Hydrogen Atom in Magnetic Field

Abstract

Some fun with adding up angular momentum.

Index Terms

Angular momentum,spin

Consider a hydrogen atom in which the electron is in the ground state. When the atom is placed in a uniform magnetic field, its Hamiltonian is given by $H = 2\mu_e eB \cdot Se_z + 4W\mathbf{Se} \cdot \mathbf{S_p}$, where $\mathbf{Se}$ and $\mathbf{S_p}$ are the spins of the electron and the proton in the atom, respectively, Se_z is the z-component of $\mathbf{Se}$, B is the strength of the magnetic field, and μ_e and W are physical constants. We want to find the eigenvalues and eigenstates of H for $B = 0$ first, and then for the general case of $B \neq 0$.

We first consider the case $B = 0$, for which the spin interaction Hamiltonian is given as:

$$H = 4W\mathbf{S_e} \cdot \mathbf{S_p} = 2W\left[(\mathbf{S_e} + \mathbf{S_p})^2 - \mathbf{S_e}^2 - \mathbf{S_p}^2\right] = 2W(\mathbf{J}^2 - \frac{3}{2}), \tag{1}$$

where $\mathbf{J} = \mathbf{S_p} + \mathbf{S_e}$ is the total angular momentum operator. Now, we need to find the spectrum of j, which is the total angular momentum quantum number, which results from addition of two spin-1/2 particles. The general rule for addition of two particles with spin S_1 and S_2 is $|S_1 - S_2| \leq j \leq S_1 + S_2$, which tells us that $j = 0, 1$ for our case. So the eigenstates are,

$$|0,0\rangle, |1,1\rangle, |1,0\rangle \,\text{and}\, |1,-1\rangle. \tag{2}$$

Note that the last three states have the same energy, W. The first state has energy $-3W$. When we turn on B, the first part of the Hamiltonian becomes effective. This part has the eigenstates,

$$|\uparrow;\downarrow,\uparrow\rangle \,\text{and}\, |\uparrow;\downarrow,\uparrow\rangle, \tag{3}$$

where we choose the first state to be the electron state, which can be up or down. The state of the proton is irrelevant for the this part of the Hamiltonian, it can be up or down. We have to find the common eigenstates for the first and second part of the Hamiltonian, which will be the eigenstates of the full Hamiltonian. For this, we may expand the states given in Eq. (2) in terms of the the individual states, $|j_e, m_e\rangle$ and $|j_p, m_p\rangle$. Two of them will be trivial to do, $|1,1\rangle = |\uparrow,\uparrow\rangle$ (both particles have to be spin up so that total spin along z is 1.) and $|1,-1\rangle = |\downarrow,\downarrow\rangle$ (both particles have to be spin down so that total spin along z is -1). For $|0,0\rangle$, we propose the form, $|0,0\rangle = \alpha|\uparrow,\downarrow\rangle + \beta|\downarrow,\uparrow\rangle$, and try the following;

$$J_-|0,0\rangle = 0 = (J_{1-} + J_{2-})\left(\alpha|\uparrow,\downarrow\rangle + \beta|\downarrow,\uparrow\rangle\right) = (\alpha + \beta)|\downarrow,\downarrow\rangle, \quad \alpha = -\beta. \tag{4}$$

Normalizing the state we get $|0,0\rangle = \frac{|\uparrow,\downarrow\rangle - |\downarrow,\uparrow\rangle}{\sqrt{2}}$.

For $|1,0\rangle$ state we can again propose, $|1,0\rangle = \alpha|\uparrow,\downarrow\rangle + \beta|\downarrow,\uparrow\rangle$. The fastest way to get α and β is to use the orthogonality of the states, namely $\langle 0,0|1,0\rangle = 0$ which results in $|1,0\rangle = \frac{|\uparrow,\downarrow\rangle + |\downarrow,\uparrow\rangle}{\sqrt{2}}$. Now we have an easy task of checking which ones of the above are eigenfunctions of S_{ez}. Clearly only $|1,1\rangle$ and $|1,-1\rangle$ have definite values for S_{ez}, 1/2 and $-1/2$ respectively (remember we choose the first state to be the electron state). So they are certainly eigenstates of the Hamiltonian, with eigenvalues $W + \mu_e B$ and $W - \mu_e B$, respectively. The states $|0,0\rangle$ and $|1,0\rangle$ don't have a definite S_{ez}. So we conclude that they are not eigenstates of the full Hamiltonian. We are not finished yet! Is there a possibility to create eigenstates as linear combinations of $|0,0\rangle$ and $|1,0\rangle$? It is clear that the combination will not be an eigenstate of J^2, and it won't be an eigenstate of S_{ez} either. But some specific combination may be the eigenstate of the full Hamiltonian. To find that combination it will be helpful to recognize the following property,

$$S_{ez}|00\rangle = \frac{1}{2}|1,0\rangle, \quad S_{ez}|1,0\rangle = \frac{1}{2}|00\rangle. \tag{5}$$

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To simplify the notation lets define, $\psi_0 = |0,0\rangle$ and $\psi_1 = |1,0\rangle$. Now if we write down Schrodinger equations for ψ_0 and ψ_1, we recognize that these two coupled equations can be put into a matrix form as follows.

$$i\frac{\partial}{\partial t}\begin{pmatrix}\psi_0\\ \psi_1\end{pmatrix} = \begin{pmatrix}-3W & \frac{\mu_e B}{2}\\ \frac{\mu_e B}{2} & W\end{pmatrix}\begin{pmatrix}\psi_0\\ \psi_1\end{pmatrix} = H\begin{pmatrix}\psi_0\\ \psi_1\end{pmatrix}. \tag{6}$$

So there are two more eigenstates, which are the eigenvectors of the above Hamiltonian. The eigenvalues can be calculated to be $\frac{-2W-\sqrt{B^2\mu_e^2+16W^2}}{2}$ and $\frac{-2W+\sqrt{B^2\mu_e^2+16W^2}}{2}$. The corresponding eigenvectors become,

$$\begin{aligned}|1\rangle &= \frac{1}{N}\left(-\frac{4W+\sqrt{B^2\mu_e^2+16W^2}}{B\mu_e}|0,0\rangle + |1,0\rangle\right),\\ |2\rangle &= \frac{1}{N}\left(-\frac{4W-\sqrt{B^2\mu_e^2+16W^2}}{B\mu_e}|0,0\rangle + |1,0\rangle\right),\end{aligned} \tag{7}$$

where N is the normalization constant. This completes the set of eigenstates, $|1,1\rangle$, $|1,-1\rangle$ and $|1\rangle$, $|2\rangle$. Note that there have to be 4 of them, since this is a system of multiplicity $(2S_e+1)\times(2S_p+1) = 4$, and eigenstates of H must form a basis.