Perturbation by an External Magnetic Field: Solution to Q23

Patrick Wang
patrick.wang@chem.ox.ac.uk

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Abstract

Here I give a step-by-step solution to Q23 of Prof Manolopoulos' Operators worksheet.

1 Magnetic Field in z Direction

We first identify that the term symbol $^1\mathrm{L}_1$ indicates that $S = 0$, $J = 1$, and $L = 1$ (which is the p orbital). The singlet state can then be written as $1s^12p^1$. We can ignore the s orbital as it has zero angular momentum. What we have left then is a triply degenerate p state with $\ell = 1$ and $m_\ell = \pm 1, 0$. In braket notation, we have states: $|1, 0\rangle$, $|1, +1\rangle$, and $|1, -1\rangle$. In this basis, we can immediately write down the unperturbed Hamiltonian $H^{(0)}$:

$$H^{(0)} = \begin{bmatrix} E & 0 & 0 \\ 0 & E & 0 \\ 0 & 0 & E \end{bmatrix} \tag{1}$$

For part (a), we are applying a linear constant magnetic field in the z direction, such that the perturbing term has the form:

$$H^{(1)} = \mu_0 B_z L_z = \mu_0 B_z \ell_{2z}. \tag{2}$$

ℓ_{2z} acting on our states give well defined eigenvalues:

$$\ell_{2z} |1, 0\rangle = 0 \tag{3}$$
$$\ell_{2z} |1, +1\rangle = \hbar |1, +1\rangle \tag{4}$$
$$\ell_{2z} |1, -1\rangle = -\hbar |1, -1\rangle \tag{5}$$

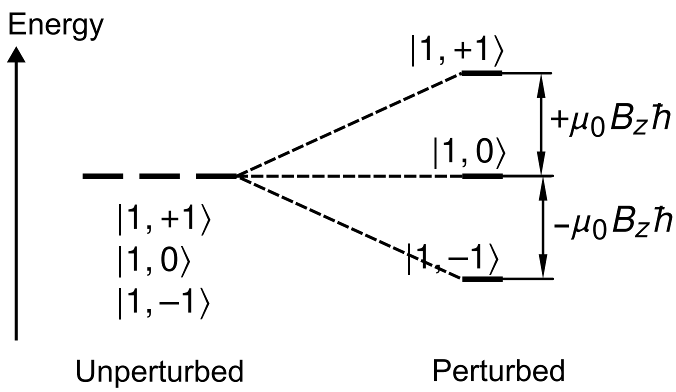

Figure 1: The energy level diagram of the states before and after perturbation the form of a magnetic field B_z applied in the z direction.

By inspection, we can write down the matrix for $H^{(1)}$:

$$H^{(1)} = \begin{bmatrix} 0 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -1 \end{bmatrix} \hbar \mu_0 B_z \tag{6}$$

which can be added to Eqn 1 to form our total Hamiltonian:

$$H = \begin{bmatrix} E & 0 & 0 \\ 0 & E + \hbar \mu_0 B & 0 \\ 0 & 0 & E - \hbar \mu_0 B \end{bmatrix} \tag{7}$$

where we can clearly see that the degeneracy has been lifted. The energy levels after perturbation are illustrated in Figure 1.

2 Magnetic Field in x Direction

Our perturbing Hamiltonian now has the form:

$$H^{(1)} = \mu_0 B_x \ell_{2x} \tag{8}$$

The problem remains very much the same but just with the added complication that we can't directly apply the x-angular momentum operator onto our basis states. To overcome this, we once again use the raising and lowering operators:

$$\ell_{2+} = \ell_{2x} + i\ell_{2y}$$
$$\ell_{2-} = \ell_{2x} - i\ell_{2y}$$

such that:

$$\ell_{2x} = \frac{1}{2}\left(\ell_{2+} + \ell_{2-}\right).$$

We can now write out the eigenvalues of each of the operators with our states:

$$\ell_{2+}\left|1, +1\right\rangle = 0 \tag{9}$$
$$\ell_{2+}\left|1, 0\right\rangle = \hbar\sqrt{2}\left|1, +1\right\rangle \tag{10}$$
$$\text{etc.} \tag{11}$$

Writing down the matrix form of the perturbing Hamiltonian in the same way as we did for the z perturbation gives:

$$H^{(1)} = \begin{bmatrix} 0 & 1 & 1 \\ 1 & 0 & 0 \\ 1 & 0 & 0 \end{bmatrix} \frac{\hbar\mu_0 B_x}{\sqrt{2}}. \tag{12}$$

We can find the shift to the energy levels by finding the eigenvalues to the addition of Eqns 1 and 12. I won't show that step here by when done correctly, you should end up with $E = E_0, E_0 \pm \frac{1}{\sqrt{2}}\hbar\mu_0 B_x$