IISER Mohali

[August 2024 Session]

PHY 403 (Atomic and molecular physics)

Midsem-II

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Max. Marks : 20

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1. Argue that in carbon atom, the configuration in which the two electrons in the $2p$ sub-shell have parallel spins is energetically more favorable than when the spins are anti-parallel.

2. Using the spectroscopic symbol $^{2S+1}[L]_J$, *obtain* all the atomic states of carbon which are possible and allowed.

3. Show that in a neutral atom, the potential energy of interactions of electrons with one another (E_3) is related to the potential energy of electrons with the nucleus (E_2) by,

$$E_3 = -\frac{1}{7}E_2 \tag{1}$$

using the Thomas-Fermi model.

4. In the Hartree-Fock method, the exchange term contribution to the energy functional is given by,

$$K = \sum_{\lambda,\mu} \langle \psi_\lambda(q_i)\psi_\mu(q_j)|\frac{1}{r_{ij}}|\psi_\mu(q_i)\psi_\lambda(q_j)\rangle\,. \tag{2}$$

Calculate its variation with respect to $\psi^*_\alpha(q_k)$.

5. Argue that in the dipole approximation, the transition probability in single electron atoms is non zero only if the spin component along the direction of quantization does not change.

Useful results

1. Thomas-Fermi model (*atomic units*)

   Fermi momentum

$$p_F = (3\pi^2\rho)^{1/3} \tag{3}$$

   For neutral atom

$$3\pi^2\rho = (2\phi)^{3/2} \quad \text{for} \quad \phi \geqslant 0 \tag{4}$$

   Thomas-Fermi equation

$$x^{1/2}\chi'' = \chi^{3/2};\ \chi(x) = \frac{r}{Z}\phi(r), r = bx \tag{5}$$

2. Matrix element relevant to absorption of external radiation

$$M_{ba} = \langle\psi_b|e^{\mathbf{ik.r}}\hat{\epsilon}.\nabla|\psi_a\rangle \tag{6}$$