LECTURE # 5

Note Title 9/10/2008

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

HUND'S RULES

① LARGEST $\vec{S}$

② LARGEST $\vec{L}$ GIVEN ①

③ $\vec{J}$: $|\vec{L} - \vec{S}|$ SHELL LESS THAN ½-FILLED

$\vec{L} + \vec{S}$ SHELL MORE THAN ½-FILLED

COMMENT ON GROUP WORK

COULOMB IN 2D

$$\rho w'' + (\overbrace{2m+1}^{\gamma} - \rho) w' - \overbrace{\left(\frac{1}{2} - M_{2p} + m\right)}^{\alpha} w = 0$$

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

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

α CAN ONLY BE $0, -1, -2, \ldots$

$\frac{1}{2} - M_{2p} + m$ CAN ONLY BE $0, -1, -2 \ldots$

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

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

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

$n = 1$

$$E_{2D} = -4 R_y^*$$

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

$$\overbrace{B\ \ C\ \ N\ \ O\ \ F\ \ Ne}^{2p\ \text{ORBITALS}}$$

Li $(1s)^2(2s)^1$

Be $(1s)^2(2s)^2$

B

$\ell_z=-1$	$\ell_z=0$	$\ell_z=+1$
		$\uparrow$

$\ell = 1$

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

$^2P_{\frac{1}{2}}$

C

-1	0	1
	↑	↑

MAX L_z POSSIBLE?

2 PARALLEL SPINS

MAX L_z IS 1 $\Rightarrow$ $L = 1$

$S = 1$

$J = |L - S|$

$^3P_0$

N

l_z -1	0	+1
↑	↑	↑

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

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

MAX L_z IS 0 $\Rightarrow$ $L = 0$

$^4S_{\frac{3}{2}}$

O

-1	0	+1
↑	↑	↑↓

$S = 1$

MAX $L_z = 1$ $\Rightarrow$ $L = 1$

$^3P_2$

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

III RULE RELATED TO SPIN-ORBIT INTERACTION

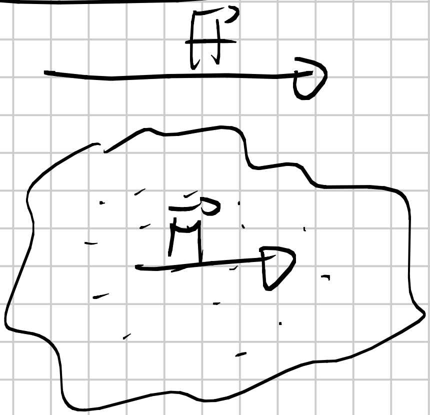
$H_{SO} \sim \alpha \vec{s}_i \cdot \vec{l}$ $\qquad \alpha > 0 \qquad \vec{J} = (\vec{s} + \vec{l})$

$H_{SO} \sim \alpha \frac{1}{2}(J^2 - s^2 - l^2)$ $\Rightarrow$ SMALLER J GIVES SMALLE SPIN ORBIT

IF I HAVE MORE THAN HALF FILLING

$\Rightarrow$ HOLES FAVOR LARGER J

MAGNETIC PROPERTIES OF SOLIDS



CHAPT 31

ASHCROFT – MERMIN

p 644 – 659

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

χ_M = MAGNETIC SUSCEPTIBILITY

$\chi_M < 0$ DIAMAGNETIC

$\chi_M > 0$ PARAMAGNETIC

$T = 0$

$$E_0(H) = E_0(H=0) + \Delta E_0(H)$$

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

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

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

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

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

AT FINITE T

$E_0 \longrightarrow F$ (FREE ENERGY)

$$e^{-\beta F} = \sum_m e^{-\beta E_m} \qquad \beta = \frac{1}{k_B T}$$

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

$$\vec{M} = -\frac{1}{V} \frac{\partial F}{\partial \vec{H}}$$

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

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

H

He