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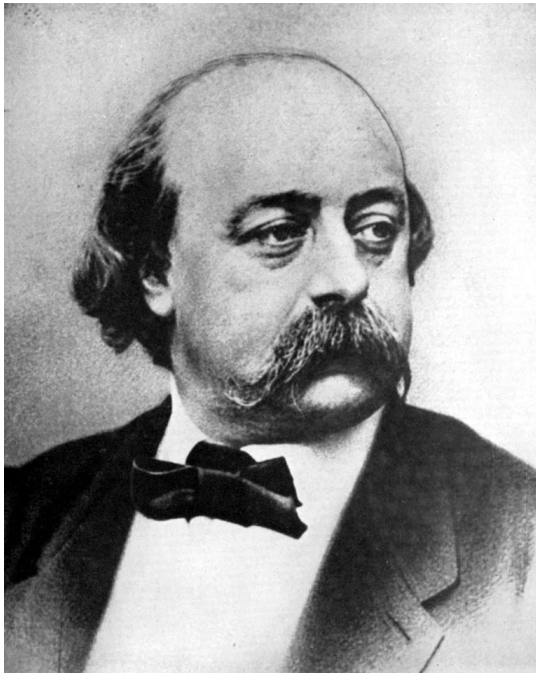


Basic Magnetism (I. Fundamentals)

A journey through Magnetism

or,

From atoms to macroscopic bodies - and back



Magnétisme: joli sujet de conversation, et qui sert à “faire des femmes”

Magnetism: an agreeable subject of conversation that can also be used to “impress women”

Gustave Flaubert, *Dictionnaire des idées reçues*, [Dictionary of Received Ideas], published 1911-13

If **one** distinctive feature of this “subject of conversation” should be stated, this could be the following one:

Magnetic phenomena involve an extremely wide variety of scales of space and time - and must be studied using a multiplicity of techniques (both experimental and theoretical)

Some examples (list not exhaustive):

- down to the atomic scale, *strictly quantum-mechanical treatment*
- *order against disorder*
- may involve *one or more phase transitions*
- *macroscopic self-organization of microscopic units*
- *single-particle and collective phenomena*
- test ground for the *physics of complex systems*

Microscopic “bricks”

- Stable magnetic moments on free atoms/ions
- Magnetic atoms/ions in solids: the crystal field
- *Why do magnetists typically speak of “spins”?* : Quenching of the angular momentum

Magnetism of free atoms and ions

1) Magnetic moment of a single orbiting electron of angular momentum ℓ : $\mu_l = -\mu_B \ell$

$$|\mu_l| = \frac{|e|\hbar}{2m_e c} [l(l+1)]^{\frac{1}{2}}$$

$$\mu_{l,z} = -\frac{|e|\hbar}{2m_e c} m_l$$
$$m_l = -l, -l+1, \dots, l-1, l$$

$$\mu_B = \frac{|e|\hbar}{2m_e c} = 0.927 \times 10^{-21} [\text{emu}]: \text{Bohr magneton}$$

2) Magnetic moment associated to electron spin s : $\mu_s = -2\mu_B s$

$$\mu_{s,z} = \pm g_s \frac{|e|\hbar}{2m_e c} \frac{1}{2} = \pm \frac{1}{2} g_s \mu_B$$
$$m_s = \pm \frac{1}{2}, \quad g_s \cong 2.0023$$

Total magnetic moment of the electron*:

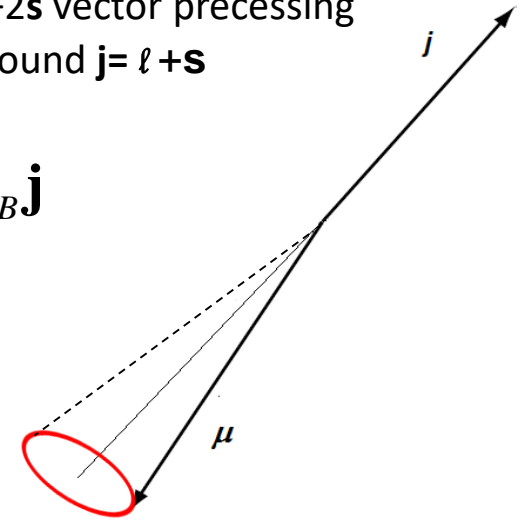
*exercise nr. 1

constant of
motion

$$\boldsymbol{\mu} = \boldsymbol{\mu}_l + \boldsymbol{\mu}_s = -\mu_B(\boldsymbol{\ell} + 2\mathbf{s}) = -g\mu_B\mathbf{j}$$

$$\mathbf{j} = \boldsymbol{\ell} + \mathbf{s}$$

$\boldsymbol{\ell} + 2\mathbf{s}$ vector precessing
around $\mathbf{j} = \boldsymbol{\ell} + \mathbf{s}$

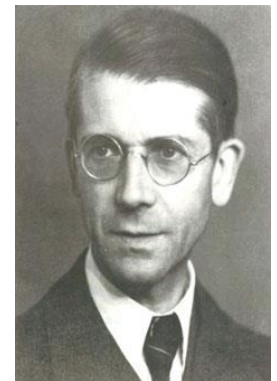


g: Landé's factor.

Magnetic moment on a multi-electron atom

Magnitude of magnetic moment is determined by
Pauli's principle + Hund's rules

- Only two electrons can occupy a single energy level [taking spin into account]
- In the ground state : (a) $\sum m_s$ takes the maximum possible value and (b) $\sum m_l$ is a maximum too (compatibly with condition [a])



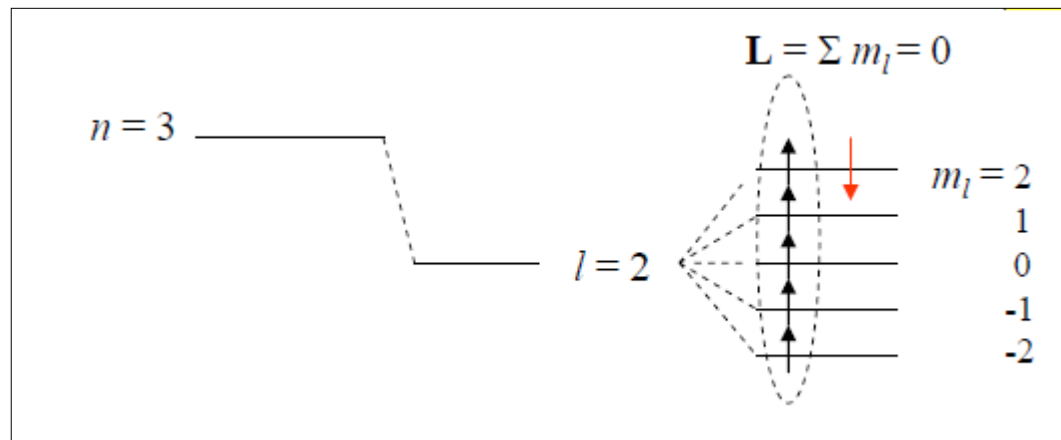
- Principal quantum number n
- Orbital angular momentum quantum number ℓ
- Magnetic quantum number m_l
- Spin quantum number m_s

$$\ell = 0, 1, 2, \dots, n-1$$

$$m_l = -\ell, -\ell + 1, -\ell + 2, \dots, \ell$$

$$m_s = +1/2, -1/2$$

Example: Fe^{2+} ion, $3d^6$



$$S = \sum m_s = \frac{1}{2} + \frac{1}{2} + \dots + \frac{1}{2} - \frac{1}{2} = \frac{4}{2} = 2$$

$$L = \sum m_l = 2 + 1 + 0 - 1 - 2 + 2 = 2$$



$$\mathbf{L = 2, S = 2}$$

In any completely filled electron shell: $S=0$, $L=0$

Russell-Saunders coupling

How do the spin and orbital angular momenta combine to form the total angular momentum of an atom ? → Central role of spin-orbit interaction

$$H_{s.o.} = \lambda \mathbf{L} \cdot \mathbf{S}$$

$$\mathbf{L} = \sum_i \boldsymbol{\ell}_i, \quad \mathbf{S} = \sum_i \mathbf{s}_i$$

Total spin feels the magnetic field resulting from the apparent motion of the nucleus' electric charge in the non-inertial frame where the electron is at rest

When spin-spin and orbit-orbit couplings dominate over spin-orbit interaction (which is treated as a perturbation):

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

$$J = (L + S), (L + S - 1), \dots, |L - S|$$

Ground state & $\lambda > 0$: \mathbf{L} and \mathbf{S} are anti-parallel for a less than half-filled shell, and $J = |L - S|$; \mathbf{L} and \mathbf{S} are parallel for a more than half-filled shell, so $J = L + S$.

Magnetic moment μ

$$\mu = -\mu_B(\mathbf{L} + 2\mathbf{S}) = -g_J\mu_B\mathbf{J}$$

$$g_J = \frac{[3J(J+1) + S(S+1) - L(L+1)]}{[] 2J(J+1)} : \text{Lande's g-factor}$$

$$\text{Effective magnetic moment } \mu_{eff} = g_J\mu_B\sqrt{J(J+1)}$$

*exercise nr. 2

$$\text{Effective number of Bohr magnetons: } p = g_J\sqrt{J(J+1)}$$

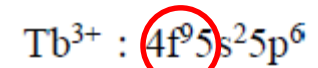
Transition metals and rare earth metals follow the Russell-Saunders coupling*

Total \mathbf{J} is a good quantum number.

*insight nr. 1

Reminder: in heavier atoms (actinides), there is a strong spin - orbit (ℓ - s) coupling for each electron; this coupling is stronger than the ℓ - ℓ or s - s coupling between different electrons \rightarrow *j-j coupling scheme*.

$$\mathbf{J} = \sum \mathbf{j}_i = \sum (\boldsymbol{\ell}_i + \mathbf{s}_i)$$



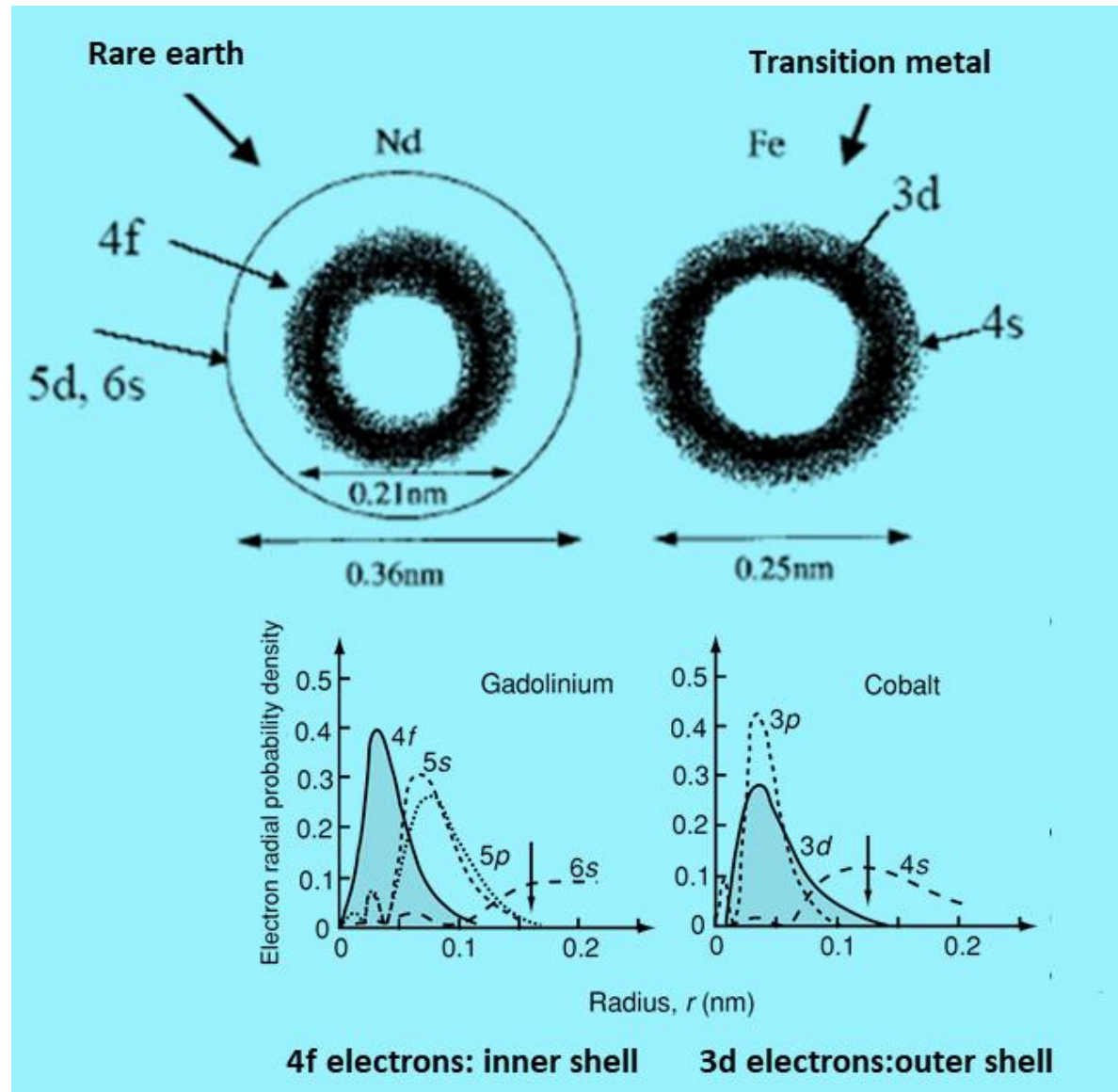
$\uparrow \downarrow$	m_l 3
$\uparrow \downarrow$	2
\uparrow	1
\uparrow	0
\uparrow	-1
\uparrow	-2
\uparrow	-3

$$\begin{aligned} L &= 5, S = 5/2 \\ J &= L + S = 15/2 \\ g &= 4/3 \\ \mu_{eff} &= 10.65 \mu_B \end{aligned}$$

Are these results still valid for magnetic atoms/ions inside crystalline solids?

$$\Psi_{nlm} = R_{nl}(r)Y_l^m(\theta, \varphi)$$

$$R_{nl}(r) \propto \exp\left(-\frac{Zr}{na_0}\right)$$

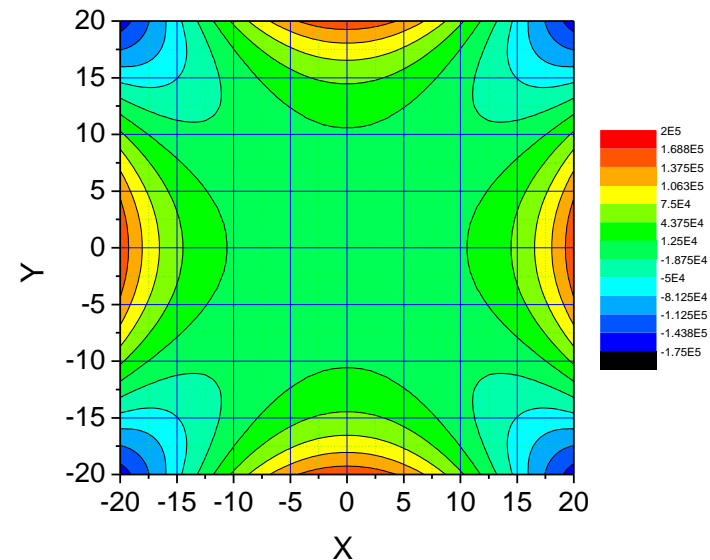
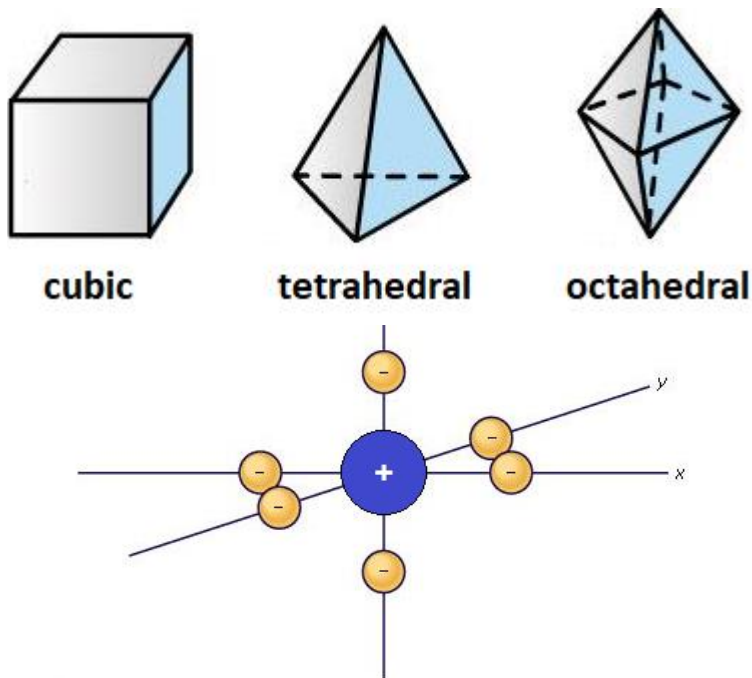


Crystal field effects

In a crystal the electrostatic potential has no longer spherical symmetry

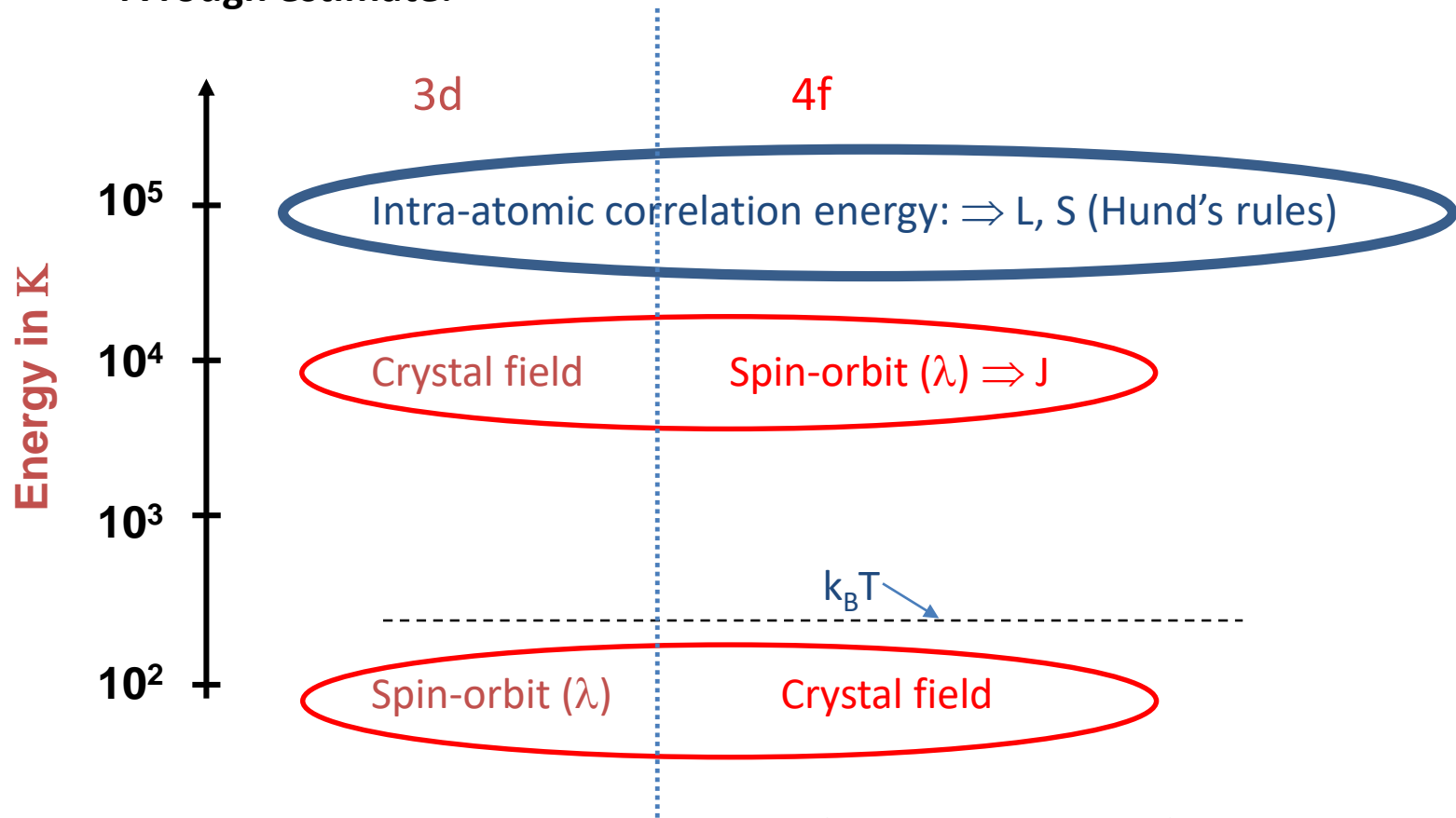
e.g., in a cubic crystal: $V_c = V_0(x^4 + y^4 + z^4 - 3x^2y^2 - 3y^2z^2 - 3z^2x^2)$

Electrostatic interaction of electron charge density with fields generated by surrounding ions



2 basic symmetries of surroundings:
cubic/octahedral & tetrahedral

A rough estimate:



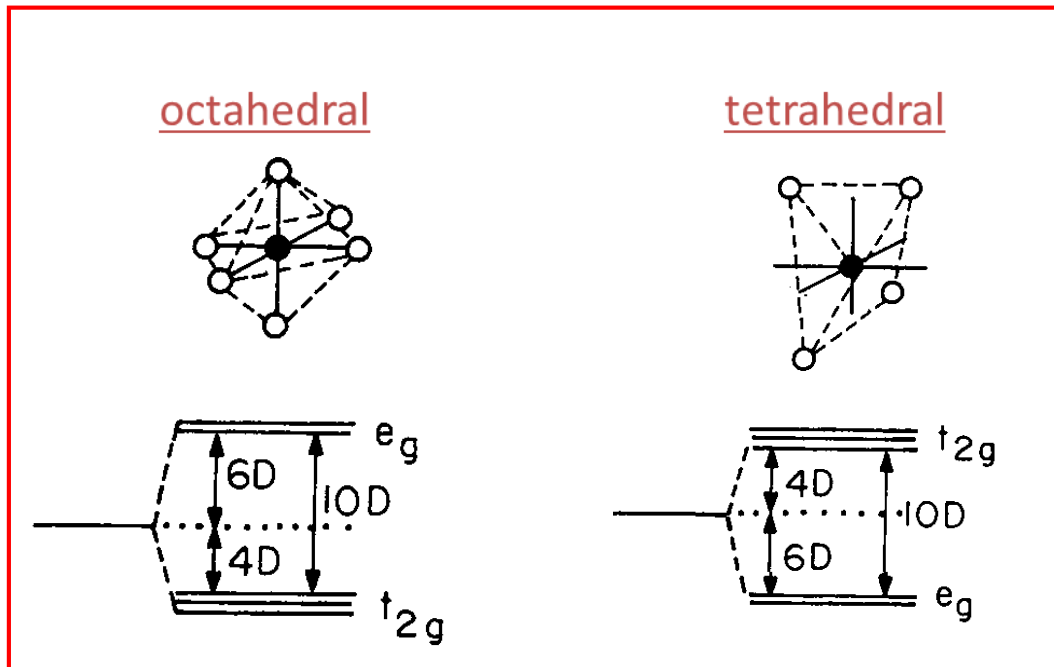
- 3d electrons less shielded than 4f electrons: crystal field larger in transition metal ions
- Spin-orbit coupling $\approx (\text{atomic number})^4$: larger in rare-earth ions

Crystal field effects in 3d ions (cubic symmetry)

In the Coulomb potential of the nucleus, the angular dependence of 3d electron wavefunction is given by the 5 spherical harmonics $Y_2^m(\theta, \varphi)$

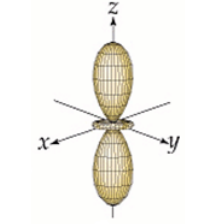
$V_c = V_0(x^4 + y^4 + z^4 - 3x^2y^2 - 3y^2z^2 - 3z^2x^2)$ adds as a perturbation term \rightarrow this breaks spherical symmetry \rightarrow new wavefunctions of 3d electrons reflect environment's symmetry

Typical environments:

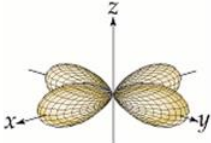


Angular part of the new angular wavefunctions - for the doublet:

$$\left\{ \begin{array}{l} Y_2^0(\theta, \varphi) \\ \frac{1}{\sqrt{2}} [Y_2^2(\theta, \varphi) + Y_2^{-2}(\theta, \varphi)] \end{array} \right\} \rightarrow \left\{ \begin{array}{l} \frac{(2z^2 - x^2 - y^2)}{r^2} \\ \frac{(x^2 - y^2)}{r^2} \end{array} \right\}$$



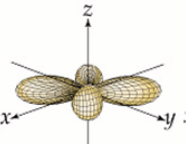
e_g¹



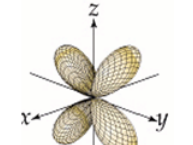
e_g²

the same for the triplet:

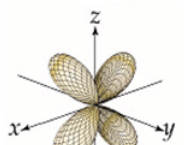
$$\left\{ \begin{array}{l} \frac{1}{\sqrt{2}} [Y_2^2(\theta, \varphi) - Y_2^{-2}(\theta, \varphi)] \\ \frac{1}{\sqrt{2}} [Y_2^1(\theta, \varphi) - Y_2^{-1}(\theta, \varphi)] \\ \frac{1}{\sqrt{2}} [Y_2^1(\theta, \varphi) + Y_2^{-1}(\theta, \varphi)] \end{array} \right\} \rightarrow \left\{ \begin{array}{l} \frac{xy}{r^2} \\ \frac{yz}{r^2} \\ \frac{zx}{r^2} \end{array} \right\}$$



t_{2g}¹



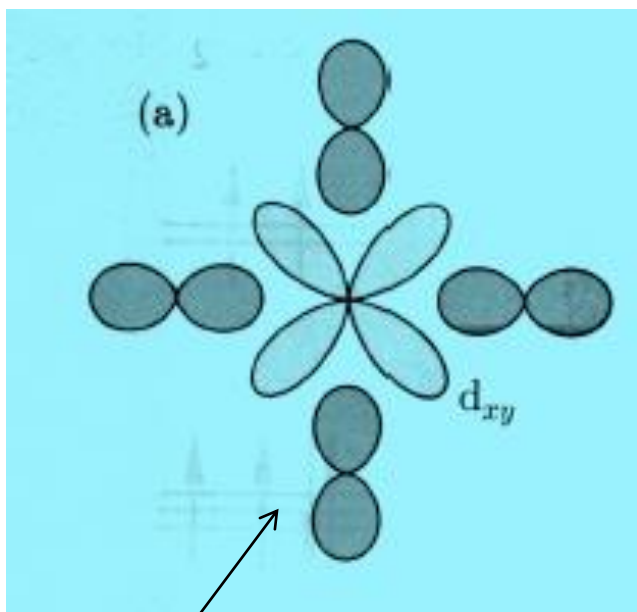
t_{2g}²



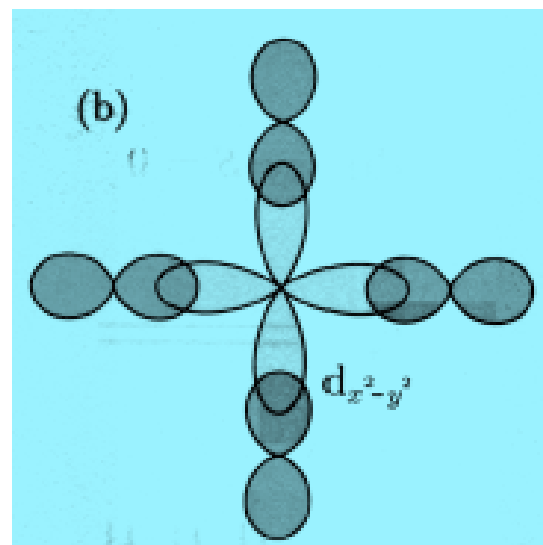
t_{2g}³

The new wavefunctions (tesseral harmonics) are **real functions** and exhibit typical **lobes** which explain the energy splitting between doublet and triplet states.

An example: in octahedral symmetry the energy associated to the orbital xy [t_{2g}^1] is lower to the energy of orbital (x^2-y^2) [e_g^2]: $E_{\text{tripl}} < E_{\text{doub}}$



Orbitals of nerest
neighbours (non
magnetic)



Larger superposition:
higher electrostatic
energy

Quenching of orbital angular momentum

Expectation value of orbital angular momentum \mathbf{L} :

a) If ground state is a doublet:

$$\langle e_g^{1,2} | L_\alpha | e_g^{1,2} \rangle = 0$$

$$\alpha = x, y, z$$

$$\mathbf{L} = -i\hbar(\mathbf{r} \times \nabla)$$

Quenching of orbital angular momentum

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$$\alpha = x, y, z$$

$$\mathbf{L} = -i\hbar(\mathbf{r} \times \nabla)$$

all matrix elements of \mathbf{L} are equal to zero: **complete quenching**

b) If ground state is a triplet:

diagonal elements still equal to zero, but non-zero off-diagonal elements exist:
partial quenching

The magnetic moment of 3d atoms/ions in a crystal structure is dominated by the spin contribution

3d ions: quenching of orbital momentum

Ion	Config- uration	Basic level	$p(\text{calc}) = g[J(J + 1)]^{1/2}$	$p(\text{calc}) = 2[S(S + 1)]^{1/2}$	$p(\text{exp})^a$
Ti ³⁺ , V ⁴⁺	3d ¹	² D _{3/2}	1.55	1.73	1.8
V ³⁺	3d ²	³ F ₂	1.63	2.83	2.8
Cr ³⁺ , V ²⁺	3d ³	⁴ F _{3/2}	0.77	3.87	3.8
Mn ³⁺ , Cr ²⁺	3d ⁴	⁵ D ₀	0	4.90	4.9
Fe ³⁺ , Mn ²⁺	3d ⁵	⁶ S _{5/2}	5.92	5.92	5.9
Fe ²⁺	3d ⁶	⁵ D ₄	6.70	4.90	5.4
Co ²⁺	3d ⁷	⁴ F _{9/2}	6.63	3.87	4.8
Ni ²⁺	3d ⁸	³ F ₄	5.59	2.83	3.2
Cu ²⁺	3d ⁹	² D _{5/2}	3.55	1.73	1.9

Effective number of Bohr magnetons:

$$p = 2\sqrt{S(S + 1)}$$

~~$$p = g\sqrt{J(J + 1)}$$~~

In most crystals of 3d elements, alloys, and compounds, electron spin is the dominant source of the magnetic moment

Looking for the effective number of Bohr magnetons per atom (ion) of the same element in different substances/arrangements can be a most surprising / frustrating experience

Example: Magnetic moment of Fe as determined by atomic rules:

$$\mu_0 = g_J \mu_B J, \mu_{\text{eff}} = g_J \mu_B (J(J+1))^{1/2}$$

$$\text{Fe}^{3+}: 3d^5 \quad L=0, S=5/2, J=5/2, g_J=2, \mu_0 = 5\mu_B, \mu_{\text{eff}} = 5.9\mu_B$$

$$\text{Fe}^{2+}: 3d^6, L=2, S=2, J=4, g_J=3/2, \mu_0 = 6\mu_B, \mu_{\text{eff}} = 6.7\mu_B$$

Fe: metal, compounds & associations:

- FeO or wüstite (Fe^{2+}): $\mu_{\text{eff}} = 5.33 \mu_B \rightarrow$ partial quenching of the orbital momentum (complete quenching would give $\mu_{\text{eff}} = 4.9 \mu_B$)

$\gamma\text{-Fe}_2\text{O}_3$ or maghemite (Fe^{3+}): $\mu_0 = 5 \mu_B$

$\alpha\text{-Fe}$ (metal): $\mu_0 = 2.2 \mu_B$

YFe_2 (intermetallic): $\mu_0 = 1.45 \mu_B$

YFe_2Si_2 : Fe apparently does not carry a magnetic moment

Fe surface: $\mu_0 = 2.8 \mu_B$

Magnetic ordering & magnetic long-range order

- Independent, localized magnetic moments: Van Vleck's Paramagnetism
- Weiss theory of Ferromagnetism: the “molecular field”
- Quantum origin of the “molecular field”
- An introduction to Paramagnetism and Ferromagnetism of metals
- Other types of magnetic long-range order

Magnetic-field sustained ordering of localized magnetic moments: Van Vleck's Paramagnetism

- Atomic magnetic moment $\boldsymbol{\mu} = - (\mathbf{L} + 2\mathbf{S}) \mu_B = - g_J \mathbf{J} \mu_B$
- No interaction between atomic moments
- Random orientation of moments at finite T and H = 0



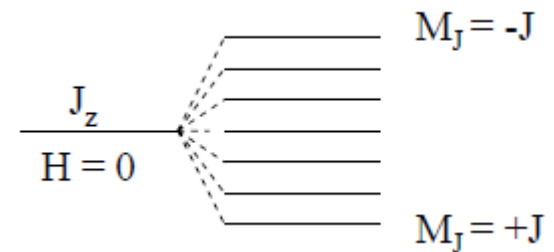
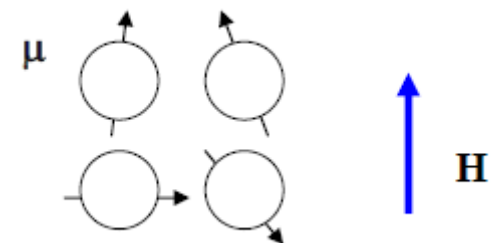
Zeeman hamiltonian & energy:

$$\mathcal{H} = - \boldsymbol{\mu} \cdot \mathbf{H} = - g \mu_B \mathbf{J} \cdot \mathbf{H}$$

$E_J = g \mu_B M_J H$ - where M_J is the eigenvalue of J_z

Probability of split-level occupancy is given

by Boltzmann statistics:
$$p(M_J) = \frac{e^{-\frac{E_J}{k_B T}}}{\sum_J e^{-\frac{E_J}{k_B T}}}$$



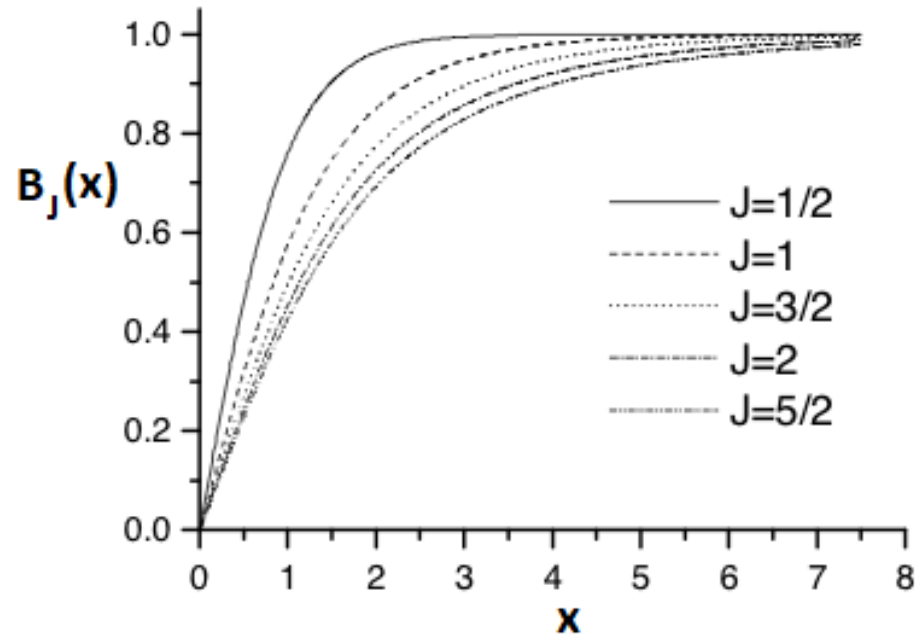
Equilibrium magnetization (Mean magnetic moment μ per unit cell)*:

$$M = N \langle \mu \rangle = Ng_J \mu_B \sum_J p(M_J) M_J = Ng_J \mu_B J B_J(x) \text{ (sum extended to } (2J+1) \text{ levels with different } M_J \text{ split by Zeeman interaction)}$$

$$B_J(x) = \frac{(2J + 1)}{2J} \coth \left[\frac{(2J + 1)}{2J} x \right] - \frac{1}{2J} \coth \left(\frac{x}{2J} \right)$$

Brillouin's function

where $x = g_J \mu_B H / k_B T$



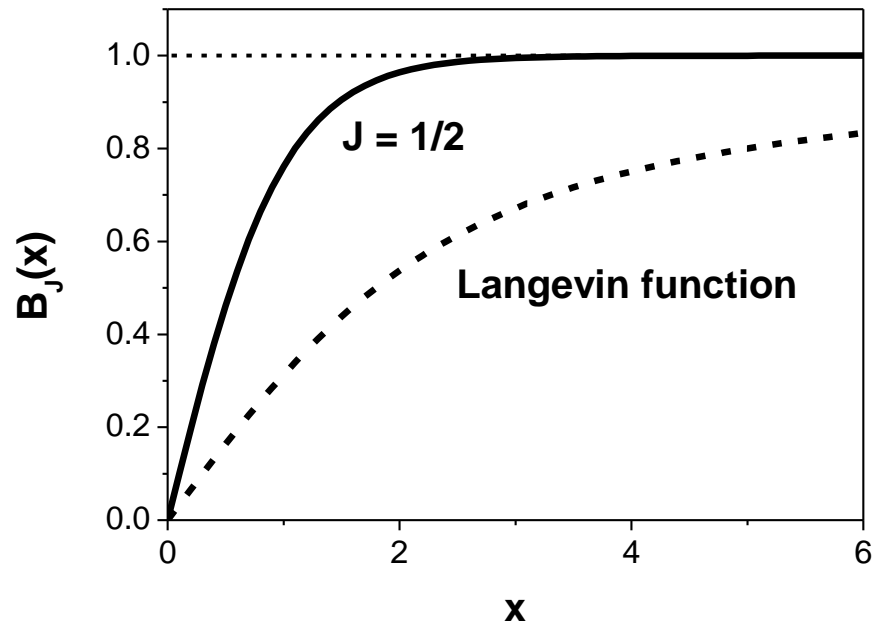
*disordering: exercise nr. 3

Classical limit ($J \rightarrow \infty$): $B_J(x) \rightarrow$ **Langevin's function**

$$L(x) = \coth(x) - \frac{1}{x} \quad \text{where } x = \mu H / kT$$

(μ : classical magnetic moment)

- Physical meaning: μ assumed to take all orientations with respect to \mathbf{H}
- Langevin's theory not suitable to describe ionic (quantum) paramagnetism. *But see later: «Langevin function revival»*



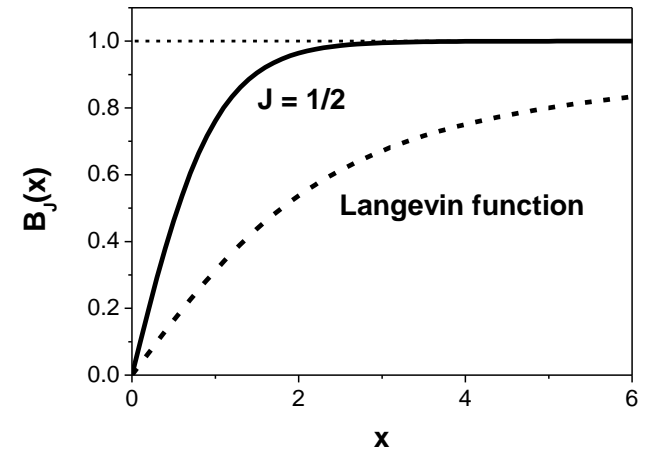
- High field limit: saturation

$$B_J(x) \rightarrow 1 \quad (H \rightarrow \infty)$$

$$M_s = N \mu_s; \quad \mu_s = g \mu_B J$$

N: Number of atoms per unit volume

all moments
become aligned



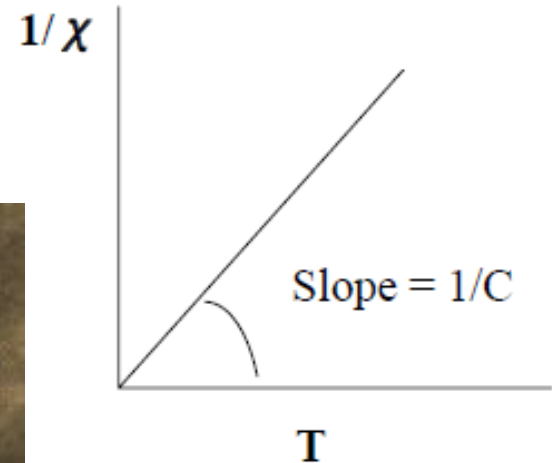
linearization

- High-temperature limit ($x \ll 1$): $B_J(x) \rightarrow [(J + 1)/3J] x$

$$M = N g_J^2 \mu_B^2 J(J + 1) H / 3k_B T = [N \mu_{\text{eff}}^2 / 3k_B T] H$$

$$\chi = M/H = C/T : \text{Curie's law}$$

$$C = N \mu_{\text{eff}}^2 / 3k_B$$



Weiss theory: Ferromagnetism of localized moments

Interaction among moments described by a “molecular” field. *This has been the first mean-field theory in history of physics.* The total magnetic field on each magnetic moment is $\mathbf{H}_T = \mathbf{H} + w \mathbf{M}$ with $w =$ positive constant, to be determined later.

$$E_j = -g_j \mu_B M_j (H + w M)$$

$$M = N \langle \mu \rangle = Ng_j \mu_B \sum_j p(M_j) M_j = Ng_j \mu_B J B_J(x) = M_0 B_J(x)$$

$$M_0 = Ng_j \mu_B J$$

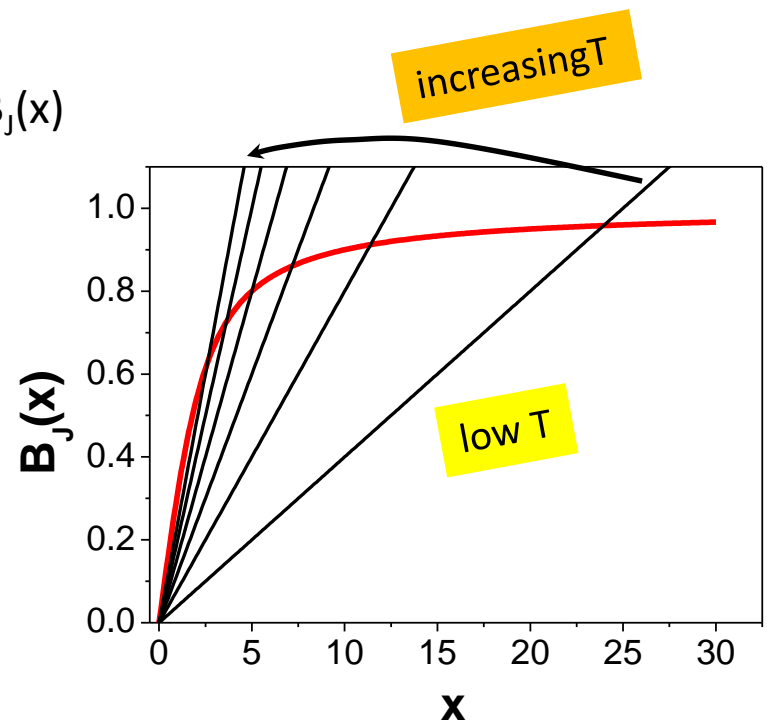
$$x = g_j J \mu_B (H + w M) / k_B T$$

When $H = 0$, a spontaneous magnetization M_s can exist below some temperature; draw:

$$M/M_0 = kT x / N(g_j \mu_B J)^2 w \text{ (slope depends on } T)$$

$$M/M_0 = B_J(x)$$

Intersect (if any) gives $M_s(T)$. **Long-range magnetic order exists below some critical temperature**



High temperature limit: $x \ll 1$

$$B_J(x) \cong (J + 1) x / 3 J$$

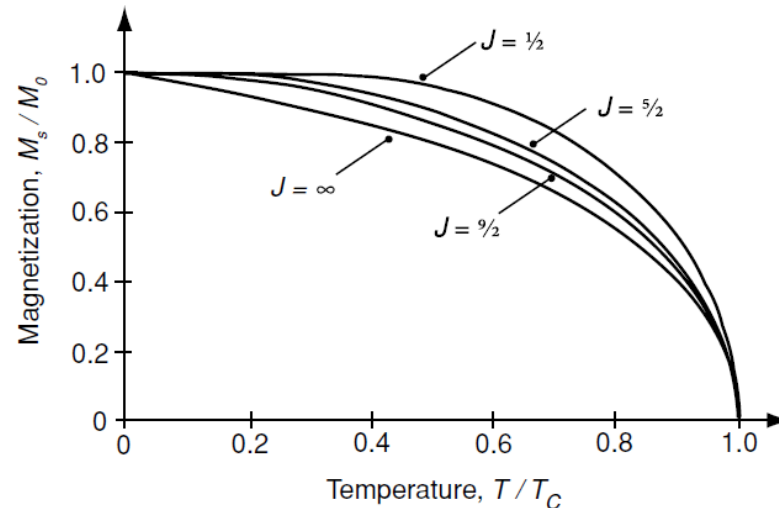
at T_c : straight line =
tangent to $B_J(x)$ in $x=0$

Define critical temperature T_c for the onset of ferromagnetism from:

$$k_B T_c / N(g_J \mu_B J)^2 w = (J + 1) / 3 J \rightarrow T_c = N(g_J \mu_B)^2 J (J + 1) w / 3 k_B = C w$$

a.k.a. *paramagnetic Curie temperature*; $T_c = N \mu_{\text{eff}}^2 w / 3 k_B$

$C = N \mu_{\text{eff}}^2 / 3 k_B$ is the Curie constant



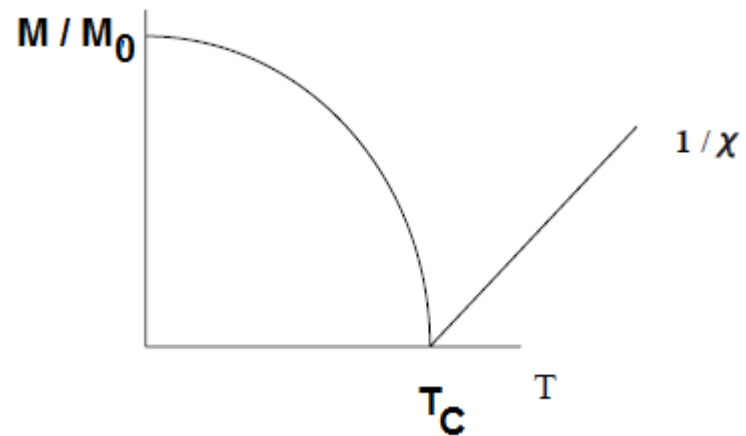
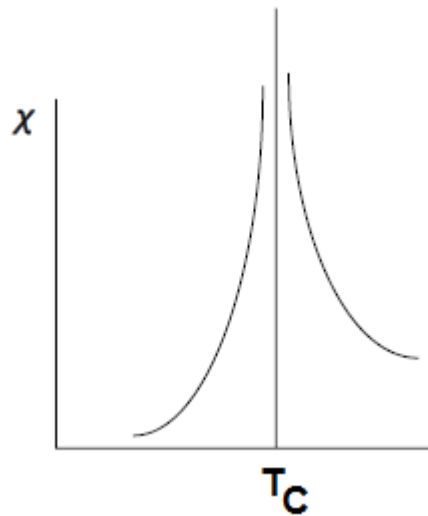
Above T_C : no *spontaneous* magnetization, no long-range order – a magnetic field is needed to induce magnetic order → paramagnetic response to applied field H :

$x \ll 1 \rightarrow$ Brillouin's function linearized

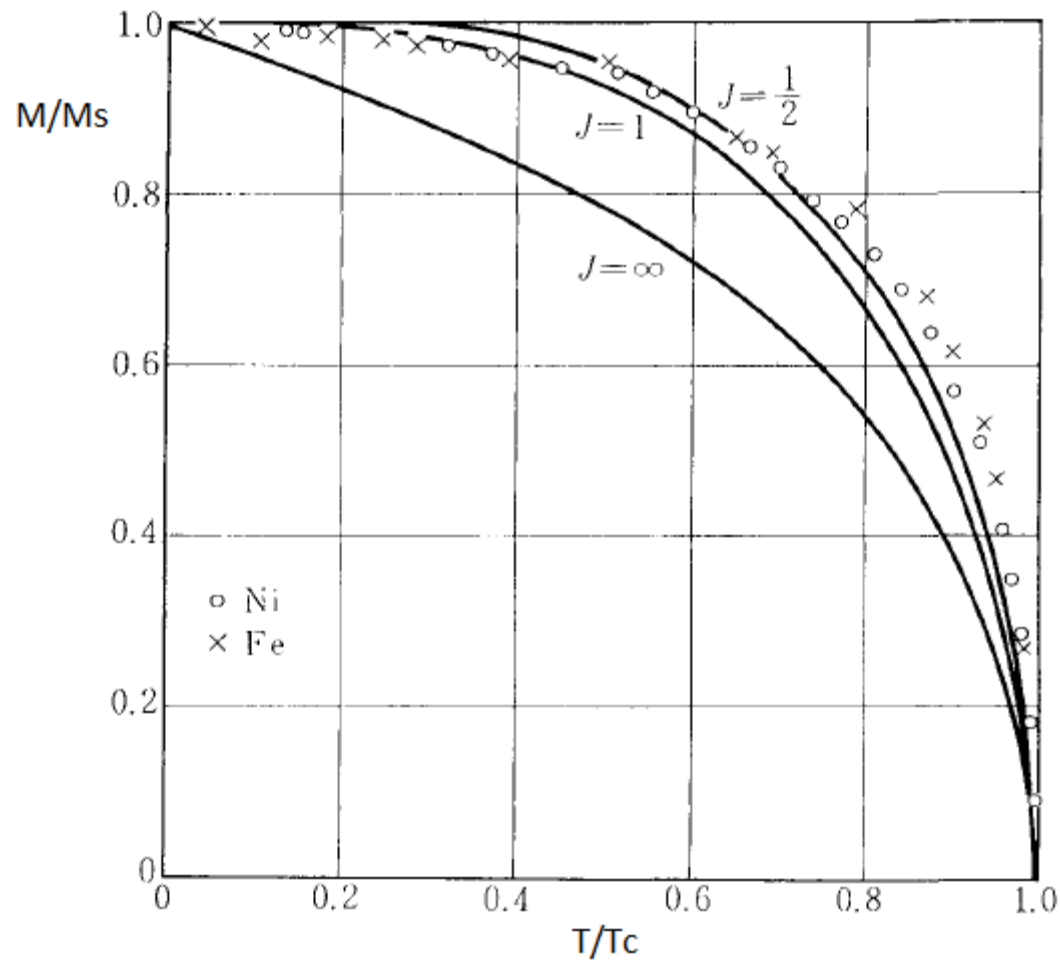
$$M \cong N g_J \mu_B J (J + 1) x / 3 = (C/T) (H + w M)$$

$$M = \frac{C}{T - Cw} H$$

$$\chi = \frac{M}{H} = \frac{C}{T - T_C} \quad \text{Curie-Weiss law}$$



Alas, the mean-field theory *fails* almost everywhere for nearly all materials...



Order-of-magnitude estimate of Weiss constant w

Values roughly appropriate to metallic Fe:

$$T_C = 1063 \text{ K}; \mu = 2.2 \mu_B, N = 8.54 \times 10^{22} / \text{cm}^3; J = S = 1$$

$$w = \frac{3k_B T_C}{N\mu^2 J(J+1)} \cong 6550 \quad (\text{a pure number in the Gaussian system of units})$$

Estimated amplitude of “molecular” field $H_m = w M = w N \mu \cong 1.1 \times 10^7 \text{ Oe}$

Typical static field generated by a standard electromagnet: $2 \times 10^4 \text{ Oe}$

Typical static field generated by a commercial superconducting magnet: $7 \times 10^4 \text{ Oe}$

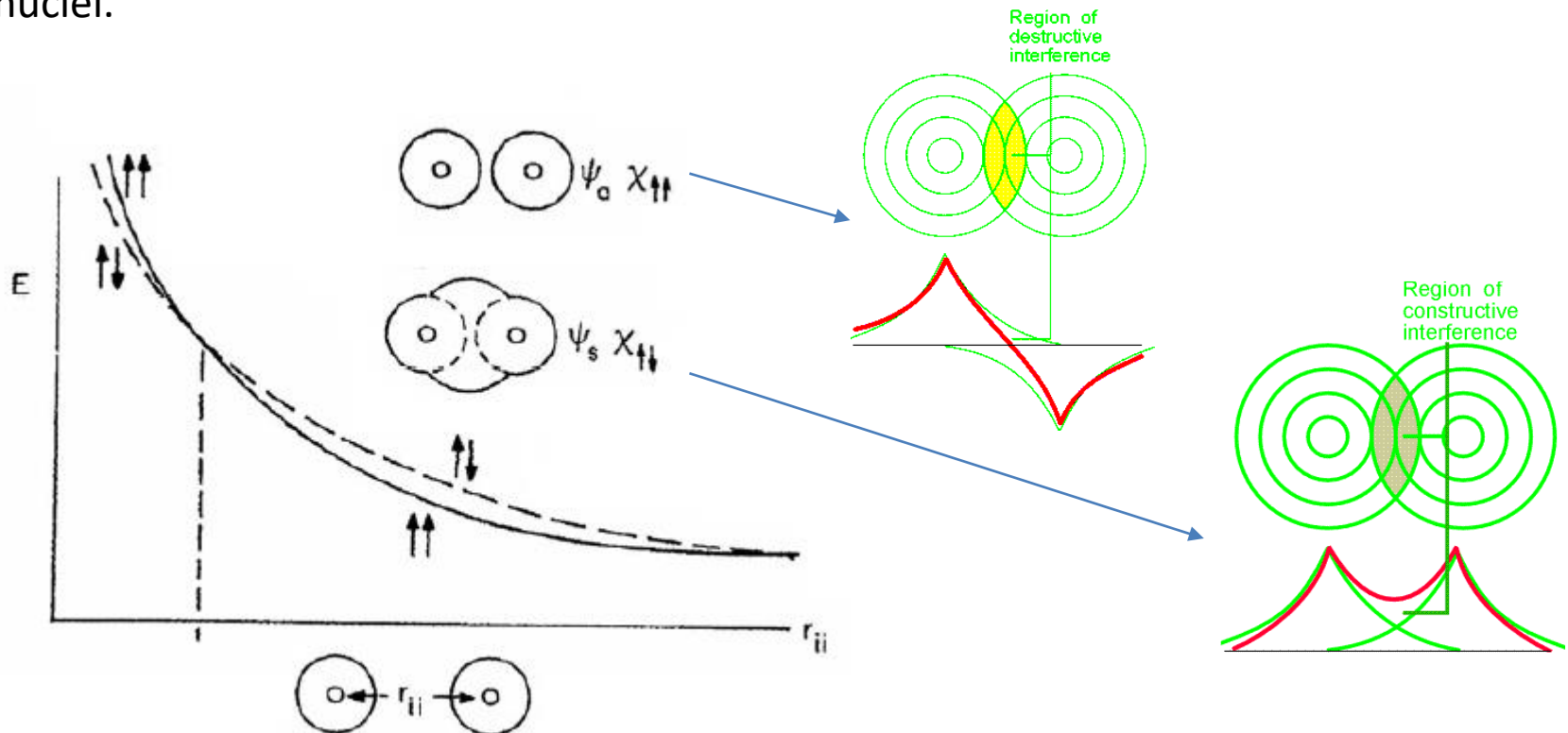
This estimate definitely rules out magnetic dipole-dipole interaction as a source of internal field.

No other classical magnetic interaction exists. The effect has fully quantum origin.

Quantum origin of the effective (“molecular”) field → exchange interaction

Coulomb repulsion of nearby electrons + Pauli principle: electrons cannot be in the same place if they are in the same spin state.

Energy difference between $\uparrow_i\downarrow_j$ and $\uparrow_i\uparrow_j$ configurations of electron spins on neighboring atoms i,j . Actual state of lowest energy depends on distance between nuclei.



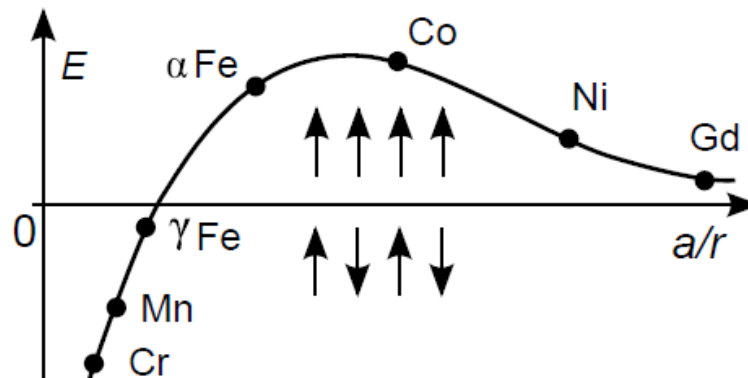
Exchange interaction is basically electrostatic and involves electron **orbits, not spins**. The starting hamiltonian contains Coulomb interaction between electrons in their orbits

However, the Pauli principle (\rightarrow *globally anti-symmetric electron wavefunction*) implies a connection between orbital and spin states.

A **spin hamiltonian** can be introduced: the Heisenberg hamiltonian, which contains the exchange integral \mathcal{J}_{ij}

$$\mathcal{H}_j = -\mathcal{J}_{ij} \mathbf{S}_i \cdot \mathbf{S}_j$$

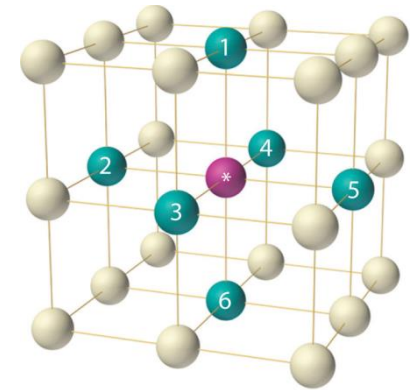
Positive \mathcal{J}_{ij} means parallel alignment of two spins; if \mathcal{J}_{ij} is negative, antiparallel alignment is favored.



In a crystal the Heisenberg hamiltonian is formally written

$$\mathcal{H} = - \sum_{i \neq j} \mathcal{J}_{ij} \mathbf{S}_i \cdot \mathbf{S}_j$$

It is often possible (mainly in insulators) to take only **nearest-neighbour interactions** in the above expression:



$$\mathcal{H} = - \sum_i \mathbf{S}_i \cdot \left(\mathcal{J} \sum_{n.n. \text{ of } i} \mathbf{S}_j \right) \rightarrow - \sum_i \mathbf{S}_i \cdot \left(\mathcal{J} \sum_{n.n. \text{ of } i} \langle \mathbf{S}_j \rangle \right) = - \sum_i \boldsymbol{\mu}_i \cdot \mathbf{H}_{eff}$$

\mathcal{J} is the same for all nn's of i

$$\boldsymbol{\mu}_i = g\mu_B \mathbf{S}_i \rightarrow \mathbf{M} = Ng\mu_B \langle \mathbf{S} \rangle$$

fluctuating \mathbf{S}_j substituted by mean value

$$\mathbf{H}_{eff} = \frac{\mathcal{J}z}{g\mu_B} \langle \mathbf{S} \rangle = \frac{\mathcal{J}z}{Ng^2\mu_B^2} \mathbf{M} = w\mathbf{M}$$

z : number of n.n.

The mean field approach in the Weiss form naturally emerges as an (over)simplified treatment of the Heisenberg hamiltonian. The Curie temperature T_C is a measure of the exchange integral:

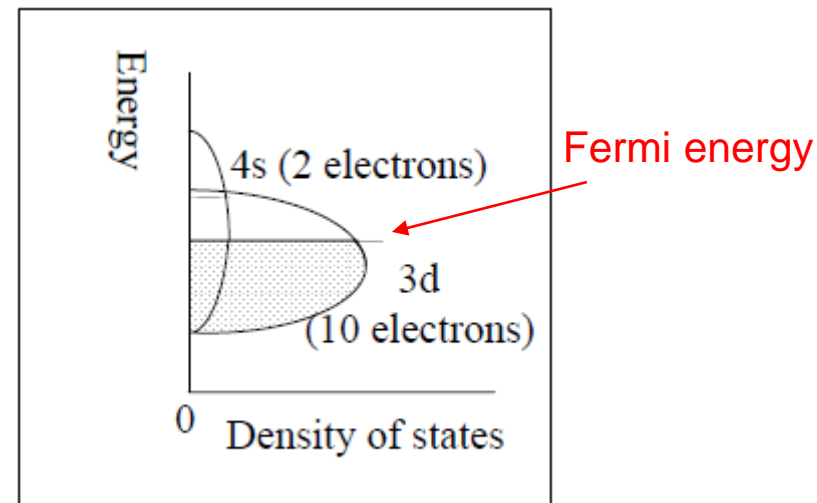
$$T_C = Cw = \frac{Ng^2\mu_B^2 S(S+1)}{3k_B} \frac{\mathcal{J}z}{Ng^2\mu_B^2} = \frac{zS(S+1)}{3k_B} \mathcal{J}$$

Magnetism and Ferromagnetism in Metals (*itinerant electron magnetism*)

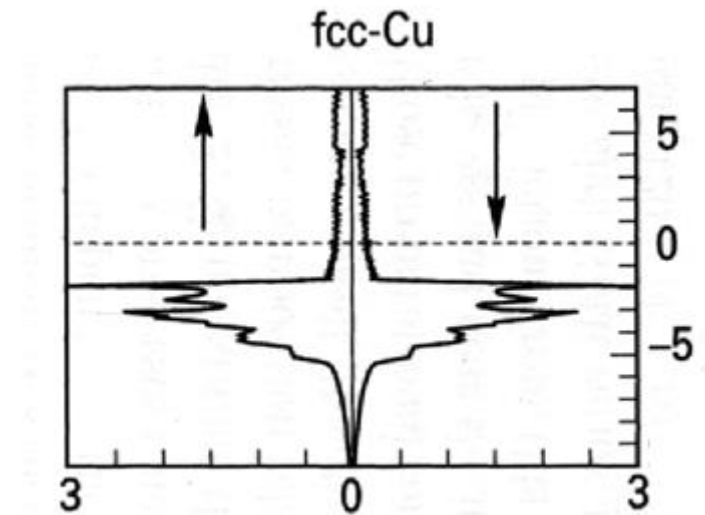
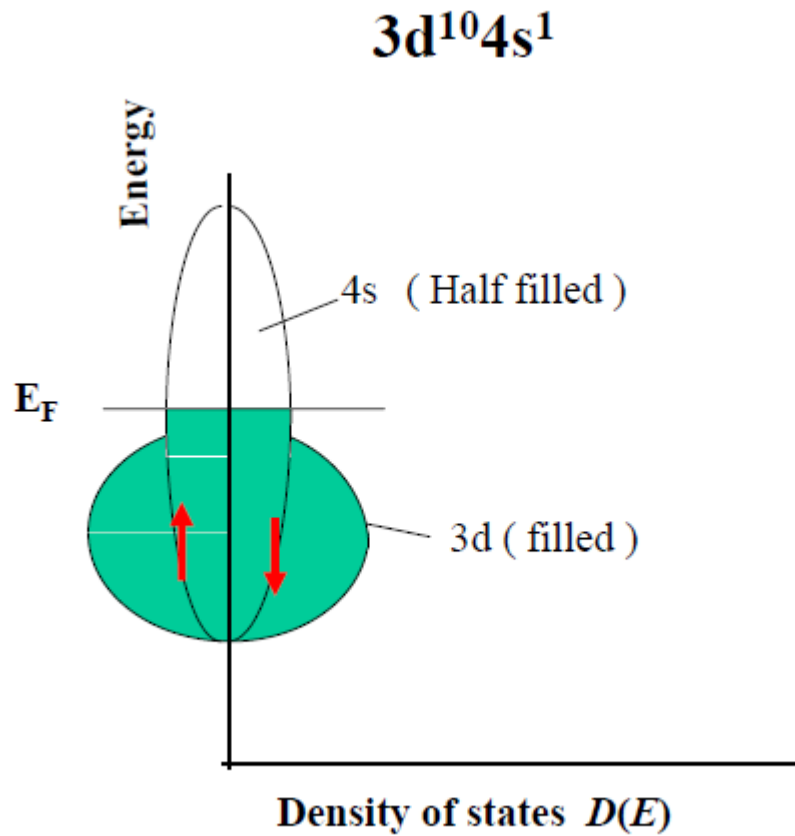
Magnetic electrons (except for the lanthanides) are usually outer electrons; in a 3d metal such as Fe, Co, Ni they are not closely bound to the atoms: they participate in the conduction mechanism. A picture of magnetism of “itinerant electrons” is needed. This involves an entirely different approach.

In 3d metals, magnetic electrons belong to a *narrow band* in opposition to 4s electrons.

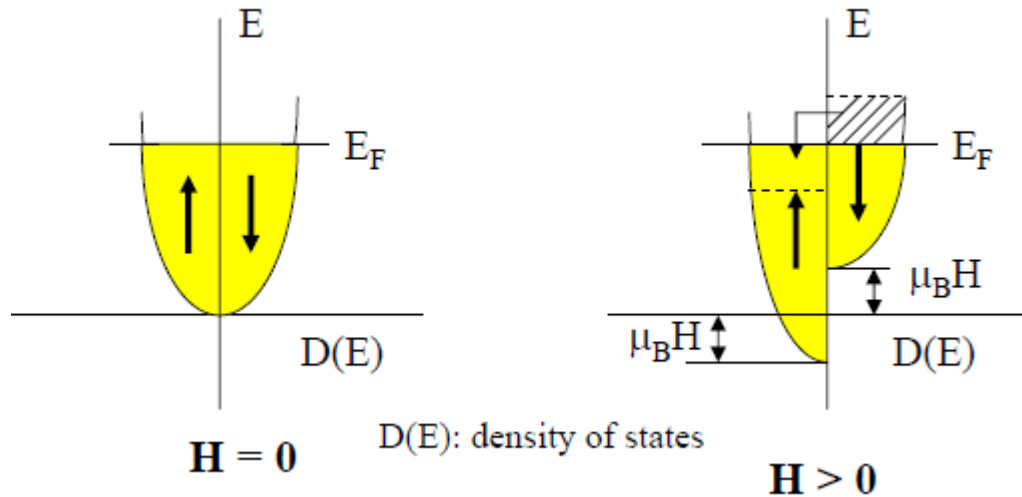
- Density of states of 3d electrons around Fermi energy is generally high
- Effective mass in 3d electrons is much higher than in 4s electrons: conduction processes are mostly ascribed to 4s electrons, however 3d electrons contribute too.



Band structure of Cu (*no net magnetic moment* → *diamagnetic metal*)



Pauli paramagnetism of free conduction electrons



Shift of subbands sustained by an external magnetic field

$$\begin{cases} \varepsilon_{\uparrow} = -\mu_B H \\ \varepsilon_{\downarrow} = +\mu_B H \end{cases}$$

- Only electrons within an energy $k_B T$ around the Fermi level are able to change spin orientation

The magnetic field produces a rigid shift of the two subbands. The numbers of spin-up /spin-down electrons become different. For simplicity, we consider the $T = 0$ case:

$$N_{\uparrow} = \frac{1}{2} \int_{-\mu_B H}^{E_F} D(E) dE \cong \frac{1}{2} \left(\int_0^{E_F} D(E) dE + \mu_B D(E_F) H \right)$$

$$N_{\downarrow} = \frac{1}{2} \int_{+\mu_B H}^{E_F} D(E) dE \cong \frac{1}{2} \left(\int_0^{E_F} D(E) dE - \mu_B D(E_F) H \right)$$

The difference is proportional to the magnetization of the system:

$$M = (N_{\uparrow} - N_{\downarrow}) \mu_B = \mu_B^2 D(E_F) H$$

density of states at E_F
(for free electrons)

$$D(E_F) = \frac{3N}{2E_F}$$

$$\chi_{Pauli} = \frac{M}{H} = \frac{3N\mu_B^2}{2E_F}$$

Pauli's paramagnetic susceptibility is very small and largely independent of T

Stoner's mean-field approach to ferromagnetic metals

Suppose now the magnetic field is the sum of the applied + an internal field (depicting the magnetic interactions among electron spins):

$$\mathbf{H}_{\text{int}} = \mathbf{H} + \mathbf{H}_{\text{exch}} = \mathbf{H} + w\mathbf{M}$$

The Pauli susceptibility in the total field is $\chi_{\text{Pauli}} = \frac{M}{(H + wM)}$ so that:

$$\chi = \frac{M}{H} = \frac{\chi_{\text{Pauli}}}{(1 - w\chi_{\text{Pauli}})}$$

Therefore, the measured susceptibility χ is enhanced with respect to the Pauli susceptibility ($w\chi_{\text{Pauli}} < 1$) and diverges when $w\chi_{\text{Pauli}} \rightarrow 1$.

The exchange energy density is: $E_{\text{exch}} = -\frac{1}{2}\mathbf{H}_{\text{exch}} \cdot \mathbf{M} = -\frac{1}{2}wM^2 = -\frac{I}{4}(N_{\uparrow} - N_{\downarrow})^2$

where the Stoner exchange integral I is a positive parameter ($w = \frac{I}{2\mu_B^2}$).

The condition for onset of a ferromagnetic order is:

$$w \chi_{\text{Pauli}} \rightarrow 1$$

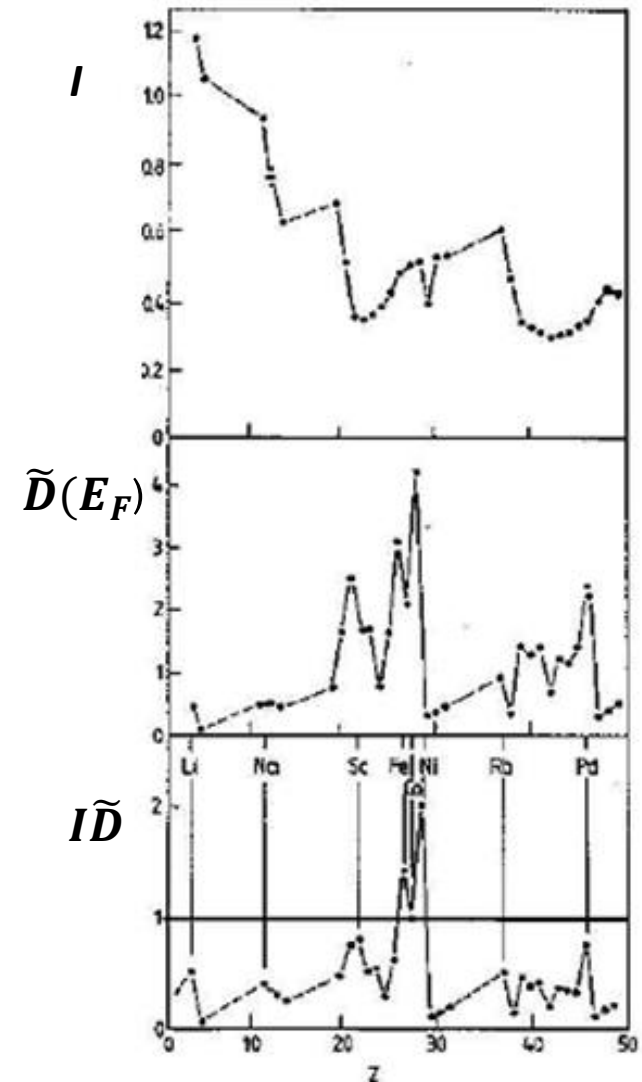
$$\mu_B^2 D(E_F) \frac{I}{2\mu_B^2} = \frac{ID(E_F)}{2} \rightarrow 1$$

Defining the average density of states per each spin subband as $\tilde{D}(E_F) = \frac{D(E_F)}{2}$ one finds the Stoner condition for the onset of itinerant ferromagnetism (= **spontaneous splitting** of subbands, sustained by the internal field only):

$$I\tilde{D}(E_F) \rightarrow 1$$

The exchange parameter has to be **large**, and the density of states at E_F **high**, in order to have spontaneous splitting of subbands.

→ Indeed, ferromagnetic metals have narrow bands and a peak in the density of states at (or near to) E_F



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$$w \chi_{\text{Pauli}} \rightarrow 1$$

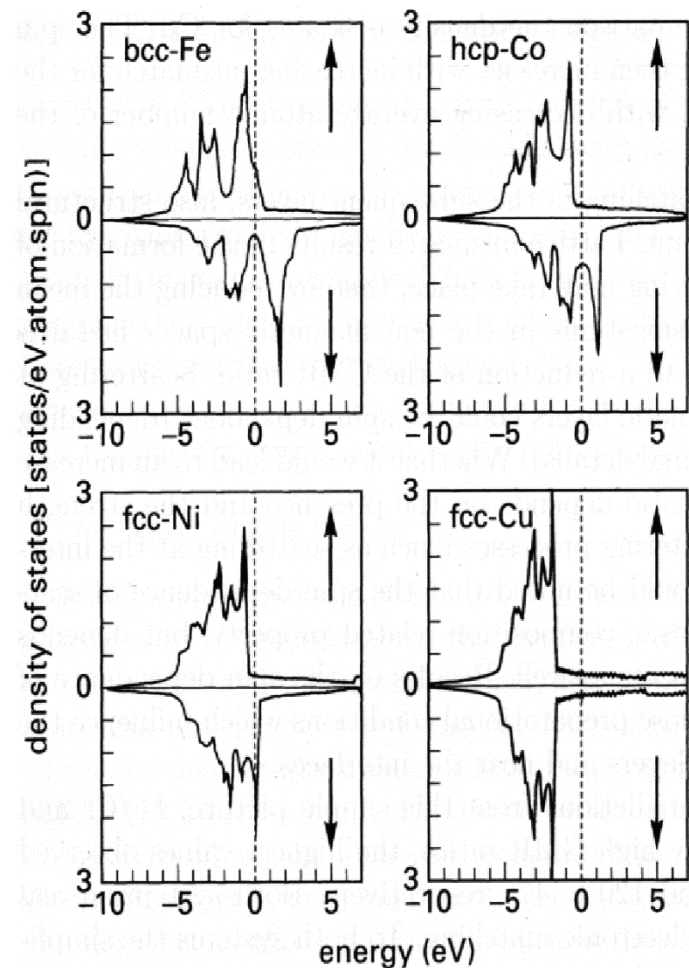
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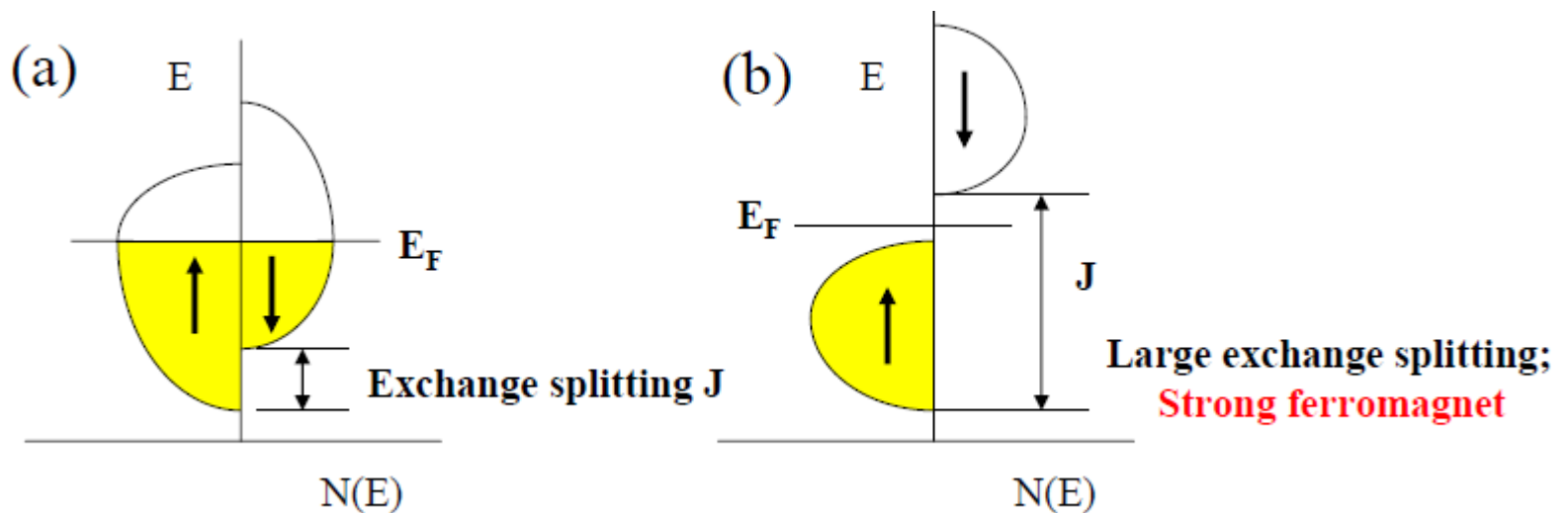
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Rigid-band approximation is just a starting point

Self-sustained 3d-subband shift: itinerant ferromagnetism



In this framework, *non-integer magnetic moments per atom* are expected (as actually measured in most 3d metals).

The larger the exchange energy, the greater the difference in energy between spin up and spin down subbands. Large exchange splitting can lead to complete separation between subbands \rightarrow *integer magnetic moments per atom*.

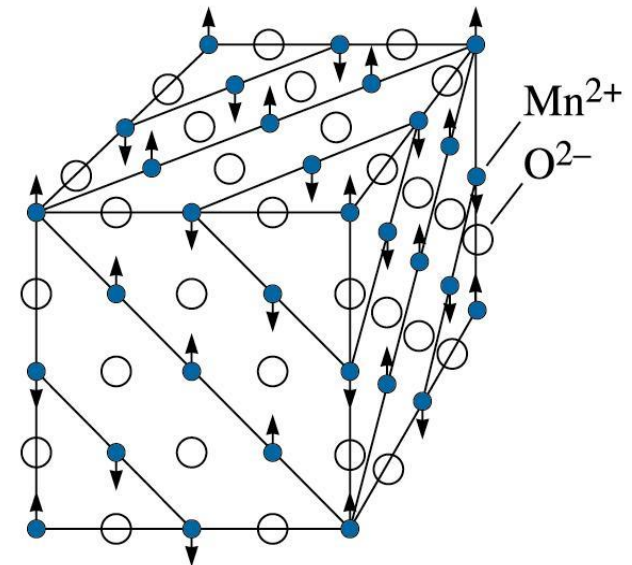
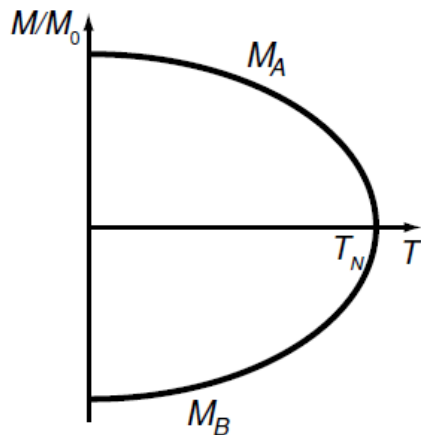
Other types of long-range magnetic order (just phenomenology)

Negative exchange $\mathcal{J} < 0$ leads to magnetic order that depends on lattice topology.

Structures with more than one magnetic sublattice include antiferromagnets and ferrimagnets

Antiferromagnetism: hidden magnetic order.

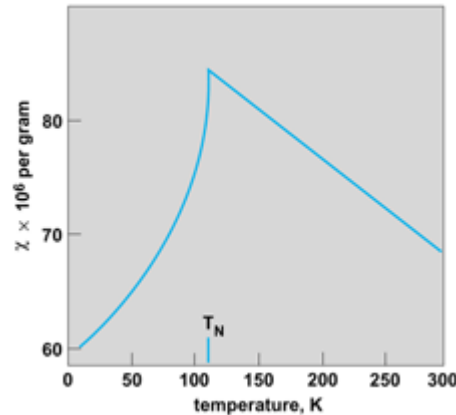
A crystal lattice is subdivided into two or more atomic sublattices which order in such a way that their net magnetization is zero.



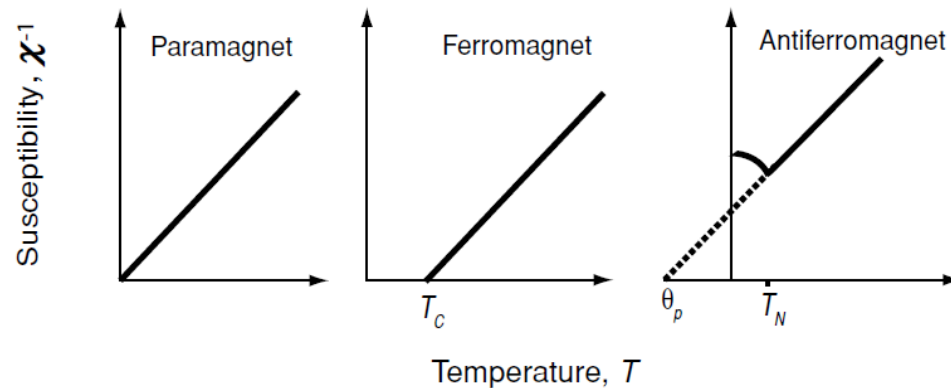
Bulk AF materials have limited applicative interest.

Renewed attention for use of AFs in modern spintronics (as anisotropy generators)

In the case of two equal and antiparallel sublattices, the antiferromagnetic ordering transition - known as *the Néel point* - is generally marked by a peak in the magnetic susceptibility

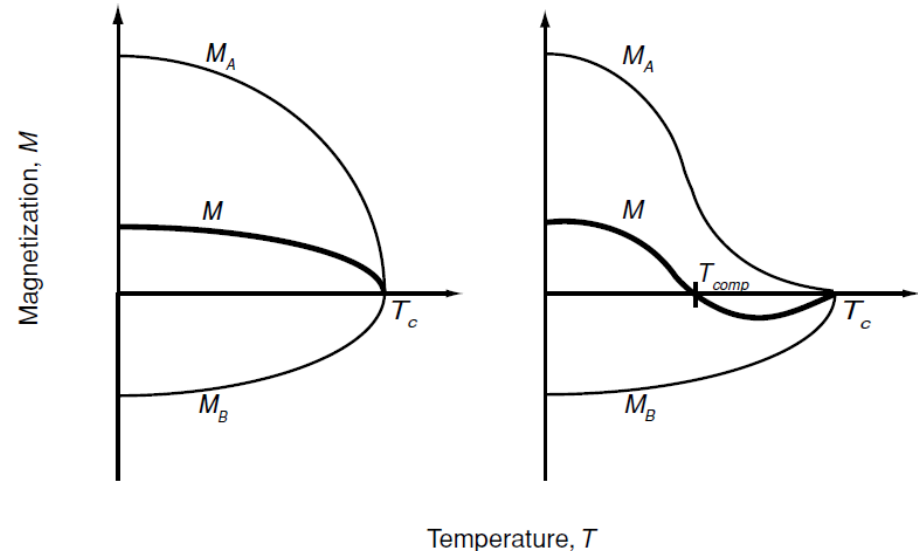
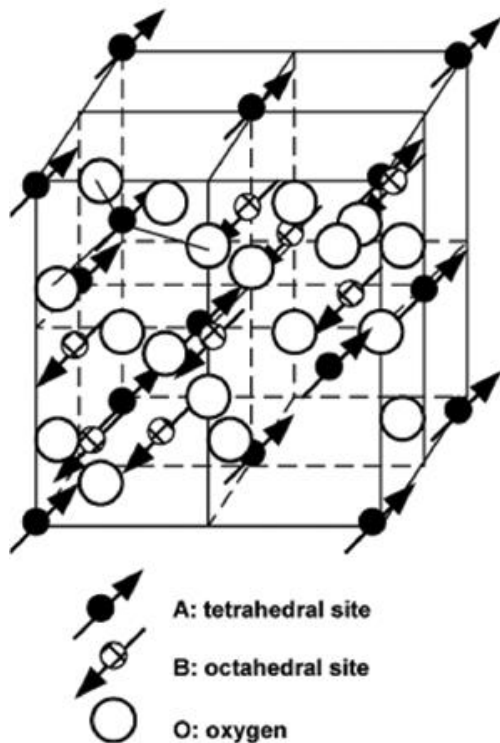


The negative exchange integral results in a Curie-Weiss curve which diverges at negative temperatures:



Ferrimagnetism: a ferrimagnet may be pictured as an antiferromagnet with two magnetically unequal, unbalanced sublattices

The commonest ferrimagnetic material is magnetite, Fe_3O_4 .



Ferrimagnets exhibit a net spontaneous magnetization below the Néel point; however, this sometimes does not vary monotonically with T .

Net magnetization + low cost + high resistivity \rightarrow high applicative interest