE


Post date: 1 Feb 2013.

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

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

and the scalar potential

$$\varphi = Kz^2$$  \hspace{1cm} (2)

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

$$\hat{i} = \hat{r}\cos\theta - \hat{\theta}\sin\theta$$  \hspace{1cm} (3)

$$\hat{j} = \hat{r}\sin\theta + \hat{\theta}\cos\theta$$  \hspace{1cm} (4)

$$\hat{k} = \hat{z}$$  \hspace{1cm} (5)

Applying this we get

$$A = \frac{B_0}{2}r\hat{\theta}$$  \hspace{1cm} (6)

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

$$B = \nabla \times A = B_0\hat{z}$$  \hspace{1cm} (7)

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

The electric field is
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\[ \mathbf{E} = -\nabla \varphi - \frac{\partial \mathbf{A}}{\partial t} \]  
\[ = -2Kz \hat{z} \] (9) (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

\[ \frac{1}{2m} \left( -\hbar^2 \nabla^2 \Psi + \frac{\hbar q}{\epsilon} (2 \mathbf{A} \cdot \nabla \Psi + \Psi \nabla \cdot \mathbf{A}) + q^2 |\mathbf{A}|^2 \right) + q \varphi \Psi = E \Psi \] (11)

From above, staying in cylindrical coordinates, we have

\[ \nabla^2 \Psi = \frac{1}{r} \frac{\partial}{\partial r} \left( r \frac{\partial \Psi}{\partial r} \right) + \frac{1}{r^2} \frac{\partial^2 \Psi}{\partial \theta^2} + \frac{\partial^2 \Psi}{\partial z^2} \] (12)
\[ = \frac{\partial^2 \Psi}{\partial r^2} + \frac{1}{r} \frac{\partial \Psi}{\partial r} + \frac{1}{r^2} \frac{\partial^2 \Psi}{\partial \theta^2} + \frac{\partial^2 \Psi}{\partial z^2} \] (13)
\[ \mathbf{A} \cdot \nabla \Psi = \frac{B_0 r}{2} \frac{\partial \Psi}{\partial \theta} \] (14)
\[ = \frac{B_0}{2} \frac{\partial \Psi}{\partial \theta} \] (15)
\[ \nabla \cdot \mathbf{A} = 0 \] (16)
\[ |\mathbf{A}|^2 = \frac{B_0^2}{4} r^2 \] (17)

We therefore have the equation

\[ \frac{-\hbar^2}{2m} \left[ \frac{\partial^2 \Psi}{\partial r^2} + \frac{1}{r} \frac{\partial \Psi}{\partial r} + \frac{1}{r^2} \frac{\partial^2 \Psi}{\partial \theta^2} + \frac{\partial^2 \Psi}{\partial z^2} \right] + \frac{i\hbar q B_0}{2m} \frac{\partial \Psi}{\partial \theta} + \frac{q^2 B_0^2}{8m} r^2 \Psi + qKz^2 \Psi = E \Psi \] (18) (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

\[ \hat{\mathbf{r}} = \cos \theta \hat{\mathbf{x}} + \sin \theta \hat{\mathbf{y}} \] (20)
\[ \hat{\theta} = -\sin \theta \hat{\mathbf{x}} + \cos \theta \hat{\mathbf{y}} \] (21)
\[ \hat{\mathbf{z}} = \hat{\mathbf{z}} \] (22)
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

$$\mathbf{R} = r\hat{\mathbf{r}} + z\hat{\mathbf{z}}$$

and the gradient is

$$\nabla = \hat{\mathbf{r}} \frac{\partial}{\partial r} + \hat{\theta} \frac{1}{r} \frac{\partial}{\partial \theta} + \hat{\mathbf{z}} \frac{\partial}{\partial z}$$

Therefore

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

$$= -i\hbar \frac{\partial}{\partial \theta}$$

We can therefore write 19 as

$$-\frac{\hbar^2}{2m} \left[ \frac{\partial^2 \Psi}{\partial r^2} + \frac{1}{r} \frac{\partial \Psi}{\partial r} + \frac{\partial^2 \Psi}{\partial z^2} \right] + \frac{L_z^2}{2mr^2} \Psi - \frac{qB_0}{2m} L_z \Psi + \frac{q^2 B_0^2}{8m} r^2 \Psi + qKz^2 \Psi = E \Psi$$

Since $L_z$ commutes with $H$, we can choose $\Psi$ 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

$$-\frac{\hbar^2}{2m} \left[ \frac{\partial^2 \Psi}{\partial r^2} + \frac{1}{r} \frac{\partial \Psi}{\partial r} + \frac{\partial^2 \Psi}{\partial z^2} \right] + \frac{\hbar^2 m_z^2}{2mr^2} \Psi - \frac{hqB_0}{2m} m_z \Psi + \frac{q^2 B_0^2}{8m} r^2 \Psi + qKz^2 \Psi = E \Psi$$

Rearranging to put the constant coefficients on the RHS we get

$$-\frac{\hbar^2}{2m} \left[ \frac{\partial^2 \Psi}{\partial r^2} + \frac{1}{r} \frac{\partial \Psi}{\partial r} + \frac{\partial^2 \Psi}{\partial z^2} \right] + \frac{\hbar^2 m_z^2}{2mr^2} \Psi + \frac{q^2 B_0^2}{8m} r^2 \Psi + qKz^2 \Psi = \left( E + \frac{hqB_0}{2m} m_z \right) \Psi$$

To solve this, we use separation of variables so that

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

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

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

where

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

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

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

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

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

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

Using the same analysis as in the harmonic oscillator case, we look at the behaviour of this equation for large $\rho$ 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
\[ R' = s' e^{-\rho^2/2} - \rho s e^{-\rho^2/2} \]  
\[ R'' = s'' e^{-\rho^2/2} - 2 \rho s' e^{-\rho^2/2} + (\rho^2 - 1) s e^{-\rho^2/2} \]  

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

\[ s'' - \left( 2 \rho + \frac{1}{\rho} \right) s' - \frac{m^2}{\rho^2} s = -\frac{4m}{qB_0\hbar} E_r s \]  

We now propose a series solution:

\[ s(\rho) = \sum_{j=0}^{\infty} c_j \rho^j \]  
\[ s'(\rho) = \sum_{j=0}^{\infty} j c_j \rho^{j-1} \]  
\[ s''(\rho) = \sum_{j=0}^{\infty} j(j-1) c_j \rho^{j-2} \]

Inserting these into \( 45 \) and equating terms for each power of \( \rho \) gives

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

This gives the recursion relation

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

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

\[ E_r = \frac{qB_0\hbar (j+1)}{m} \]  

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
\[
E = E_z + E_r - \frac{\hbar q B_0}{2m} m_z \\
= \left( n_z + \frac{1}{2} \right) \hbar \omega_z + \hbar \omega_r \left( n_r + \frac{1}{2} \right) \\
\]

\[
n_r = \frac{j - m_z}{2} \\
\omega_z = \sqrt{2qK/m} \\
\omega_r = \frac{qB_0}{m}
\]

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.