22.3.2: ii. Exercises

Q1

Show that the configuration (determinant) corresponding to the $Li^{+}1s(\alpha)1s(\alpha)$ state vanishes.

Q2

Construct the 3 triplet and 1 singlet wavefunctions for the $Li^{+}1s^{1}2s^{1}$ configuration. Show that each state is a proper eigenfunction of S^2 and S_z (use raising and lowering operators for S^2)

Q3

Construct wavefunctions for each of the following states of CH_2 :

$$a.) \quad {}^{1}B_1(1_{a1}^2 2_{a1}^2 1_{b2}^2 3_{a1}^1 1_{b1}^1) \tag{22.3.2.1}$$
$$b.) \quad {}^{3}B_1(1_{a1}^2 2_{a1}^2 1_{b2}^2 3_{a1}^1 1_{b1}^1) \tag{22.3.2.2}$$
$$c.) \quad {}^{1}A_1(1_{a1}^2 2_{a1}^2 1_{b2}^2 3_{a1}^2) \tag{22.3.2.3}$$

Q4

Construct wavefunctions for each state of the $1\sigma^2 2\sigma^2 3\sigma^2 1\pi^2$ configuration of NH.

Q5

Construct wavefunctions for each state of the $1s^1 2s^1 3s^1$ configuration of Li.

Q6

Determine all term symbols that arise from the $1s^2 2s^2 2p^2 3d^1$ configuration of the excited N atom.

Q7

Calculate the energy (using Slater Condon rules) associated with the ep valence electrons for the following states of the C atom.

i. ${}^{3}P(M_L = 1, M_S = 1)$,
ii. ${}^{3}P(M_L = 0, M_S = 0)$,
iii. ${}^{1}S(M_L = 0, M_S = 0)$, and
iv. ${}^{1}D(M_L = 0, M_S = 0)$.

Q8

Calculate the energy (using Slater Condon rules) associated with the π valence electrons for the following states of the NH molecule.
i. ${}^{1}\Delta(M_L = 2, M_S = 0)$,
ii. ${}^{1}\Sigma(M_L = 0, M_S = 0)$, and
iii. ${}^{3}\Sigma(M_L = 0, M_S = 0)$.