IISER Mohali

[August 2024 Session]

PHY 403 (Atomic and molecular physics)

EndSem

Instructor: Ambresh Shivaji (**email:** ashivaji, **office:** 2F6-AB1)

Max. Marks : 50

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1. Working in the central field approximation and neglecting L-S coupling, answer the following for Li atom.

   (a) Write down the ground state wave function ψ_g.

   (b) What is the energy E_g of this state?

   (c) What is the explicit form of the Hamiltonian H, which satisfies, $H\psi_g = E_g\psi_g$?

   (d) What would be E_g if electrons have spin zero?

   [2+1+1+1]

2. Write down the quantum numbers of the states described in the spectroscopic notation as ${}^2S_{3/2}$, ${}^3D_2$ and ${}^5P_3$. Determine if any of these states are impossible, and if so explain why.

   [3+2]

3. Which of the following transitions are allowed by the electric dipole selection rules?

   (a) ${}^2D_{3/2} \rightarrow {}^2P_{1/2}$

   (b) ${}^3P_1 \rightarrow {}^2S_{1/2}$

   (c) ${}^3F_3 \rightarrow {}^3P_2$

   (d) ${}^4F_{7/2} \rightarrow {}^4D_{5/2}$

   State the reason for the forbidden transitions.

   [1+1+1+1]

4. The hyperfine structure of the Thallium-81 D_1 : ${}^2P_{1/2} \rightarrow {}^2S_{1/2}$ line (377.7 nm) contains, three components 377.6888 nm, 377.6830 nm and 377.6720 nm. Taking $I = \frac{1}{2}$, estimate the hyperfine constants in eV for the states involved in D_1 transition.

   [5]

5. We observe a radiative transition in a Helium-4 ion [${}^4_2He^+$]. Its wavelength is approximately equal to the first line of the Balmer series in Hydrogen atom. Which atomic levels of the ${}^4_2He^+$ ion are involved in this transition? What is the corresponding photon wavelength in nm?

   [5]

6. The fine structure formula for the Hydrogen atom obtained by solving Dirac equation exactly is given by,

$$E_{nj} = m_e c^2 \left\{ \left[1 + \left(\frac{\alpha}{n - (j + \frac{1}{2}) + \sqrt{(j + \frac{1}{2})^2 - \alpha^2}} \right)^2 \right]^{-1/2} - 1 \right\}.$$

Noting that $\alpha << 1$, obtain the fine structure correction at $\mathcal{O}(\alpha^4)$ in terms of $E_n^0 = -\frac{1}{2} m_e c^2 \frac{\alpha^2}{n^2}$.

[6]

7. A $L-S$ level multiplet is observed with spacings in the ratio of 3:5. What are possible values of L and S?

[5]

8. Calculate the ratio of the number of hydrogen molecules at the first excited vibrational level to the number of molecules at the first excited rotational level at $T = 8.75 \times 10^5$ K. For hydrogen molecule take $\omega = 8.25 \times 10^{14}\ \text{s}^{-1}$ and $B = \frac{\hbar^2}{2I} = 1.3 \times 10^{-3}$ eV.

[5]

9. Into what number of sublevels are the following states split in a weak magnetic field: (a) $^3P_0$; (b) $^2F_{5/2}$; (c) $^4D_{1/2}$?

[3]

10. Discuss the splitting of level corresponding to nd^2 configuration in j-j coupling scheme. Label the allowed states using the notation $(j_1, j_2)_J$. What is the total number of allowed states?

[7]

Useful results

1. Fundamental constants

$$h = 6.63\times10^{-34}\ \text{J s};\ c = 3\times10^{8}\ \text{m/s};\ k_B = 1.38\times10^{-23}\ \text{J/K};\ e = 1.6\times10^{-19}\ \text{C}$$
$$m_e = 9.1\times10^{-31}\ \text{kg} = 0.511\ \text{MeV};\ m_p = 1.673\times10^{-27}\ \text{kg} = 938.3\ \text{MeV}$$
$$m_n = 1.675\times10^{-27}\ \text{kg} = 938.6\ \text{MeV};\ \alpha = \frac{e^2}{\hbar c} \simeq \frac{1}{137}$$

2. Zeeman shift in weak magnetic field

$$\Delta E = g_J \mu_B B_0 M_J;\ g_J = 1 + \frac{\mathbf{L.S}}{\mathbf{J}^2} \tag{1}$$

3. Fine structure energy shift

$$\Delta E = A_f[J(J+1) - L(L+1) - S(S+1)] \tag{2}$$

where A_f is a constant for a given $L-S$ level multiplet.

4. Hyperfine interaction in atoms,

$$\delta H = \frac{A_{hf}}{\hbar^2}\ \mathbf{I.J};\ \ A > 0 \tag{3}$$

where A_{hf} depends on L, S and J. The vector sum of $\mathbf{I}$ and $\mathbf{J}$ defines the total angular momentum $\mathbf{F}$ of the atom. The selection rules for F are same as those for J.