Condensed Matter Physics I

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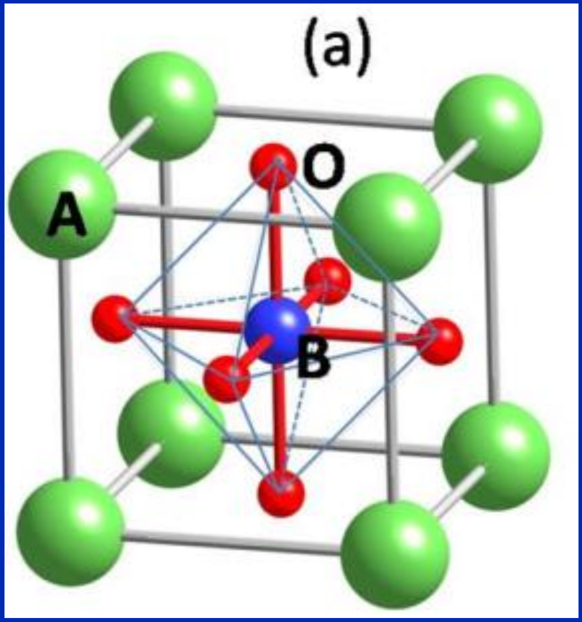
Last time

Langevin diamagnetism

Moments

- Free ions
- LS couping
- Hund's rules
- Spectroscopic splitting factor
- Crystal field effects



Today

Paramagnetism

- Curie paramagnetism
- van Vleck magnetism
- Pauli paramagnetism

PARAMAGNETISM

Non-ordering magnetism

Orbital magnetism $\vec{p} \rightarrow \vec{p} + \frac{e}{c}\vec{A}$

Spin magnetism $g_o \mu_B \vec{H} \cdot \vec{S}$

$$E_B \approx \mu_B g_j \vec{H} \cdot \langle n | \vec{J} | n \rangle + \sum_{n \neq n'} \frac{\left[g_j \mu_B \vec{H} \cdot \langle n | \vec{J} | n' \rangle \right]^2}{E_n - E_{n'}} + \frac{e^2}{8mc^2} H^2 \left\langle n \left| \sum_i \left(x_i^2 + y_i^2 \right) \right| n \right\rangle$$

↳ Curie (para)

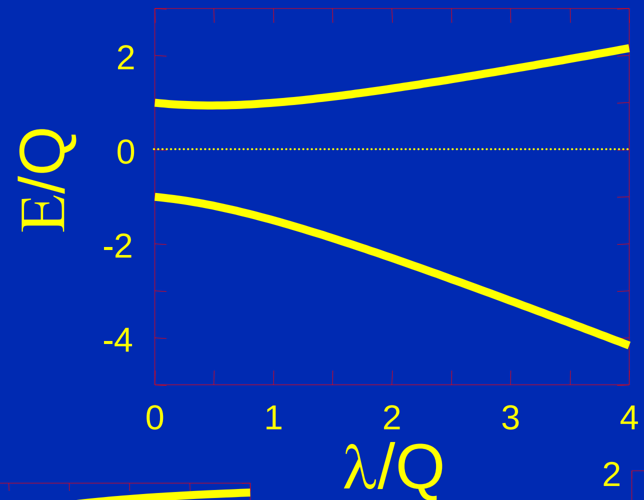
↳ van Vleck (para)

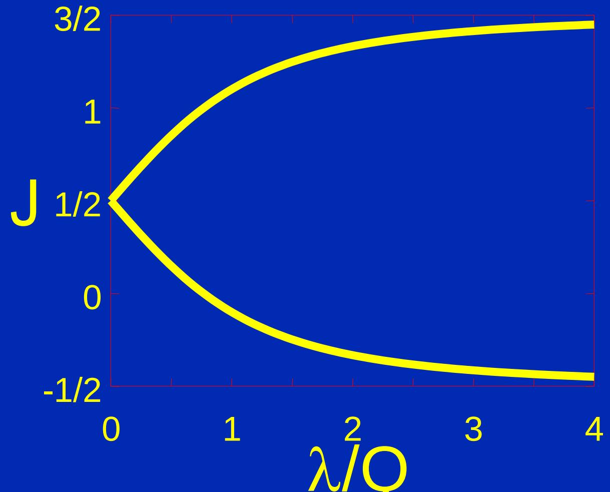
↳ Langevin (dia)

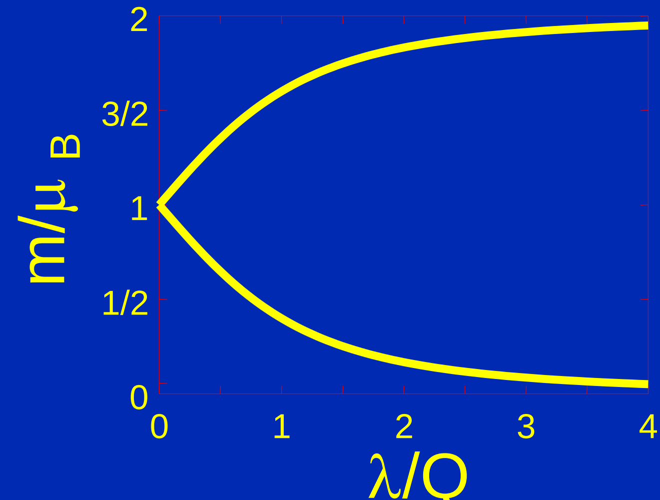
Spin-orbit coupling
Russel-Saunders, Hund’s rules
Crystal field splitting

Crystal field + spin-orbit

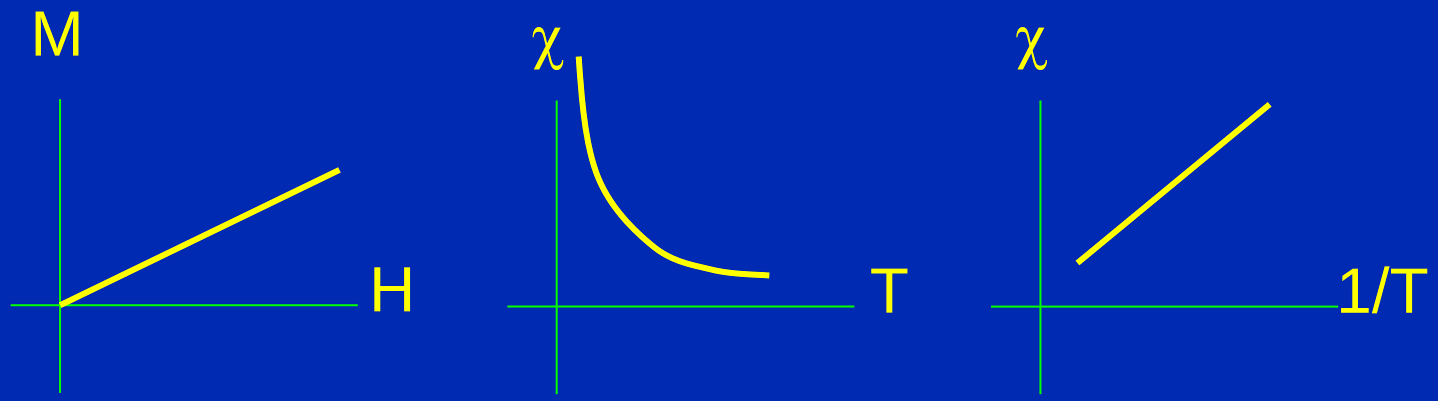
$$H = H_o + QV_{CF} + \lambda \vec{L} \cdot \vec{S}$$







Paramagnetism



- “Alignment” of weakly interacting magnetic moments
- Magnetic moments = spin, orbit
- Ground state splitting (Curie)
- **Curie law** $\chi = C/T$
- Low lying excited states (**van Vleck**)
- Metals: Density of states effects (**Pauli magnetism**)

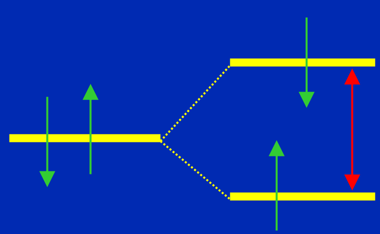
Curie law: G.S.

$$E_B \approx g_j \mu_B \vec{H} \cdot \langle n | \vec{J} | n \rangle + \sum_{n \neq n'} \frac{\left[g_j \mu_B \vec{H} \cdot \langle n | \vec{J} | n' \rangle \right]^2}{E_n - E_{n'}} + \frac{e^2}{8mc^2} H^2 \left\langle n \left| \sum_i \left(x_i^2 + y_i^2 \right) \right| n \right\rangle$$

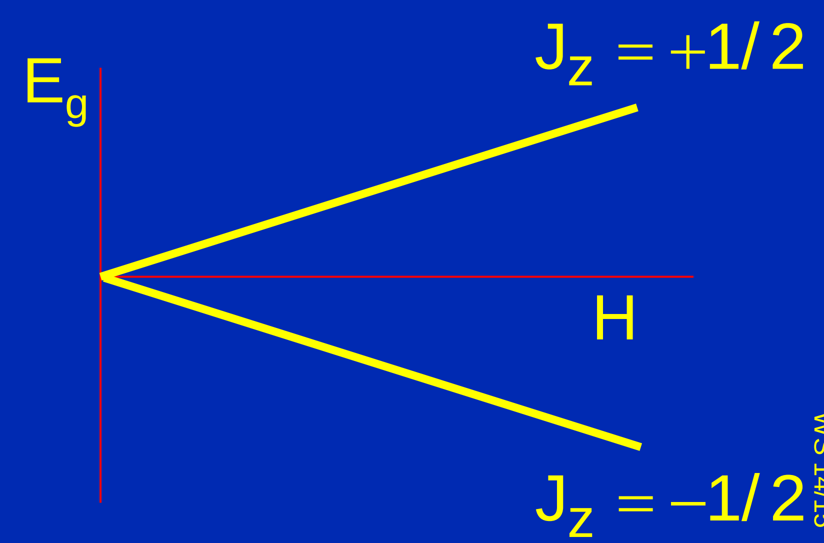
Magnetic ground state

Ground state splitting: $E_B = g_j \mu_B H_z J_z$

L=0; S=1/2

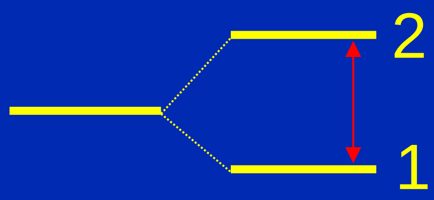


$2\Delta = \mu_B H_z$



Curie law: J=1/2

For J=1/2:



$2\Delta = g_j \mu_B H_z$

Thermal occupation N_i/N of the two states:

$$\frac{N_1}{N} = \frac{e^{\Delta/\tau}}{e^{\Delta/\tau} + e^{-\Delta/\tau}} \qquad \frac{N_2}{N} = \frac{e^{-\Delta/\tau}}{e^{\Delta/\tau} + e^{-\Delta/\tau}}$$

Magnetization M:

$$M = \frac{(N_1 - N_2)}{V} g_j \mu_B |J_z| = n\mu \cdot \tanh\left(\frac{\mu H}{kT}\right)$$

$$\frac{\mu H}{kT} << 1 \quad \rightarrow \quad M = n\mu \cdot \frac{\mu H}{kT} \quad \text{and} \quad \chi = \frac{n\mu^2}{kT} = \frac{C}{T}$$

Curie Law: J

More general: for G.S. with J: 2J+1 equi-spaced levels

$$M = n\langle M\rangle = n\frac{\sum_{J_z=-J}^{J} g_j\mu_B J e^{-g_j\mu_B J_z H/kT}}{\sum_{J_z=-J}^{J} e^{-g_j\mu_B J_z H/kT}} = n g_j \mu_B J B_J(x)$$

With Brillouin function B_J:

$$B_J(x) = \frac{2J+1}{2J}\coth\left(\frac{2J+1}{2J}x\right) - \frac{1}{2J}\coth\left(\frac{x}{2J}\right) \qquad x = \frac{g_j \mu_B J H}{kT}$$

Curie Law: $kT >> \mu_B H$

$$x << 1 \ (\mu H << kT):$$

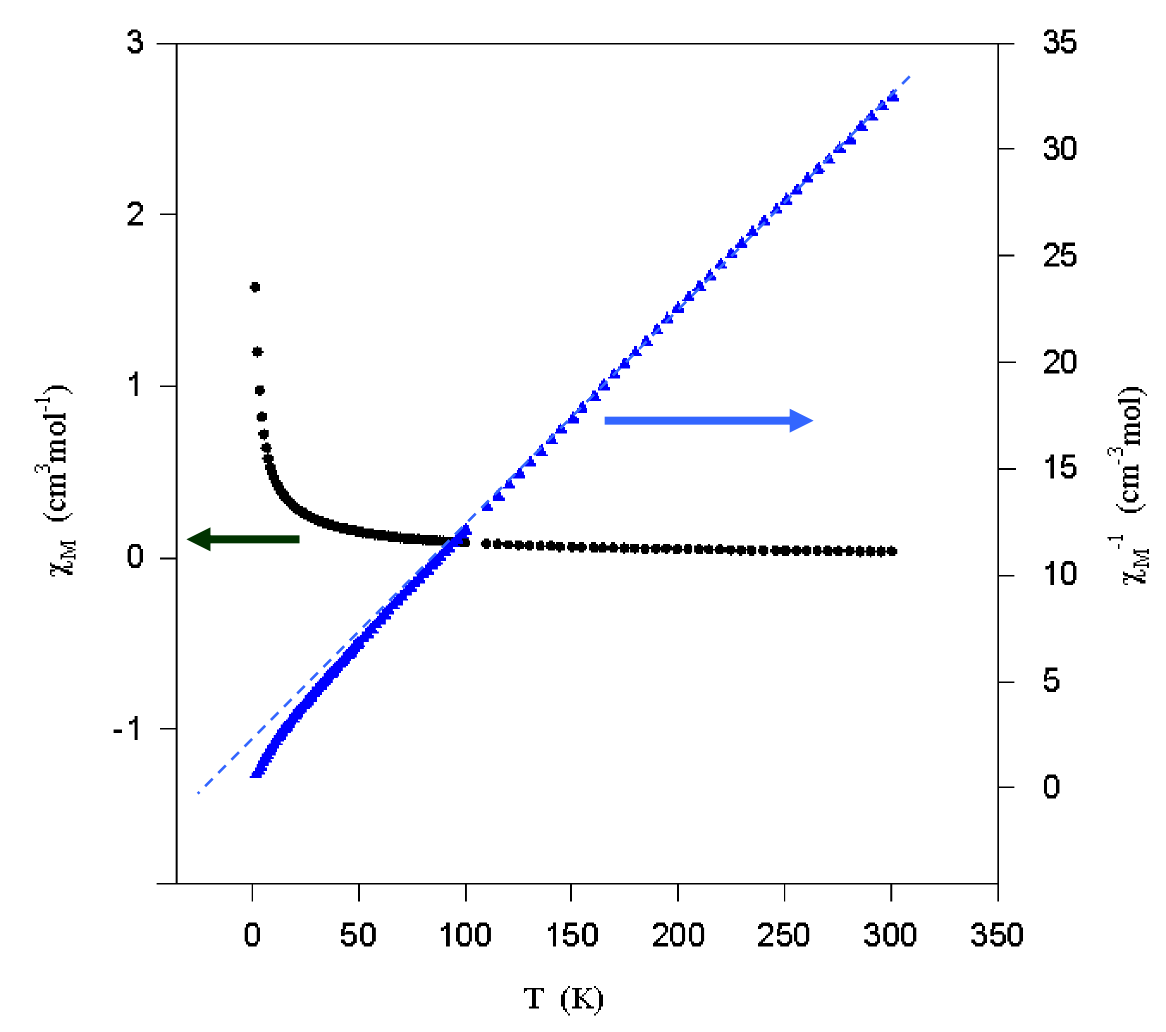
$$\coth(x) = 1/x + x/3 + x^3/45 + \ldots$$

$$\frac{M}{H} = \chi \cong \frac{Np^2\mu_B^2}{3kT} = \frac{C}{T} \qquad p = g_j\sqrt{J(J+1)}$$

p: effective magneton number

C: Curie constant

$(C_4H_{12}N_2)_2Mn_2Ga_5(H_2O)(PO_4)_8$



Curie law & Xtal field

Rare earth's: 4f shell's small ('inner' electrons)

=> p experimental $\approx$ p calculated

except for Eu^{3+} and Sm^{3+}

where low lying states mix in

Iron group: 3d shell's on the outside

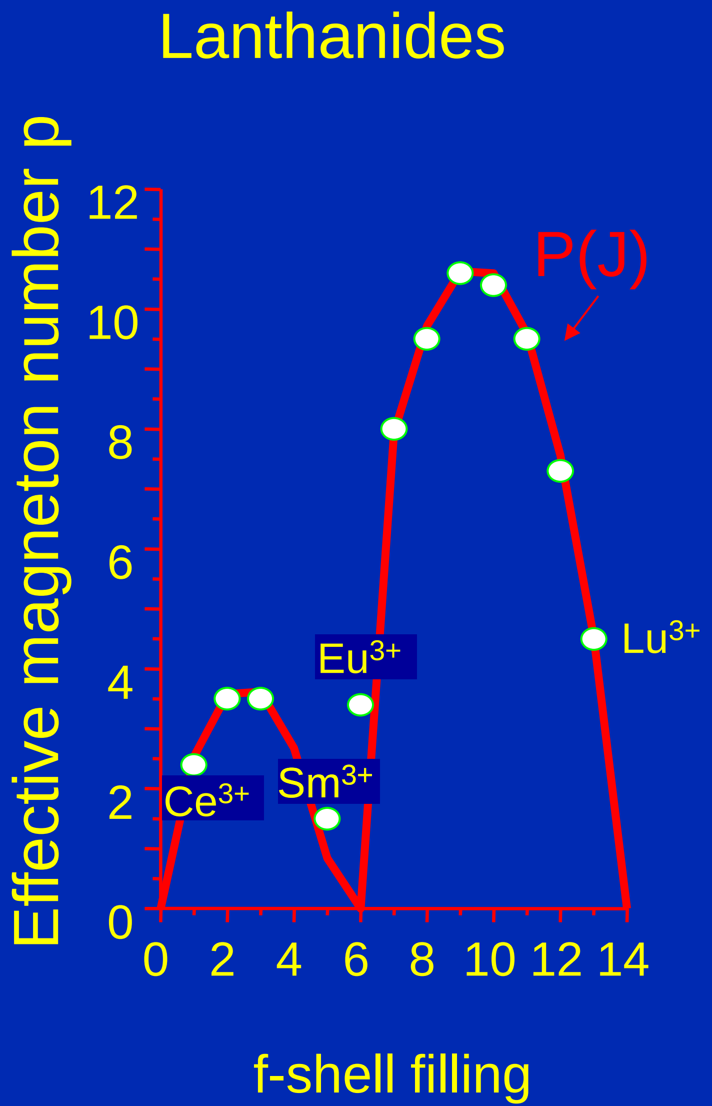
=> Crystal field important

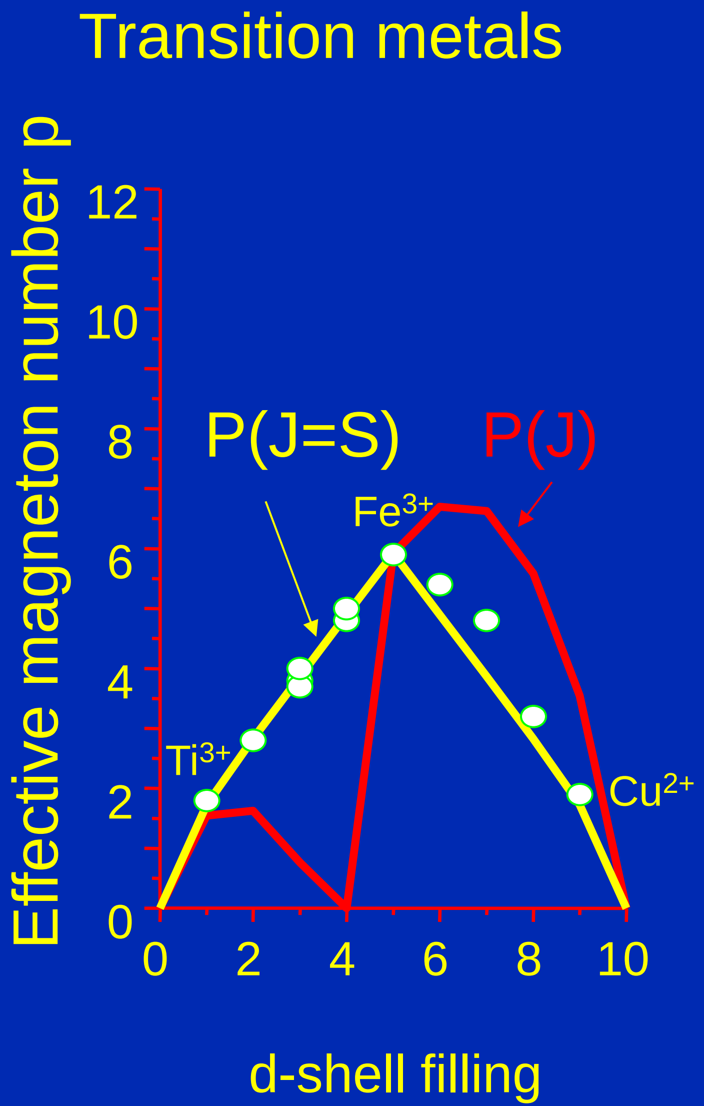
p experimental $\neq$ p calculated

$$p \cong 2\sqrt{S(S+1)} \Rightarrow p^2 = 3 \text{ for } S = 1/2$$

as if L_z=0 (quenching)

Effective magneton numbers





van Vleck paramagnetism

$$E_B \approx g_j \mu_B \vec{H} \cdot \langle n | \vec{J} | n \rangle + \sum_{n \neq n'} \frac{\left[g_j \mu_B \vec{H} \cdot \langle n | \vec{J} | n' \rangle \right]^2}{E_n - E_{n'}} + \frac{e^2}{8mc^2} H^2 \left\langle n \left| \sum_i \left(x_i^2 + y_i^2 \right) \right| n \right\rangle$$

Non-magnetic groundstate $|0\rangle$

$$\chi = -\frac{N}{V} \frac{\partial^2 E_{B,0}}{\partial H^2} = 2 \frac{N}{V} \sum_{n \neq 0} \frac{\left(g_j \mu_B \langle n | J_z | 0 \rangle \right)^2}{E_n - E_0} - \frac{e^2}{4mc^2} \frac{N}{V} \left\langle 0 \left| \sum_i \left(x_i^2 + y_i^2 \right) \right| 0 \right\rangle$$

Only one excited state Δ above GS,

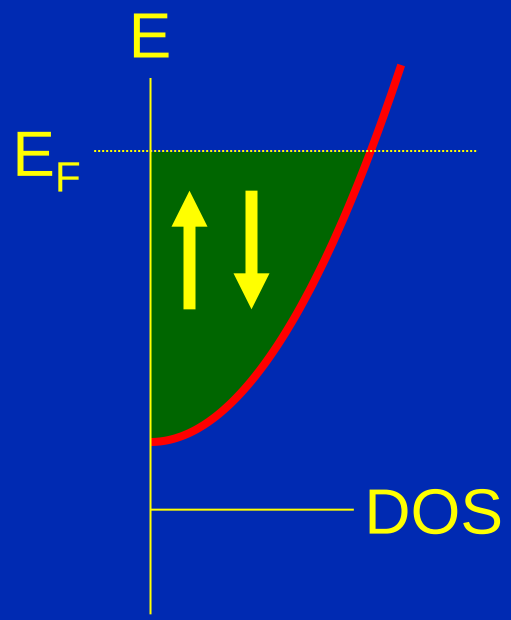
kT<< Δ $\quad \chi = 2n \dfrac{\left(g_j \mu_B \langle n | J_z | 0 \rangle \right)^2}{\Delta} + \chi_{dia}$

kT>> Δ: $\quad \chi = n \dfrac{\left(g_j \mu_B \langle n | J_z | 0 \rangle \right)^2}{kT} + \chi_{dia}$

Competition between van Vleck and Langevin

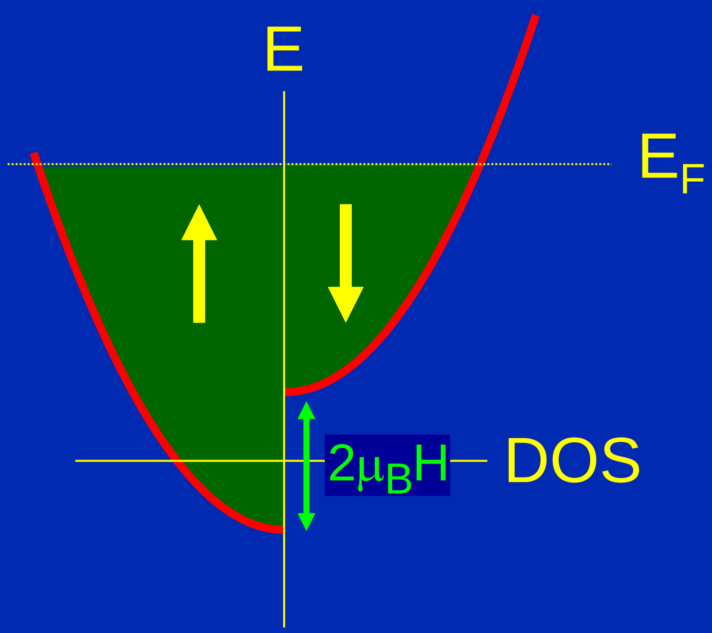
Conduction electrons: Pauli paramagnetism

No field: $E = \frac{\hbar^2 k^2}{2m^*}$ $E_F = \frac{\hbar^2}{2m^*}\left(3\pi^2 n\right)^{2/3}$ $D(E) = \frac{1}{2\pi^2}\left(\frac{2m^*}{\hbar^2}\right)^{3/2}\sqrt{E}$



Pauli paramagnetism

$$H \neq 0: \quad E = \frac{\hbar^2 k^2}{2m^*} \pm \frac{1}{2} g_o \mu_B H$$



$$N_\uparrow = \frac{1}{2} \int_{-\mu_B}^{E_F} D(E + \mu_B H)\, dE$$

$$\approx \frac{1}{2} \left(\int_0^{E_F} D(E)\, dE + \mu_B H \cdot D(E_F) \right)$$

$$N_\downarrow \approx \frac{1}{2} \left(\int_0^{E_F} D(E)\, dE - \mu_B H \cdot D(E_F) \right)$$

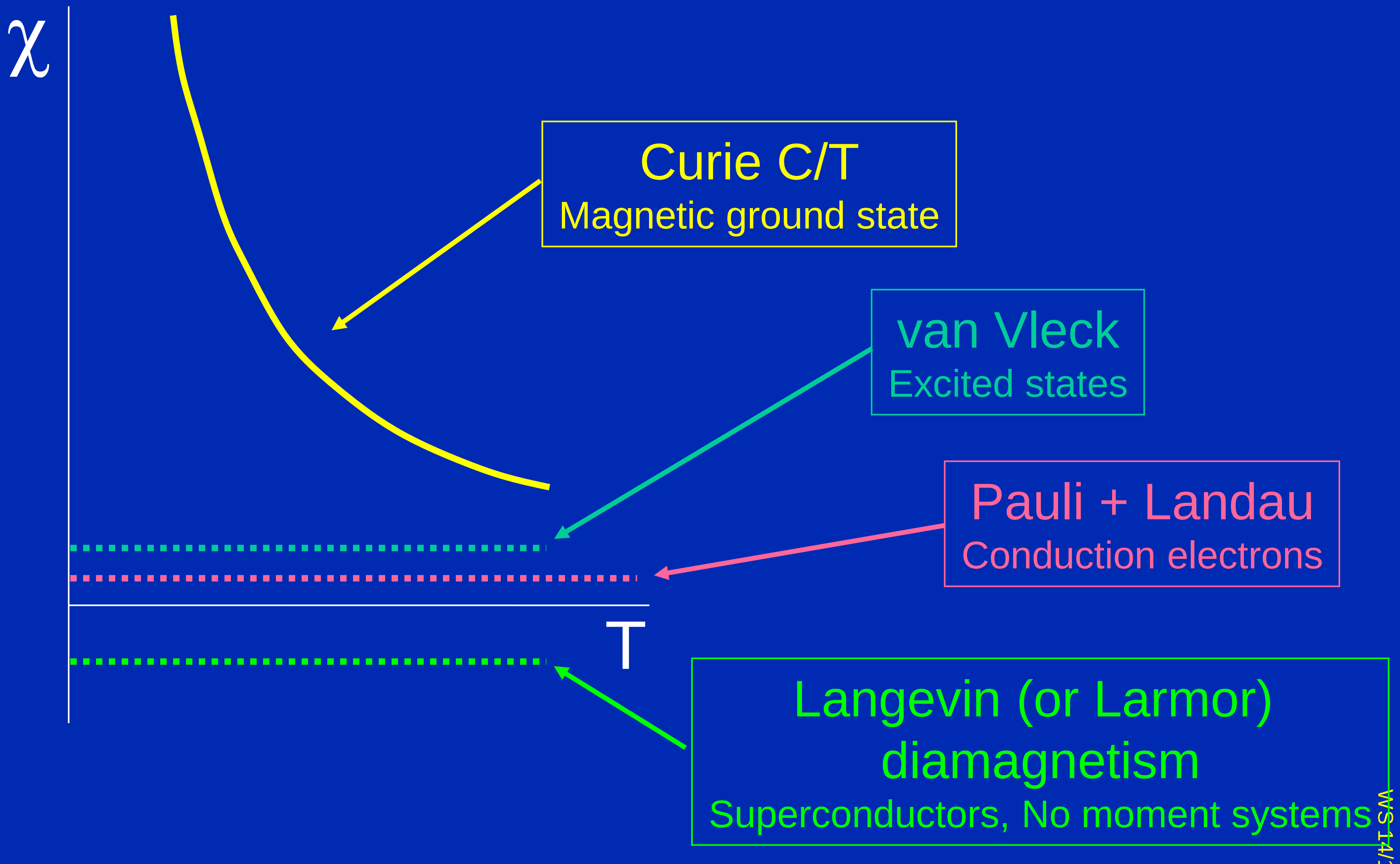
Pauli: $M = \mu_B (N_\uparrow - N_\downarrow)$

$$= \mu_B^2 D(E_F)\, H = \frac{3n\mu_B^2}{2kT_F} H$$

Landau (dia): $M = -\dfrac{n\mu_B^2}{2kT_F} H$

$$\Longrightarrow \quad \boxed{\chi_e = \frac{n\mu_B^2}{kT_F}}$$

Overview para/diamagnetism



Magnetism

Diamagnetism:

- No magnetic moments
- No magnetic interaction
- Response due to induced currents
- Magnetization opposite to field

- Ideal gases
- Superconductors

Paramagnetism:

- Magnetic moments (spin, orbit)
- Weak magnetic interactions
- Response due to orientation
- Magnetization in field direction

- Metals
- ‘odd electron’ systems
- O_2, biradicals

Ordered magnetism:

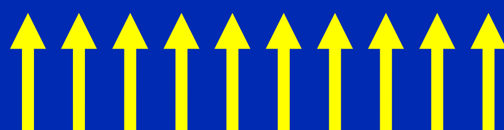
- Magnetic moments
- Strong magnetic interactions
- Response due to polarization
- Ferro-, antiferro-, ferrimagnetic

- Fe, Ni, Co, Gd, Dy
- CoO, FeO, high-T_c (CuO systems)

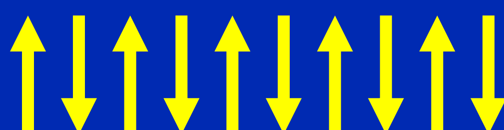
Ordered Magnetism

What if there is a strong interaction between moments ?

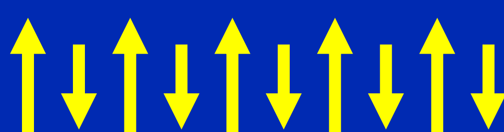
$$H_{i,j} = -2J_{i,j}\vec{S}_i \cdot \vec{S}_j$$



Ferromagnetism

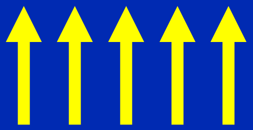


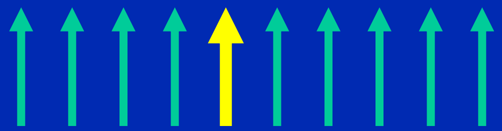
Antiferromagnetism

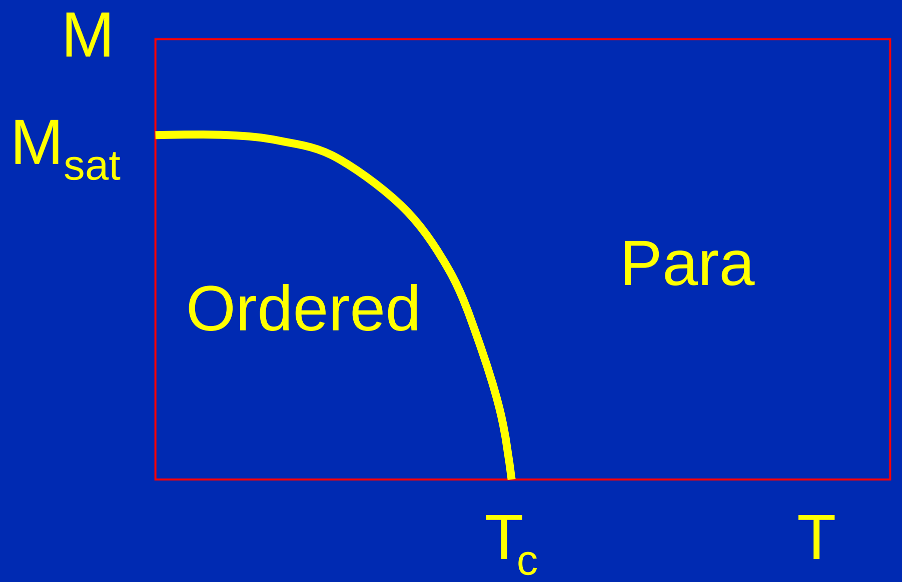


Ferrimagnetism

Ferromagnetic order







Mean field approximation:

Each moment experiences an additional "field" proportional to the magnetization due to the presence of all other moments.

$$H_{mf} = \lambda M$$

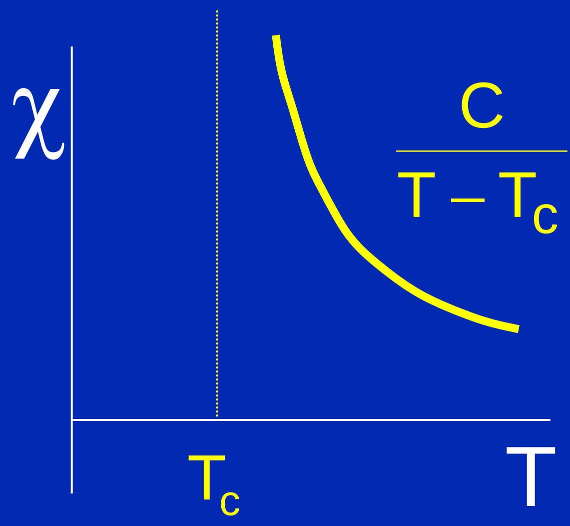
Mean field approach

Curie-Weiss Law

$T > T_c$: No ordering, paramagnetic

$$M = \chi_{para}(H_{ext} + H_{mf})$$

$$\chi = \frac{M}{H_{ext}} = \frac{C}{T}\frac{(H_{ext} + \lambda M)}{H_{ext}} = \frac{C}{T - C\lambda} = \frac{C}{T - T_c}$$



More precise

$$\chi \propto (T - T_c)^{-\gamma} \qquad \gamma \approx 1.33$$

Mean field approach

$T < T_c$: Ordering, spontaneous ferromagnetic moment

For S=1/2 (Brouillin function, neglect external field):

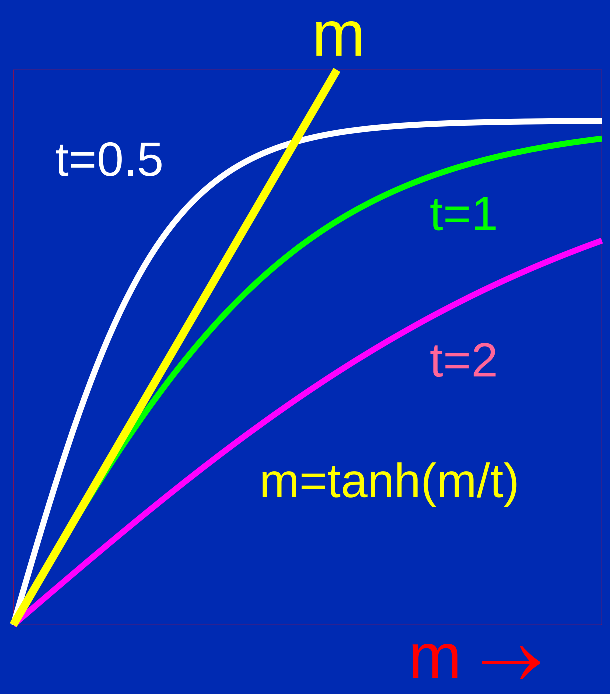
$$M = n\mu_B \tanh\left(\frac{\mu_B H}{kT}\right) = n\mu_B \tanh\left(\frac{\mu_B \lambda M}{kT}\right)$$

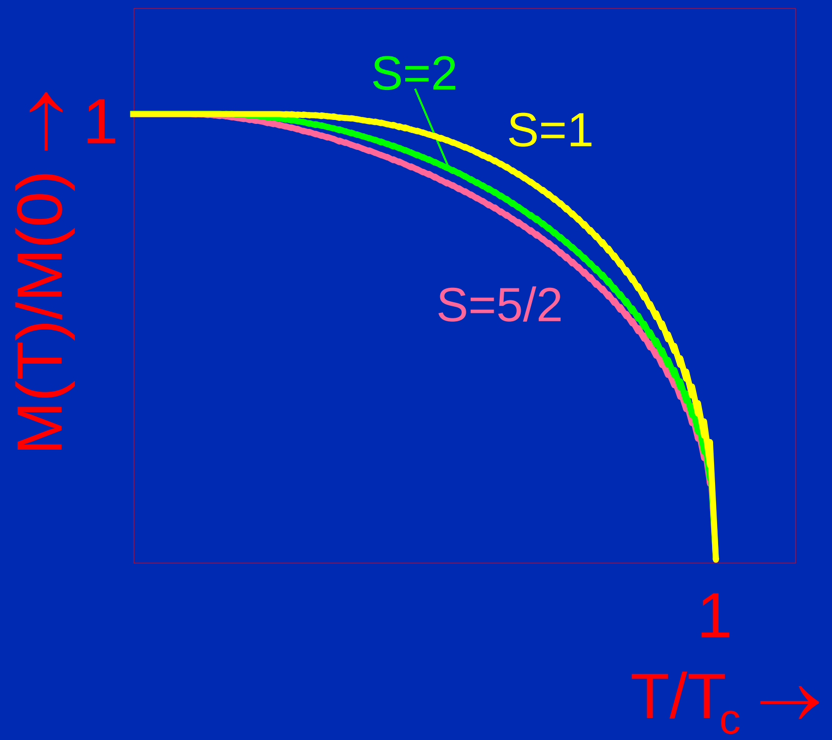
$$\left.\begin{array}{l} t = kT/\lambda n \mu_B{}^2 \\ m = M/n\mu_B \end{array}\right\} \quad m = \tanh(m/t)$$

$$m/t \gg 1: \quad m = 1 - 2e^{-2m/t}$$

$$\rightarrow M = M(0) - 2n\mu_B e^{-2\lambda n \mu_B{}^2/kT}$$

Spontaneous magnetization





$Sm_{(3-x)}Ho_xFe_5O_{12}$ (x=2.4)

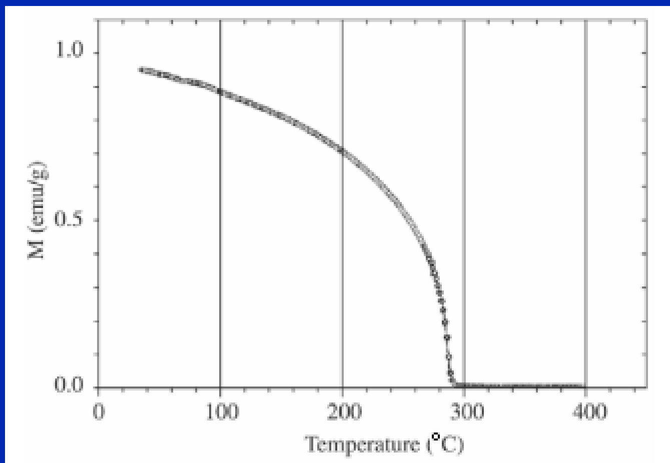


Figure 8. Magnetization-temperature curve of the powder calcined at 1450 °C when subsequently subjected to a 240 Oe magnetic field.

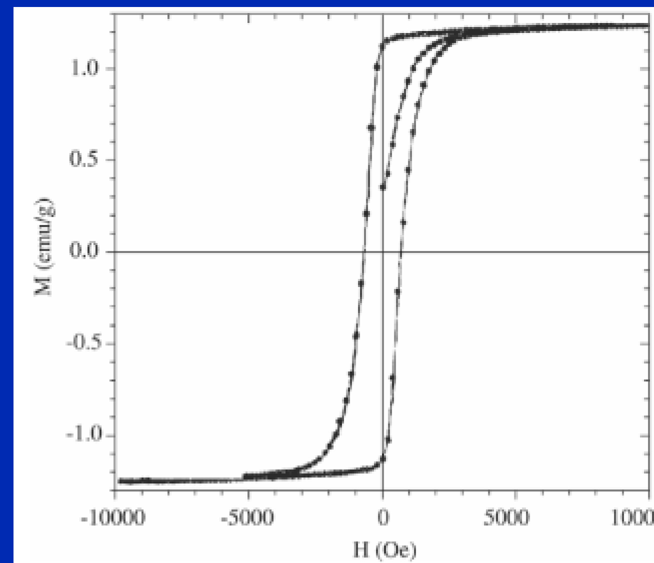


Figure 7. Hysteresis loop of the powder calcined at 1450 °C.

V. da Rocha Caffarena, T. Ogasawara, Mat. Res. 2003