

LECTURE # 5

Note Title

9/10/2008

- VARIATIONAL METHOD
- ELECTRONIC CONFIGURATION FOR $N-e$ ATOM
- EQUIVALENT CONFIGURATION

HUND'S RULES

① LARGEST S



② LARGEST L GIVEN ①

③ \vec{J} $|\vec{L} - \vec{S}|$ SHELL LESS THAN $1/2$ -FILLED
 $\vec{L} + \vec{S}$ SHELL MORE THAN $1/2$ -FILLED

A diagram showing a vector \vec{J} on the left. Two arrows originate from a point: one pointing up and to the right, and another pointing down and to the right. The vector \vec{J} is the resultant of these two arrows, pointing up and to the right. This illustrates the addition of orbital angular momentum L and spin angular momentum S to form total angular momentum J .

COMMENT ON GROUP WORK

COULOMBS IN 2 D

$$\rho w'' + (2m + 1 - \rho) w' - \left(\frac{1}{2} - M_{2\rho} + M \right) w = 0$$

$$x f'' + (r - x) f' - \alpha f = 0$$

$$F \sim 1 + \frac{\alpha x}{\dots} + \frac{\alpha(\alpha+1)x^2}{\dots} + \frac{\alpha(\alpha+1)(\alpha+2)x^3}{\dots}$$

α CAN ONLY BE $0, -1, -2, \dots$

$\frac{1}{2} - M_{2\rho} + M$ CAN ONLY BE $0, -1, -2, \dots$

$$E_{2D} = -\frac{1}{(n - \frac{1}{2})^2} R_y^{\#}$$

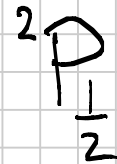
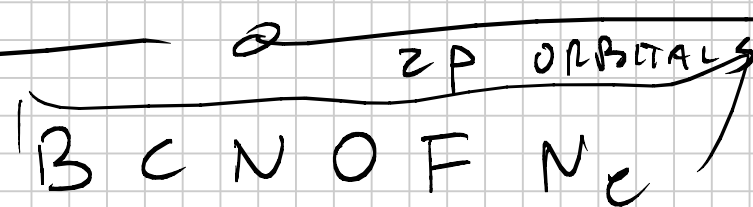
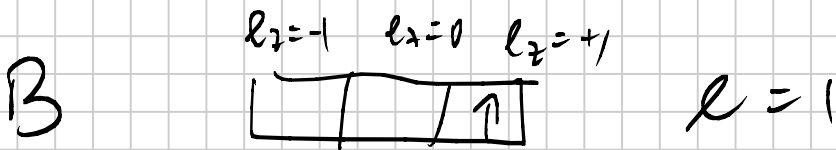
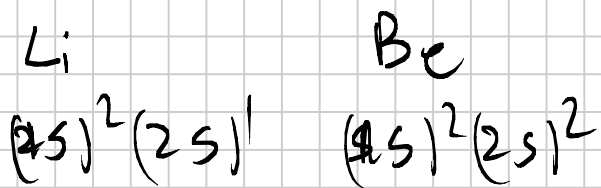
$$E_{3D} = -\frac{1}{n^2} R_y^{\#}$$

$$n = \underline{1}, 2, 3, 4, \dots$$

$$n=1$$

$$E_{2D} = -4 R_y^{\#}$$

$$E_{3D} \sim -1 R_y^{\#}$$



$$J = |1 - \frac{1}{2}|$$



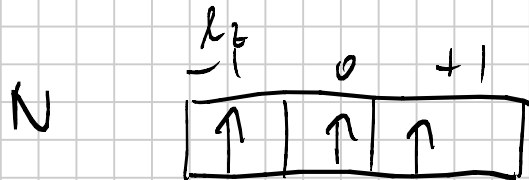
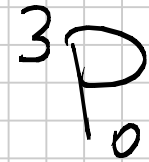
MAX L_z POSSIBLE?

2 PARALLEL SPINS

MAX L_z IS 1 $\Rightarrow L = 1$

$S = 1$

$J = |L - S|$



$S = \frac{3}{2}$

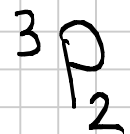
$L_z = l_z^1 + l_z^2 + l_z^3$

MAX L_z IS 0 $\Rightarrow L = 0$



$S = 1$

MAX $L_z = 1 \Rightarrow L = 1$



$\vec{J} = \vec{L} + \vec{S}$

III RULE RELATED TO SPIN-ORBIT INTERACTION

$$H_{SO} \sim \alpha \vec{s}_i \cdot \vec{l}' \quad \alpha > 0 \quad \vec{J} = (\vec{s}' + \vec{l}')$$

$$H_{SO} \sim \alpha \left(\frac{J^2 - S^2 - L^2}{2} \right) \Rightarrow \text{SMALLER } J$$

GIVES SMALLER SPIN ORBIT

IF I HAVE MORE THAN HALF FILLING

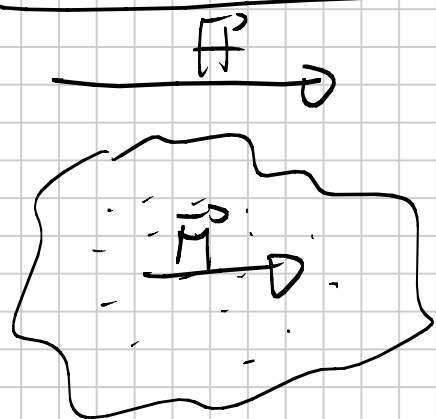
$S=0 \quad L=0$

$$|\uparrow_k | \uparrow_k | \uparrow | = |\uparrow_k | \uparrow_k | \uparrow_k | - |\quad | \quad | \downarrow_k | = + |\quad | \quad | \quad | \uparrow |$$

↑ HOLE

\Rightarrow HOLES FAVOR LARGER J

MAGNETIC PROPERTIES OF SOLIDS



$$\vec{M}^0 = \chi_M \vec{H}^0$$

CHAPT 31

ASCROFT-MERMIN

p644 - 659

χ_M = MAGNETIC SUSCEPTIBILITY

$\chi_M < 0$ DIAMAGNETIC

$T = 0$ $E_0(H) = E_0(H=0) + \Delta E_0(H)$ $\chi_M > 0$ PARAMAGNETIC

$$\Delta E_0 = - \int \vec{M}^0 \cdot \vec{H}^0 dV$$

$$\vec{M}^0 = - \frac{1}{V} \frac{\partial E_0}{\partial \vec{H}^0}$$

$$M_x = - \frac{1}{V} \frac{\partial E_0}{\partial H_x}$$

$$M_y = - \frac{1}{V} \frac{\partial E_0}{\partial H_y}$$

$$\chi_M = - \frac{1}{V} \frac{\partial^2 E_0}{\partial H^2} \quad (\vec{M}^0 \parallel \vec{H}^0)$$

AT FINITE T

$E_0 \rightarrow F$ (FREE ENERGY)

$$e^{-\beta F} = \sum_m N e^{-\beta E_m}$$

$$\beta = \frac{1}{k_B T}$$

$E_m(H)$ = ENERGY LEVELS
OF ADDM IN
PRESENCE OF H

$$\langle H \rangle = - \frac{1}{V} \frac{\partial F}{\partial H}$$

$$\chi_m = - \frac{1}{V} \frac{\partial^2 F}{\partial H^2}$$

$$M(H, T) = \frac{\sum_m M_m(H) e^{-\beta E_m}}{\sum_m e^{-\beta E_m}}$$

H

H₂