

PC3233 Assignment 4

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1 Dipole-Dipole Interaction

1.1 Part A

The interaction energy, E , between two magnetic dipole, $\vec{\mu}_1$ and $\vec{\mu}_2$, is given by:

$$E = +\frac{\mu_0}{4\pi} \frac{\vec{\mu}_1 \cdot \vec{\mu}_2 - 3(\vec{\mu}_1 \cdot \hat{r})(\vec{\mu}_2 \cdot \hat{r})}{r^3} \quad (1)$$

Since the energy is magnetic potential energy is given by:

$$E = -\vec{m} \cdot \vec{B} \quad (2)$$

Therefore, we can extract the magnetic field of magnetic dipole, \vec{B}_i , from the interaction energy, E :

$$\vec{B}_i(\vec{r}) = -\frac{\mu_0}{4\pi} \frac{3(\vec{\mu}_i \cdot \vec{r})\vec{r}}{r^5} - \frac{\vec{\mu}_i}{r^3} \quad (3)$$

Hence, in order for $E = 0$ for any given $|\vec{r}|$, \vec{B}_i must be orthornormal to $\vec{\mu}_j$.

1.2 Part B

For parallel moments, we can expand the dot product of E as:

$$E = \frac{\mu_0}{4\pi} \frac{\mu_1 \mu_2}{r^3} (1 - 3 \cos^2 \theta) \quad (4)$$

Then, we can obtain the following:

$$\begin{cases} E_{min} = -\frac{\mu_0}{2\pi} \frac{\mu_1 \mu_2}{r^3} & \text{if } \theta = 0, \pi \\ E_{max} = +\frac{\mu_0}{4\pi} \frac{\mu_1 \mu_2}{r^3} & \text{if } \theta = \frac{\pi}{2} \end{cases} \quad (5)$$

1.3 Part C

For case (b) with $|\vec{r}| = 2\text{\AA}$. We can calculate the interaction energy, E , as follows using the formula we obtain from the previous section:

For electron-electron case, we have:

$$\begin{cases} E_{min} = -\frac{\mu_0}{2\pi} \frac{\mu_B^2}{r^3} = -6.4505 \times 10^{-24} \text{J} & \text{if } \theta = 0, \pi \\ E_{max} = +\frac{\mu_0}{4\pi} \frac{\mu_B^2}{r^3} = 3.22527 \times 10^{-24} \text{J} & \text{if } \theta = \frac{\pi}{2} \end{cases} \quad (6)$$

For proton-proton case ($\mu_{proton} = 1.4 \times 10^{-26} \text{\AA m}^2$), we have:

$$\begin{cases} E_{min} = -\frac{\mu_0}{2\pi} \frac{\mu_{proton}^2}{r^3} = -4.90 \times 10^{-30} \text{J} & \text{if } \theta = 0, \pi \\ E_{max} = +\frac{\mu_0}{4\pi} \frac{\mu_{proton}^2}{r^3} = 2.45 \times 10^{-30} \text{J} & \text{if } \theta = \frac{\pi}{2} \end{cases} \quad (7)$$

To compute the magnetic field, \vec{B} , we can rearranged the formula we obtained in part (a):

$$\begin{aligned} E = -\vec{\mu} \cdot \vec{B} &\implies E = -|\mu||B| \cos \theta \\ &\implies |B| = \frac{E}{|\mu|} \quad \text{since } \mu \text{ always align to the } \vec{B} \end{aligned}$$

Hence, we can compute the magnetic field, B , for the electron-electron as follows:

$$\begin{cases} |B| = \frac{E}{|\mu|} = 0.4016 \text{T} & \text{if } \theta = 0, \pi \\ |B| = \frac{E}{|\mu|} = 0.2007 \text{T} & \text{if } \theta = \frac{\pi}{2} \end{cases} \quad (8)$$

For proton-proton case, we have:

$$\begin{cases} |B| = \frac{E}{|\mu|} = 3.5 \times 10^{-4} \text{T} & \text{if } \theta = 0, \pi \\ |B| = \frac{E}{|\mu|} = 1.75 \times 10^{-4} \text{T} & \text{if } \theta = \frac{\pi}{2} \end{cases} \quad (9)$$

1.4 Part D

Express the interaction energy, E , in the previous section in terms of J , cm^{-1} , and μK .

For electron-electron case, we have:

$$\begin{cases} E_{min} = -\frac{\mu_0}{2\pi} \frac{\mu_B^2}{r^3} = -6.4505 \times 10^{-24} J = -32.47 cm^{-1} = -467211 \mu K & \text{if } \theta = 0, \pi \\ E_{max} = +\frac{\mu_0}{4\pi} \frac{\mu_B^2}{r^3} = 3.22527 \times 10^{-24} J = 16.24 cm^{-1} = 233605 \mu K & \text{if } \theta = \frac{\pi}{2} \end{cases} \quad (10)$$

For proton-proton case, we have:

$$\begin{cases} E_{min} = -\frac{\mu_0}{2\pi} \frac{\mu_{proton}^2}{r^3} = -4.90 \times 10^{-30} J = -2.4667 cm^{-1} = -0.355 \mu K & \text{if } \theta = 0, \pi \\ E_{max} = +\frac{\mu_0}{4\pi} \frac{\mu_{proton}^2}{r^3} = 2.45 \times 10^{-30} J = 1.2334 cm^{-1} = 0.177 \mu K & \text{if } \theta = \frac{\pi}{2} \end{cases} \quad (11)$$

2 Mathematical Relationships

Consider the following matrix:

$$M = \begin{pmatrix} a & b \\ c & d \end{pmatrix} \quad (12)$$

2.1 Analytic Expression of Eigenvalues

To diagonalize the matrix, we solve for the eigenvalues, λ , by solving the following equation:

$$\det(M - \lambda I) = 0 \quad (13)$$

Then, we have:

$$\det \begin{pmatrix} a - \lambda & b \\ c & d - \lambda \end{pmatrix} = 0$$

Then compute the determinant:

$$\begin{aligned} (a - \lambda)(d - \lambda) - bc &= 0 \\ \lambda^2 - (a + d)\lambda + ad - bc &= 0 \end{aligned}$$

Since the eigenvalues are the roots of the characteristic equation, which is quadratic, we get the analytic expression for λ using the quadratic formula:

$$\lambda = \frac{-(a+d) \pm \sqrt{(a+d)^2 - 4(ad-bc)}}{2} \quad (14)$$

2.2 Generalized $n \times n$ Eigenvalues

The degree of polynomial of the characteristic equation is n , where n is the dimension of the matrix.

According to Abel-Ruffini theorem, there is no general solution for the roots of a polynomial of degree $n \geq 5$.

For degree $n = 2, 3, 4$, we can solve for the roots of the characteristic equation using the quadratic, cubic, and quartic formulae respectively.

3 Atoms in Magnetic Field

3.1 Part A

Given a Li^{++} with $I = 1$. The energy levels due to fine structure splitting is given by:

$$E_{n,j} = E_n \left[1 + \frac{Z^2 \alpha^2}{n} \left(\frac{1}{j + \frac{1}{2}} - \frac{3}{4n} \right) \right] \quad (15)$$

Hence we can determine the following:

$$\begin{cases} E_{1, \frac{1}{2}} &= E_1 \left[1 + \frac{Z^2 \alpha^2}{4} \right] \\ E_{2, \frac{1}{2}} &= E_2 \left[1 + \frac{5Z^2 \alpha^2}{16} \right] \\ E_{2, \frac{3}{2}} &= E_3 \left[1 + \frac{Z^2 \alpha^2}{16} \right] \end{cases} \quad (16)$$

The energy levels shift due to Hyperfine structure is given by:

$$\Delta H_{HF} = \frac{g_i \mu_k B}{2\sqrt{j(j+1)}} [F(F+1) - I(I+1) - j(j+1)] \quad (17)$$

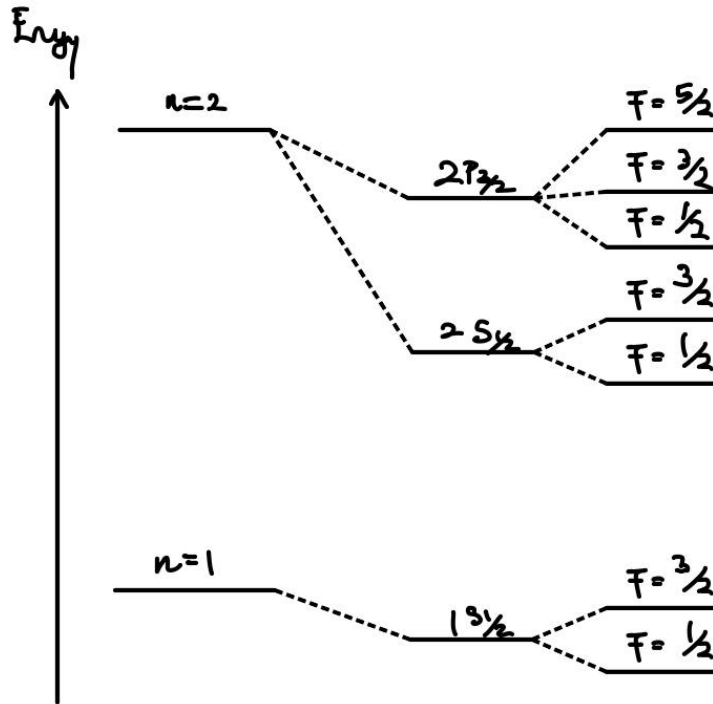
The possible value of total angular momentum, is given by:

$$F = |j - I|, |j - I + 1|, \dots, |j + I| \quad (18)$$

Hence, by setting $g_i \mu_k B = 1$, we can compute the energy levels shift due to hyperfine structure.

$$\left\{ \begin{array}{ll} \Delta H_{HF} = \frac{-2\sqrt{3}}{3} & \text{if } F = \frac{1}{2}, j = \frac{1}{2}, 1s \\ \Delta H_{HF} = \frac{2\sqrt{6}}{3} & \text{if } F = \frac{3}{2}, j = \frac{1}{2}, 1s \\ \Delta H_{HF} = -\frac{2\sqrt{3}}{3} & \text{if } F = \frac{1}{2}, j = \frac{1}{2}, 2s \\ \Delta H_{HF} = \frac{\sqrt{3}}{3} & \text{if } F = \frac{3}{2}, j = \frac{1}{2}, 2s \\ \Delta H_{HF} = -\frac{\sqrt{15}}{3} & \text{if } F = \frac{1}{2}, j = \frac{3}{2}, 2p \\ \Delta H_{HF} = \frac{2\sqrt{15}}{15} & \text{if } F = \frac{3}{2}, j = \frac{3}{2}, 2p \\ \Delta H_{HF} = -\frac{\sqrt{15}}{5} & \text{if } F = \frac{5}{2}, j = \frac{3}{2}, 2p \end{array} \right. \quad (19)$$

Hence we can draw the energy level diagram for the fine and hyperfine structure states as below.



3.2 Part B: Compute Lande Factor

For Lande factor, g_j , is given by:

$$g_j = 1 + \frac{j(j+1) - l(l+1) + s(s+1)}{2j(j+1)} \quad (20)$$

Hence, for g_j for all fine structure states up to $n = 2$ is given in the below:

$$\begin{cases} g_j = \frac{1}{3} & \text{if } j = \frac{1}{2}, l = 1, s = \frac{1}{2} \\ g_j = \frac{4}{3} & \text{if } j = \frac{3}{2}, l = 1, s = \frac{1}{2} \end{cases} \quad (21)$$

3.3 Part C: Zeeman Effect

The Zeeman effect energy splitting, ΔE , is given by:

$$\Delta E = \mu_j g_j \mu_B B \quad (22)$$

Hence for lowest Zeeman states, we have:

$$\Delta E = m_j g_j \mu_B B = \Delta m_j \frac{1}{3} \mu_B B = 1.0304 \times 10^{-24} \text{J} \quad (23)$$