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

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

and the scalar potential

$$\varphi=Kz^2 \tag{2}$$

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

$$\begin{aligned}
\hat{\mathbf{i}} &= \hat{\mathbf{r}}\cos\theta-\hat{\theta}\sin\theta && (3)\\
\hat{\mathbf{j}} &= \hat{\mathbf{r}}\sin\theta+\hat{\theta}\cos\theta && (4)\\
\hat{\mathbf{k}} &= \hat{\mathbf{z}} && (5)
\end{aligned}$$

Applying this we get

$$\mathbf{A}=\frac{B_0}{2}r\hat{\theta} \tag{6}$$

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

$$\begin{aligned}
\mathbf{B} &= \nabla\times\mathbf{A} && (7)\\
&= B_0\hat{\mathbf{z}} && (8)
\end{aligned}$$

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

The electric field is

$$\begin{aligned}
\mathbf{E} &= -\nabla\varphi-\frac{\partial\mathbf{A}}{\partial t} && (9)\\
&= -2Kz\hat{\mathbf{z}} && (10)
\end{aligned}$$

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

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

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

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

$$\frac{i\hbar qB_0}{2m}\frac{\partial\Psi}{\partial\theta}+\frac{q^2B_0^2}{8m}r^2\Psi+qKz^2\Psi = E\Psi \quad (19)$$

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

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

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

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

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

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

and the gradient is

$$\nabla = \hat{\mathbf{r}}\frac{\partial}{\partial r} + \hat{\theta}\frac{1}{r}\frac{\partial}{\partial \theta} + \hat{\mathbf{z}}\frac{\partial}{\partial z} \tag{24}$$

Therefore

$$\begin{aligned} L_z &= \left[-i\hbar \mathbf{R} \times \nabla\right]_z && (25) \\ &= -i\hbar\frac{\partial}{\partial \theta} && (26) \end{aligned}$$

We can therefore write 19 as

$$\begin{aligned} -\frac{\hbar^2}{2m}\left[\frac{\partial^2\Psi}{\partial r^2} + \frac{1}{r}\frac{\partial \Psi}{\partial r} + \frac{\partial^2\Psi}{\partial z^2}\right] + \frac{L_z^2}{2mr^2}\Psi - && (27) \\ \frac{qB_0}{2m}L_z\Psi + \frac{q^2B_0^2}{8m}r^2\Psi + qKz^2\Psi &= E\Psi && (28) \end{aligned}$$

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

$$\begin{aligned} -\frac{\hbar^2}{2m}\left[\frac{\partial^2\Psi}{\partial r^2} + \frac{1}{r}\frac{\partial \Psi}{\partial r} + \frac{\partial^2\Psi}{\partial z^2}\right] + \frac{\hbar^2 m_z^2}{2mr^2}\Psi - && (29) \\ \frac{\hbar qB_0}{2m}m_z\Psi + \frac{q^2B_0^2}{8m}r^2\Psi + qKz^2\Psi &= E\Psi && (30) \end{aligned}$$

Rearranging to put the constant coefficients on the RHS we get

$$\begin{aligned} -\frac{\hbar^2}{2m}\left[\frac{\partial^2\Psi}{\partial r^2} + \frac{1}{r}\frac{\partial \Psi}{\partial r} + \frac{\partial^2\Psi}{\partial z^2}\right] + \frac{\hbar^2 m_z^2}{2mr^2}\Psi && (31) \\ +\frac{q^2B_0^2}{8m}r^2\Psi + qKz^2\Psi = \left(E + \frac{\hbar qB_0}{2m}m_z\right)\Psi && (32) \end{aligned}$$

To solve this, we use separation of variables so that

$$\Psi(r,\theta,z) \equiv R(r)\Theta(\theta)Z(z) \tag{33}$$

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:

$$
\begin{aligned}
-\frac{\hbar^2}{2m}\left[R''+\frac{1}{r}R'-\frac{m_z^2}{r^2}R\right]+\frac{q^2B_0^2}{8m}r^2R &= E_rR \qquad (34)\\
-\frac{\hbar^2}{2m}Z''+qKz^2Z &= E_zZ \qquad (35)
\end{aligned}
$$

where

$$E_r+E_z=E+\frac{\hbar qB_0}{2m}m_z \tag{36}$$

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

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

where the angular frequency is

$$\omega_z\equiv\sqrt{\frac{2qK}{m}} \tag{38}$$

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

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

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

$$
\begin{aligned}
x^2R''+\frac{x^2}{\rho}R'-x^2\frac{m_z^2}{\rho^2}R-x^2\rho^2R &= -\frac{2mE_r}{\hbar^2}R \qquad (40)\\
R''+\frac{1}{\rho}R'-\frac{m_z^2}{\rho^2}R-\rho^2R &= -\frac{4mE_r}{qB_0\hbar}R \qquad (41)
\end{aligned}
$$

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

$$R''\approx\rho^2R \tag{42}$$

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

$$R' = s' e^{-\rho^2/2} - \rho s e^{-\rho^2/2} \tag{43}$$

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

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

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

We now propose a series solution:

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

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

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

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

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

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

This gives the recursion relation

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

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

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

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 js are even and from 36 and 37 the total energy is

The total energy is therefore

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

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

$$n_r = \frac{j - m_z}{2} \tag{55}$$

$$\omega_z = \sqrt{2qK/m} \tag{56}$$

$$\omega_r = qB_0/m \tag{57}$$

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.