

ATOMS, MOLECULES & REACTIONS
 QUANTUM MECHANICS, WEEK 3, SPRING 2006

Chapter 13

(33) $\frac{1\ell}{1s} \frac{1\ell}{2s}$

$$\psi_{\text{Be}} (1s^2 2s^2) = \frac{1}{\sqrt{4!}} \begin{pmatrix} 1s(1)\alpha(1) & 1s(1)\beta(1) & 2s(1)\alpha(1) & 2s(1)\beta(1) \\ 1s(2)\alpha(2) & 1s(2)\beta(2) & 2s(2)\alpha(2) & 2s(2)\beta(2) \\ 1s(3)\alpha(3) & 1s(3)\beta(3) & 2s(3)\alpha(3) & 2s(3)\beta(3) \\ 1s(4)\alpha(4) & 1s(4)\beta(4) & 2s(4)\alpha(4) & 2s(4)\beta(4) \end{pmatrix}$$

(36) C $1s^2 2s^2 2p^1 3p^1$

The text has worked out the possible terms arising from this configuration to be

3D , 1D , 3P , 1P , 3S and 1S (page 744 of Raff)

of these, the ^{lowest energy} ~~ground~~ state is 3D

(38) - (40)

~~(38)~~ These ~~were~~ ^{were} assigned in error. Don't have to do these.

HW sheet

(29)

$$\psi = \begin{vmatrix} \psi_A(1) & \psi_A(2) \\ \psi_B(1) & \psi_B(2) \end{vmatrix} = \psi_A(1)\psi_B(2) - \psi_A(2)\psi_B(1)$$

(a)

if we interchange the rows we get

$$\psi_1 = \begin{vmatrix} \psi_B(1) & \psi_B(2) \\ \psi_A(1) & \psi_A(2) \end{vmatrix} = \psi_B(1)\psi_A(2) - \psi_B(2)\psi_A(1) \\ = -\psi$$

(b)

if we interchange the columns we get

$$\psi_2 = \begin{vmatrix} \psi_A(2) & \psi_A(1) \\ \psi_B(2) & \psi_B(1) \end{vmatrix} = \psi_A(2)\psi_B(1) - \psi_B(2)\psi_A(1) \\ = -\psi$$

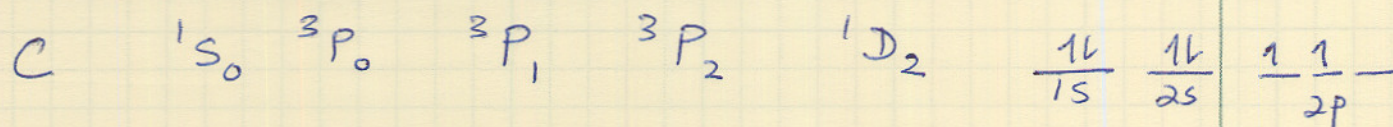
∴ Interchanging the columns or the rows changes the sign of the wavefunction.

(c) If two electrons have the same spin orbital (say electron 2 has the spin orbital ~~ψ_B~~ ψ_A)

$$\text{then } \psi = \begin{vmatrix} \psi_A(1) & \psi_A(2) \\ \psi_A(1) & \psi_A(2) \end{vmatrix} = \psi_A(1)\psi_A(2) - \psi_A(1)\psi_A(2) \\ = 0$$

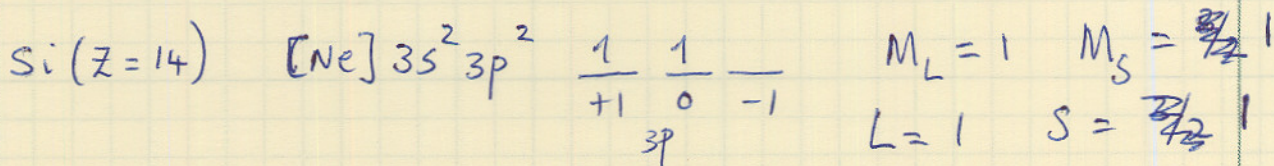
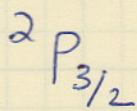
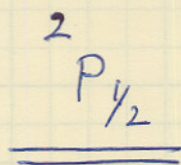
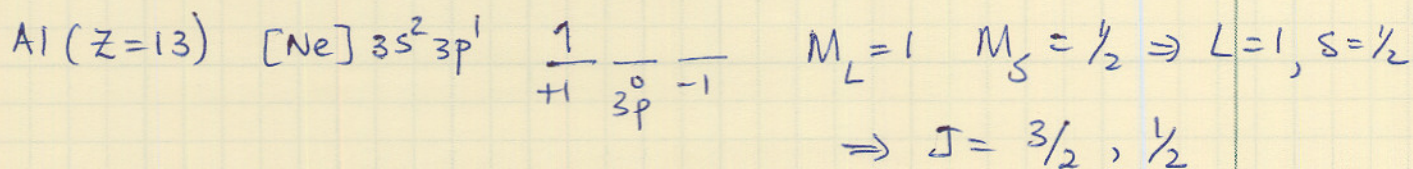
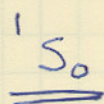
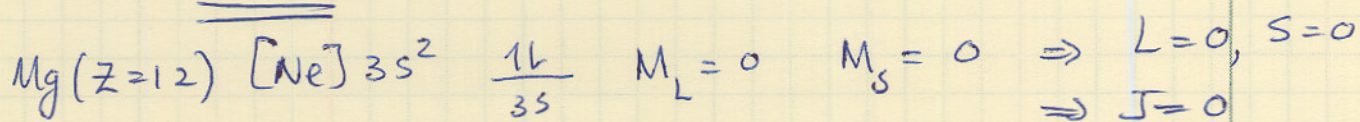
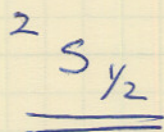
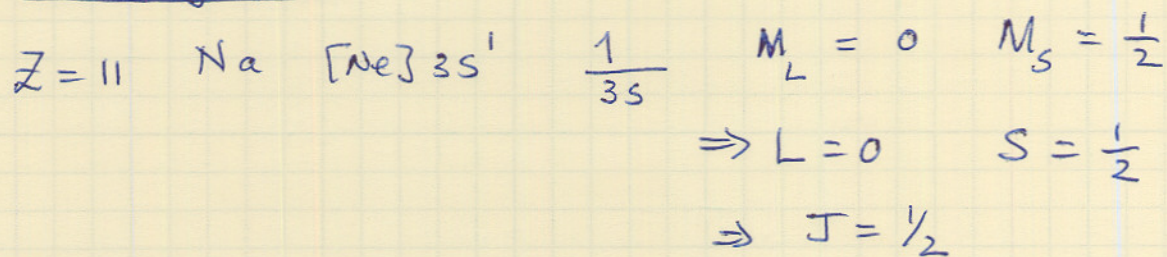
∴ wavefunction ceases to exist if the 2 electrons have the same spin orbital.

(39)

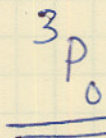
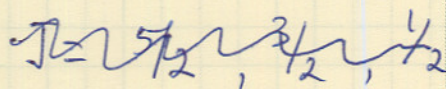
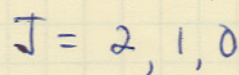


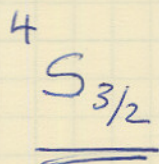
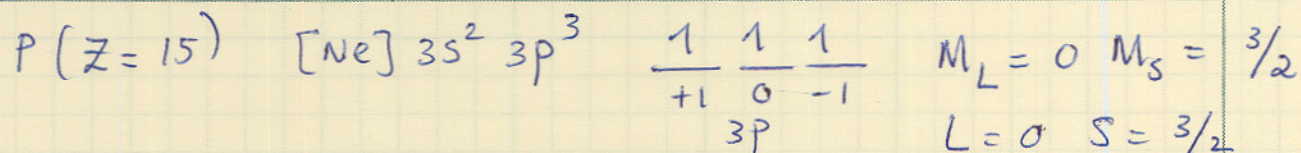
according to Hund's rules, the ground state is $3p_0$

Term symbols

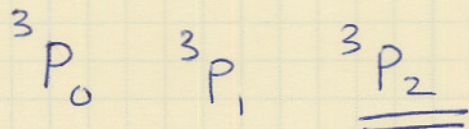
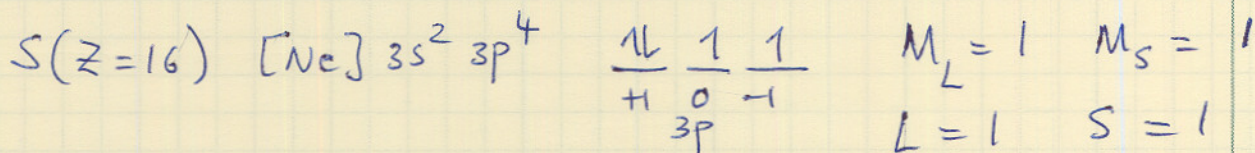


~~$2p_{3/2}$~~

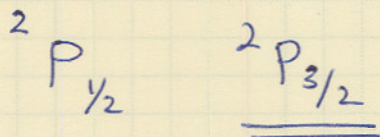
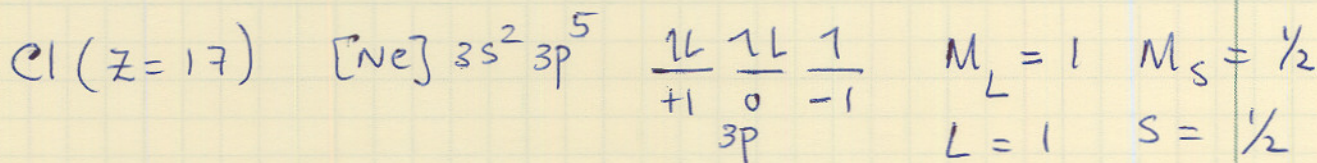




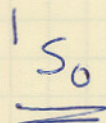
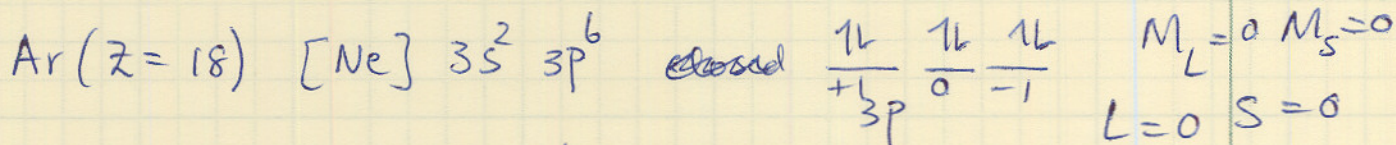
$J = 3/2$



$J = 2, 1, 0$



$J = 3/2, 1/2$



$J = 0$

