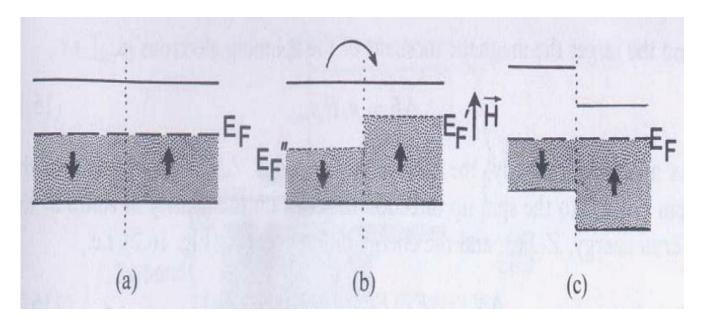
13

Quantum Mechanical Considerations

13.1 Paramagnetism and Diamagnetism

* Paramagnetism



Magnetic moment of the spinning electrons: dominant contribution to paramagnetism

Susceptibilities for paramagnetic metals based on the energy theory

Potential energy:
$$E_p = -\mu_0 \mathbf{m} \cdot \mathbf{H}$$

$$\Delta E = \mu_0 H \mu_{ms}$$

$$\Delta N = \Delta E Z(E_F)$$
$$= \mu_0 H \mu_{ms} Z(E_F)$$

$$M = \frac{\mu_m}{V}$$

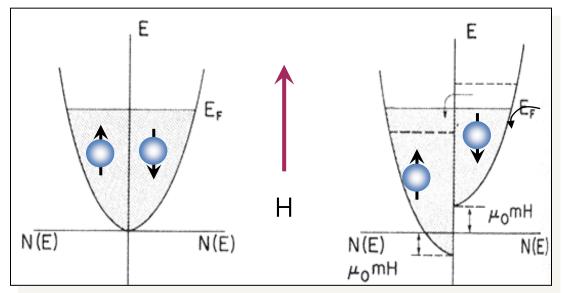
$$M = \frac{\mu_{ms}}{V} \Delta N = \frac{\mu^{2}_{ms} \mu_{0} HZ (E_{F})}{V}$$

$$\chi = \frac{M}{H} = \frac{\mu^2_{ms} \mu_0 Z(E_F)}{V}$$



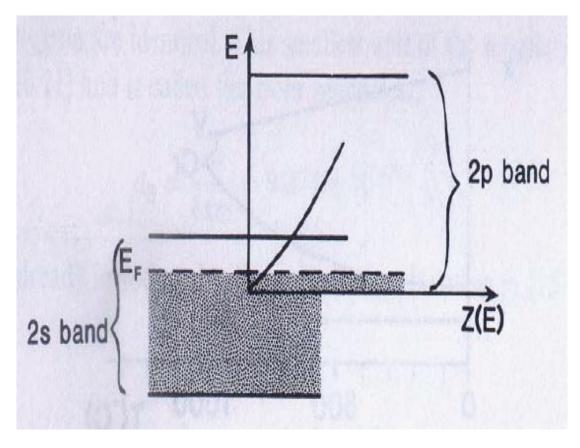
$$H = 0$$





$$\chi_{spin,para} = \frac{\mu_B^2 \mu_0 Z(E_F)}{V}$$

* Diamagnetism





$$\chi_{dia} = -\frac{e^2 Z r^2 \mu_0}{6 m V}$$

$$\mu_m = I \times A = \frac{e}{t} A = \frac{e}{s/v} A = \frac{ev\pi r^2}{2\pi r} = \frac{evr}{2} \qquad \text{(A= area of loop)}$$

$$2\pi r = n\lambda = n\frac{h}{p}$$

$$rp = \frac{h}{2\pi}n = \hbar n$$

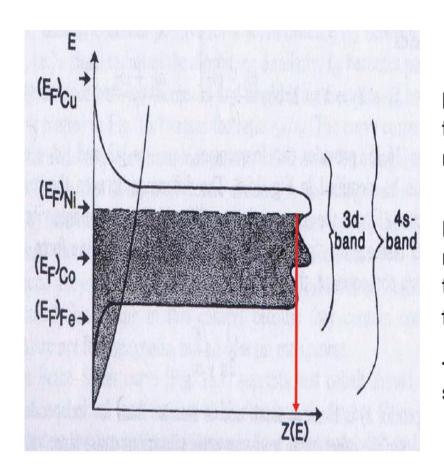
$$mvr = \hbar n = \frac{nh}{2\pi}$$

For
$$n=1$$
, $\mu_m = \frac{eh}{4\pi m}$

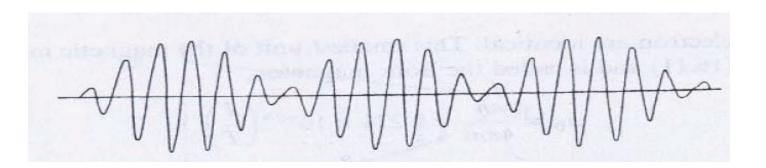
$$\mu_B = \frac{eh}{4\pi m} = 9.274 \times 10^{-24} \left(\frac{J}{T}\right)$$

Bohr Magneton

13.2 Ferromagnetism and Antiferromagnetism



- d-bands overlap the next higher s-band. dband can accommodate up to ten electrons, so that the density of states for a d-band is relatively large
- For instance, the density of states of Ni near Fermi energy are comparatively large, one needs only a relatively small amount of energy to transfer a considerable number of electrons from spin down into spin up configurations.
- only minimum energy is needed to change spin direction in the ferromagnetic metals.



$$X_1 = b \sin w_1 t$$

$$X_2 = b\sin w_2 t$$

$$X_1 + X_2 = X = 2b\cos\frac{w_1 - w_2}{2}t\sin\frac{w_1 + w_2}{2}t$$

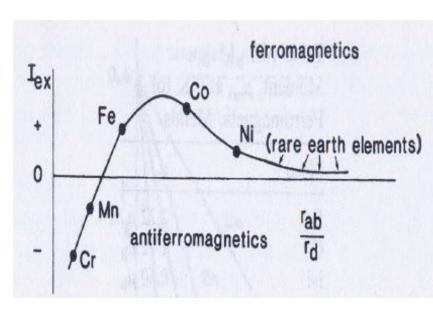
The difference of frequencies is larger, the stronger the coupling.

If the two pendula vibrate in a parallel fashing, the restoring force, *kx*, is small. As a result, the frequency is smaller than for independent vibration

$$v_0 = \frac{1}{2\pi} \sqrt{\frac{k}{m}}$$

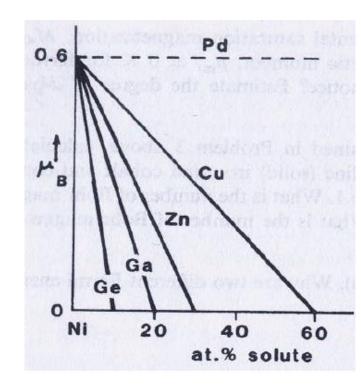
$$I_{ex} = \int \psi_a(1)\psi_b(2)\psi_a(2)\psi_b(1) \left[\frac{1}{r_{ab}} - \frac{1}{r_{ab}} - \frac{1}{r_{b1}} + \frac{1}{r_{12}} \right] d\tau$$

- I_{ex} is positive \rightarrow parallel spins are energetically more favorable than antiparallel spins. (vice versa)



- I_{ex} becomes positive for a small distance r_{12} between the electrons, i.e., a small radius of the d-orbit, r_{d} . Similarly, I_{ex} becomes positive for a large distance between the nuclei and neighboring electrons r_{a2} and r_{b1} .

- For Cu, no "unfilled d- or f-band", the condition for ferromagnetism.
- If copper is alloyed to nickel, the extra copper electrons progressively fill the *d*-band and compensate some of the unsaturated spins of nickel → the magnetic moment per atom of this alloy is reduced.



- The *3d* - band of Ni is filled by only 9.4 electrons (0.6 electron lacks per atom). Thus, about 60% copper atoms are needed until the magnetic moment of Ni has reached a zero value.