Introduction to magnetism
Part I - Moments

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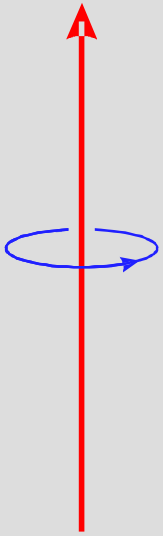
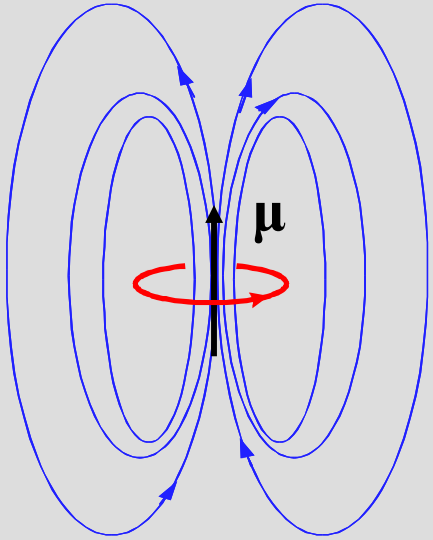
Oersted field



$$B = \frac{\mu_0 I}{2\pi r}$$

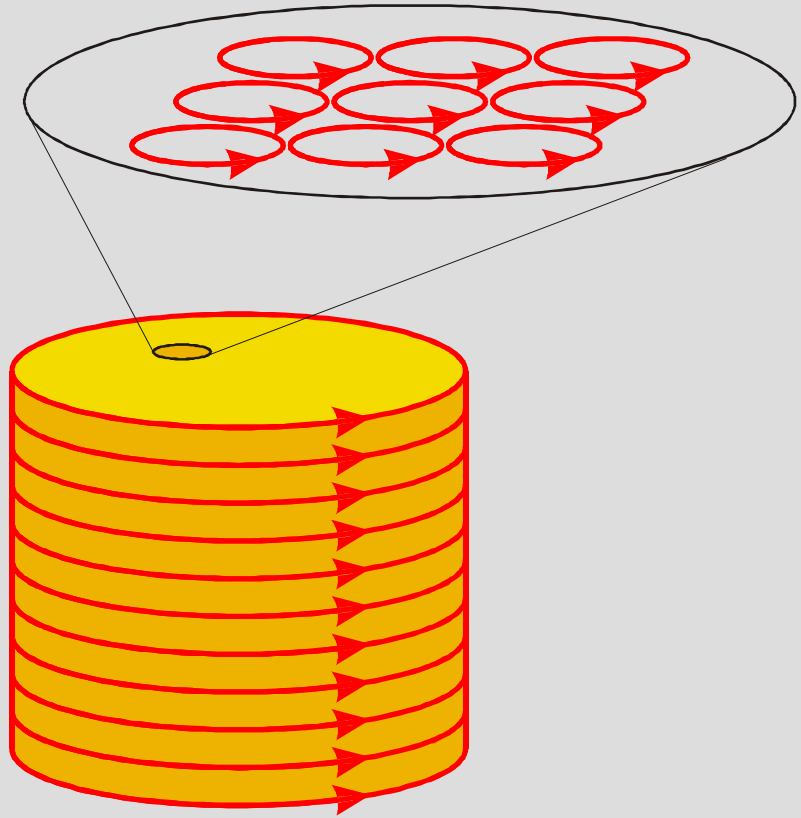
Magnetic dipole



$$B = \frac{\mu_0}{4\pi r^3} \times \left[\frac{3}{r^2}(\boldsymbol{\mu}.\mathbf{r})\mathbf{r} - \boldsymbol{\mu} \right]$$

Magnetic dipole: A.m²

Magnetic material



Magnetization: A.m^{-1}

Magnetic moment: A.m²

Manipulation of magnetic materials:
↳ Application of a magnetic field

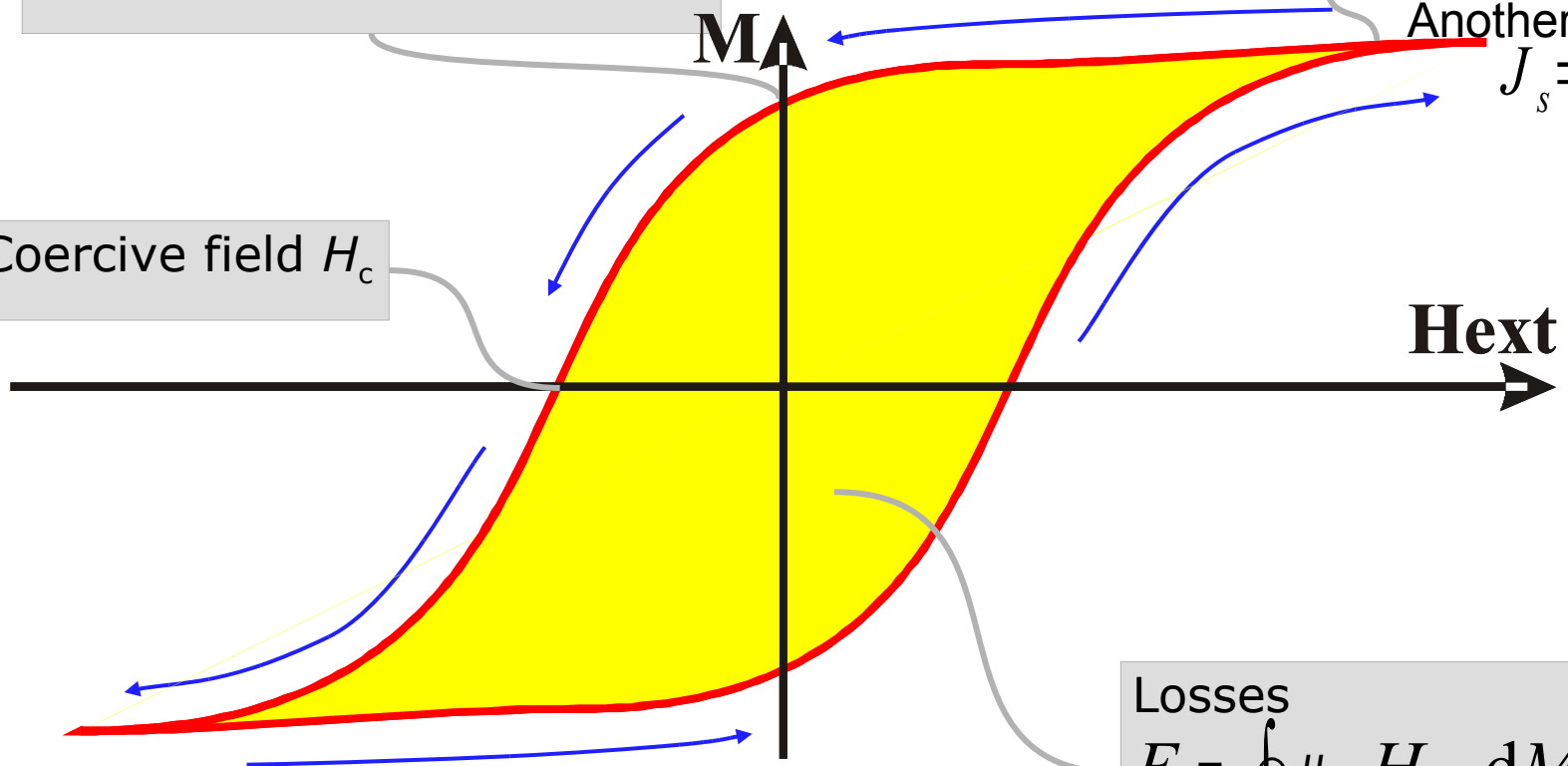
Zeeman energy: $E_Z = -\mu_0 \mathbf{H}.\mathbf{M}_s$

Spontaneous ≠ **S**aturation

Spontaneous magnetization M_s

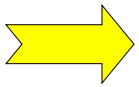
Remanent magnetization M_r

Another notation
$J_s = \mu_0 M_s$

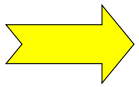


Coercive field H_c

Losses
$E = \oint \mu_0 H_{ext} dM$



1. Magnetic moments



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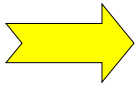
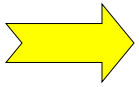
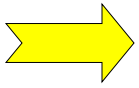


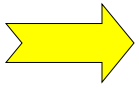
3. Moments in fields



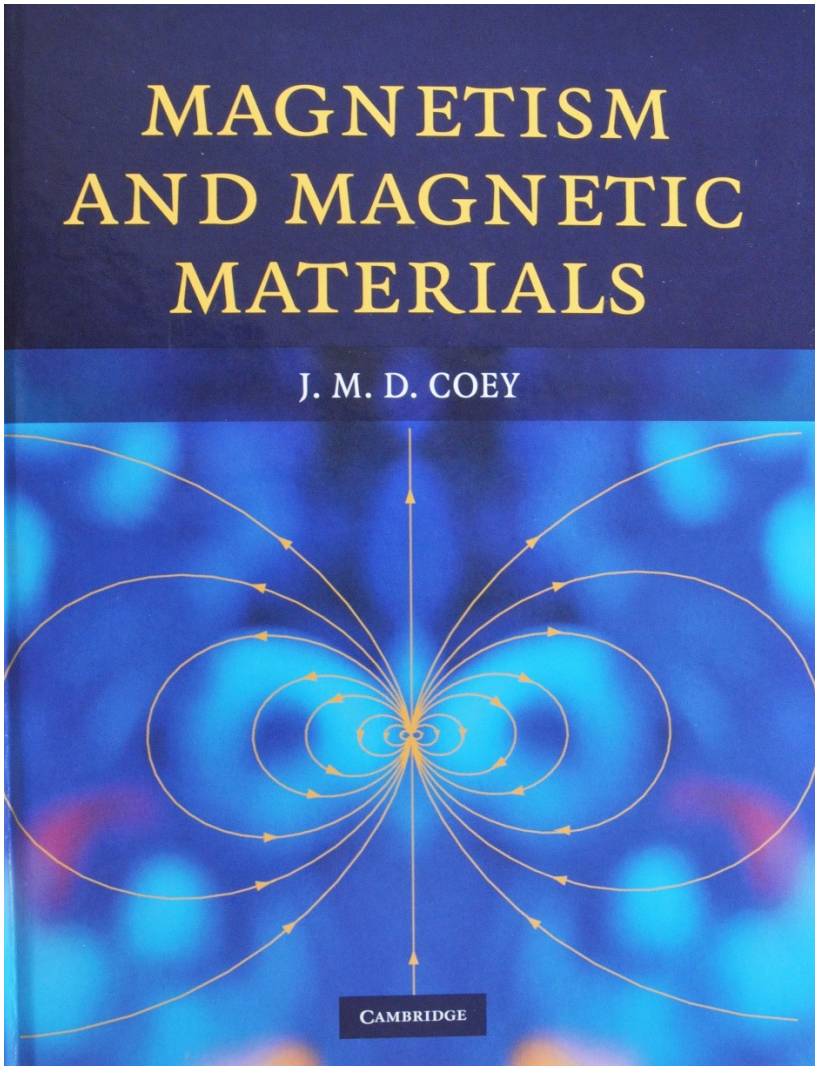
4. Magnetic ordering

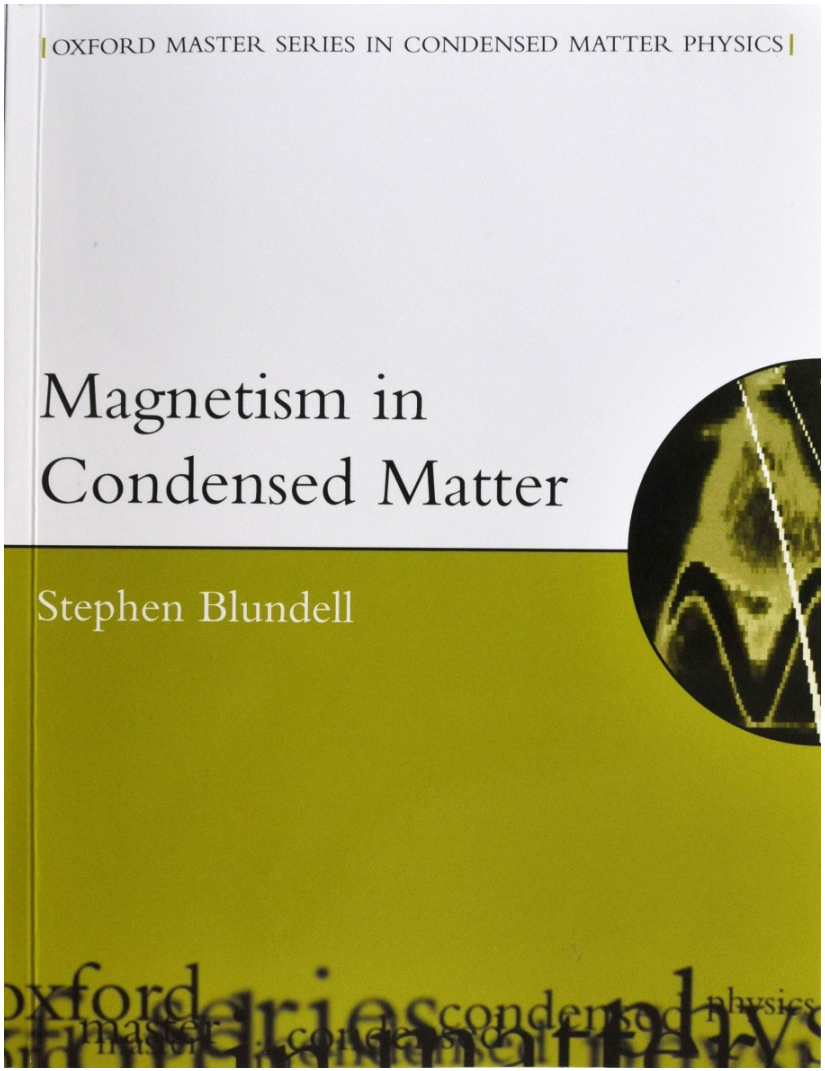


5. Magnetism in metals



6. Magnetic anisotropy





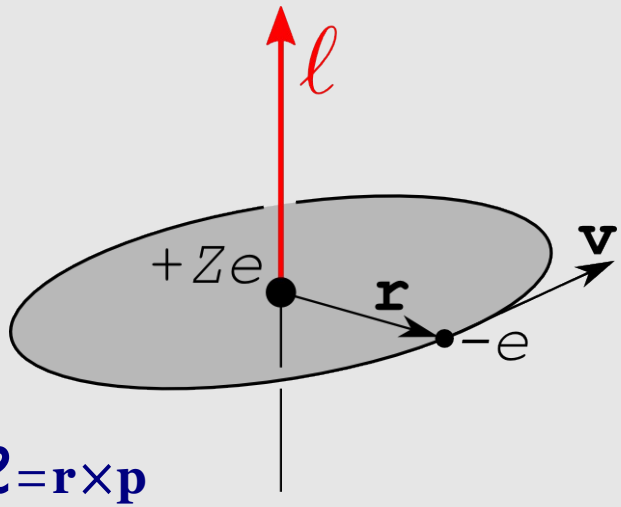
Repository of lectures of the European School on Magnetism: http://esm.neel.cnrs.fr

Classical physics

General definition

$$\boldsymbol{\ell} = \iiint \rho(\mathbf{r}).\mathbf{r}\times\mathbf{v}(\mathbf{r}).\mathrm{d}\mathbf{r}$$

Electron orbiting around a charged nucleus



$\boldsymbol{\ell} = \mathbf{r}\times\mathbf{p}$

➡ $\ell = m_e r v$

$m_e = 9.109\times10^{-31}$ kg

Quantum mechanics

Heisenberg uncertainty principle:

$\Delta r.\Delta p \geq \hbar/2$

$h = 6.626\times10^{-34}$ J.s

$\hbar = h/2\pi = 1.0546\times10^{-34}$ J.s

➡ $\hbar$ is a natural measure for angular momenta. Niels Bohr's postulate, quantization of angular momentum

$|\mathbf{r}\times\mathbf{p}| \in \hbar\mathbb{Z}$

Figures

Newton's law: $Ze^2/4\pi\epsilon_0 r^2 = m_e v^2/r$

Quantized ℓ: $\ell = m_e r v = \ell\hbar$

➡ $r = n^2 a_0/Z$ with Bohr radius $a_0 = \dfrac{4\pi\epsilon_0\hbar^2}{m_e e^2}$

$a_0 = 0.529$ Å

➡ $\alpha = \hbar/m_e a_0 c \approx 1/137.04$ (fine structure cte)

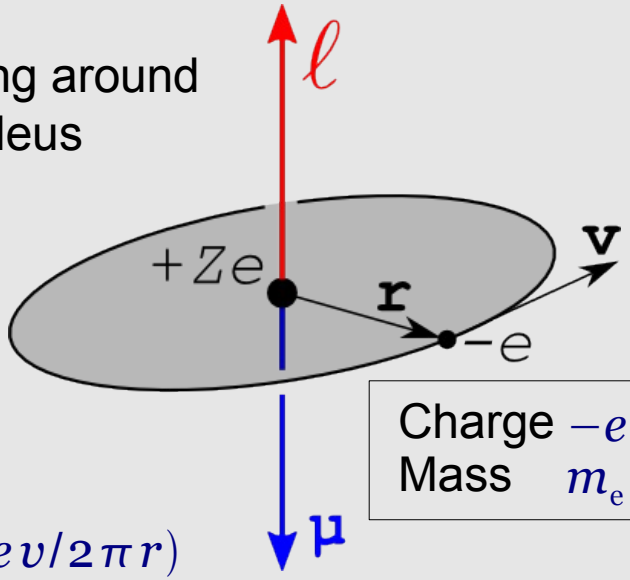
Electrons are largely not relativistic

Classical physics

General definition

$$\mu = \frac{1}{2}\iiint \mathbf{r}\times\mathbf{j}(\mathbf{r})\,\mathrm{d}\mathbf{r}$$

Electron orbiting around a charged nucleus



$$\mu = I\,\mathcal{S}$$

$$\begin{aligned}\mu &= \pi r^2 I \\ &= \pi r^2(-ev/2\pi r) \\ &= -erv/2\end{aligned}$$

Charge $-e$
Mass m_e

$e = 1.6\times10^{-19}$ C

Quantum mechanics

$|\boldsymbol{\ell}| = \ell\hbar$ with $\ell \in \mathbb{Z}$

ℓ is an orbital magnetic quantum number.

$$\Rightarrow \quad \mu_B = \gamma\hbar = -\frac{e}{2m_e}\hbar$$

is Bohr magneton, the quantum for magnetic moments

$$\Rightarrow \quad \mu_z = m_\ell \mu_B = m_\ell\left(\frac{-e}{2m_e}\right)\hbar$$

$m_\ell \in [-\ell\,;\ell]$

$\Rightarrow \quad \mu = \gamma\boldsymbol{\ell}$ with γ : gyromagnetic ratio

$\gamma = -\dfrac{e}{2m_e}$ for orbital motion of electrons

Figures

$\mu_B = 9.274\times10^{-24}$ A.m^2

Spin angular momentum

Spin = intrinsic quantized angular momentum

Electrons are fermions (half-integer spin)

with spin quantum number $s=\pm\frac{1}{2}$

➡ Angular momentum $s\hbar=\pm\frac{\hbar}{2}$

Spin magnetic moment

Electron radius $r_e\approx 2.818\times10^{-15}$ m

$|\boldsymbol{\ell}|=r.p=\hbar/2$ ➡ Relativistic, Dirac equation

➡ $\mu_e=\left(\frac{-eg}{2m_e}\right)m_s$ with $m_s=\pm\frac{1}{2}$

and $g=2.0023\approx 2$ Landé factor

Electrons carry a spin magnetic moment $\approx\mu_B$

Overview

Landé factor g is a dimensionless version of γ: $\frac{|\boldsymbol{\mu}|}{\mu_B}=g\frac{|\boldsymbol{\ell}|}{\hbar}$ or $\gamma=-\frac{eg}{2m_e}$

➡ Orbital moment: $g=1$ $\gamma=-\frac{e}{2m_e}$

➡ Electron spin: $g\approx 2$ $\gamma\approx-\frac{e}{m_e}$

Figures

With $n\approx 8.4\times10^{28}$ atoms/m^3 (for Fe)

➡ $n\mu_B\approx 7.8\times10^5$ A/m

Measured: $M_{s,Fe}\approx 1.73\times10^6$ A/m

➡ $\approx 2.2\,\mu_B$ atom^{-1} (Z=26)

Few electrons involved in ferromagn.

$|\gamma|\approx e/m$

➡ Nucleon spin moment is weak and will be neglected here

Semi-classical picture

The nucleaus is orbiting in the sitting framework of the electron, inducing

Current of the 'orbiting' nucleus'

$$I_n = +Zev/r$$

$$m_e r v \sim n\hbar$$

$$B_{so} = \frac{\mu_0 I_n}{2r}$$

For the spin of one electron:

$$\epsilon_{so} = -\mu_B B_{so} \sim \frac{\mu_0 \mu_B^2 Z^4}{4\pi a_0^3}$$

Figures

Spin-orbit is larger for heavy elements

Reminder:

$\mu_0 = 4\pi \times 10^{-7}$ S.I.

$\mu_B = 9.274 \times 10^{-24}$ A.m^2

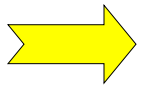
$a_0 = 0.529$ Å

$$\frac{\mu_0 \mu_B^2}{4\pi a_0^3} \sim 4.2 \text{ K}/Z^4$$

$$\sim 0.36 \text{ meV}/Z^4$$

⇨ Screening and details of electrons in atoms are required

⇨ In the range 10-1000meV for magnetic elements



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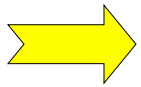

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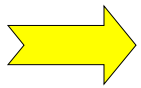
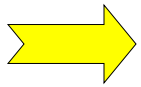


3. Moments in fields



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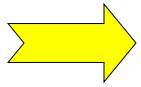

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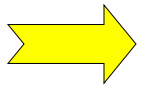


6. Magnetic anisotropy

Framework

Charged nucleus + Z electrons

➡ N-body problem → untractable

➡ Seek one electron solutions + perturbation theory (→ Hund's rules etc.)

Schrödinger equation $\mathcal{H}\,\psi_i = \epsilon_i \psi_i$ with hamitonian $\mathcal{H} = -\frac{\hbar^2}{2m_e}\nabla^2 - \frac{Ze^2}{4\pi\epsilon_0 r}$

Seek solutions: $\psi(r,\theta,\phi) = R(r)\Theta(\theta)\Phi(\phi)$

Electronic orbitals

$R_n^\ell(r)$ and $Y_\ell^{m_\ell}(\theta,\phi) = P_\ell^{m_\ell}(\theta)e^{i m_\ell \phi}$ with:		# of states
n	Principal quantum number → Sets the main energy levels	$\in \mathbb{N}$
ℓ	Secondary quantum number → Orbital moment	$n-1$
m_ℓ	Magnetic quantum number → z component of orbital moment	$2\ell+1$
m_s	Spin quantum number	2

Labeling the levels

Series

⇨ K (n=1), L (n=2), M (n=3), N (n=4) etc.

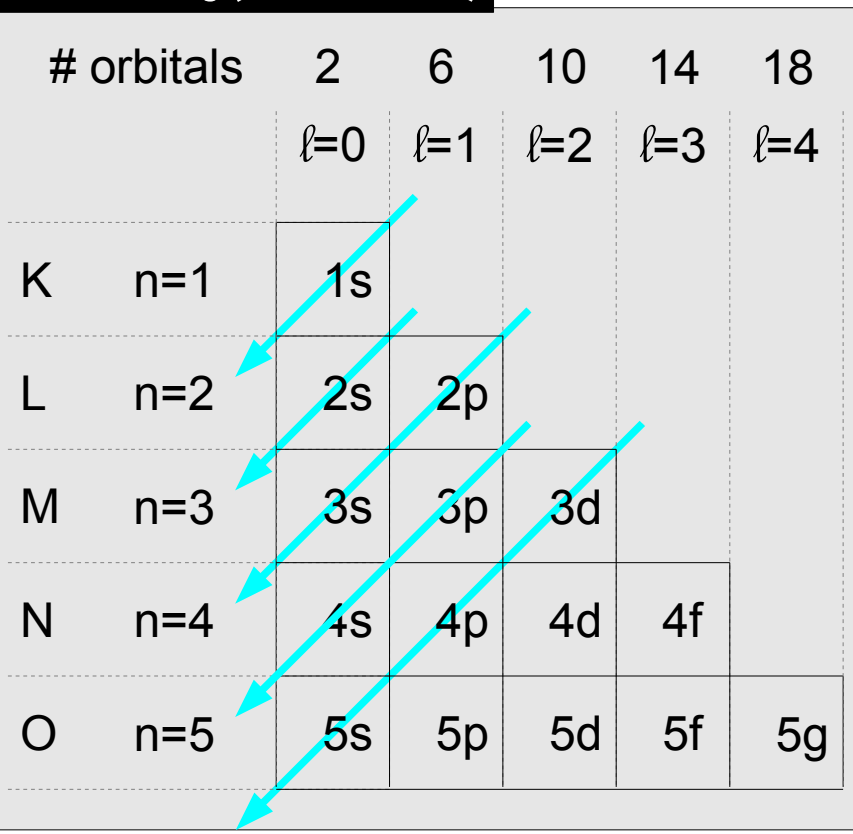
⇨ s (ℓ=0), p (ℓ=1), d (ℓ=2), f (ℓ=3), g (ℓ=4) etc.

Usage

Spectroscopy

Chemical-physical properties

n and ℓ filling (Hartree-Fock)



Examples

Fe, Z=26

➡ $1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^6\ 4s^2\ 3d^6$

2 2 6 2 6 2 6

Ion Fe2+

➡ $3 + 1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^6\ 4s^0\ 3d^6$

Ion Fe3+

➡ $3 + 1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^6\ 4s^0\ 3d^5$

Combination of momenta and moments

Angular and spin momenta from all electrons add up:

$$\mathbf{L}=\sum \boldsymbol{\ell}_i \quad \text{and} \quad \mathbf{S}=\sum \boldsymbol{s}_i \qquad \mathbf{J}=\mathbf{L}+\mathbf{S}$$

$$\mathbf{S}^2=S(S+1)$$
$$\mathbf{L}^2=L(L+1)$$
$$\mathbf{J}^2=J(J+1)$$

Resulting magnetic moment:

$$\boldsymbol{\mu} = (-\mu_B/\hbar)(\mathbf{L}+2\mathbf{S})$$
$$= g(-\mu_B/\hbar)\mathbf{J}$$

Landé factor

$$g=\frac{3}{2}+[S(S+1)-L(L+1)]/2\mathbf{J}(J+1)$$

Only partly filled shells may display angular momentum and magnetic moment.

Hund's rules

Or: empirical rules for populating the last partly filled shell

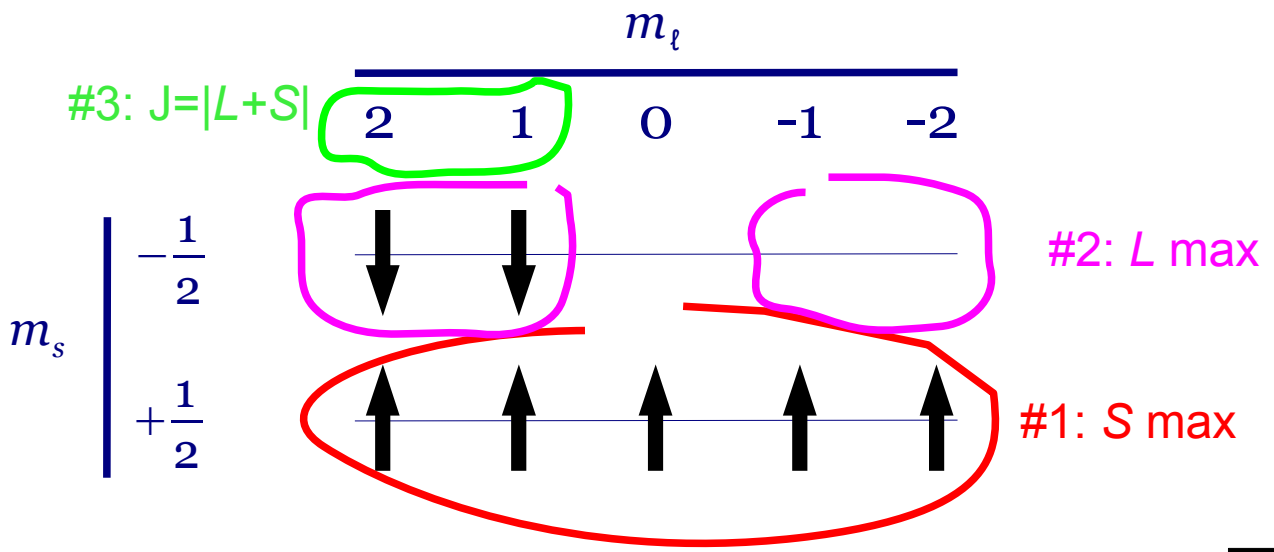
Rule	Arises from...
1. Maximize S	Coulomb interaction and Pauli principle
2. Maximize L consistent with S	Coulomb; electrons orbiting same sense
3. J=|L-S| for less than half-filled shells J=L+S for more than half-filled shells → $M_J \in [-J, J]$	Spin-orbit coupling

Co, Z=27 ⇒ $1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^6\ 4s^2\ 3d^7$ (2 2 6 2 6 2 7)

Filled subshells

7 electrons to fit

$\ell = 2 \rightarrow m_\ell \in [-2,2]$



$S = +\frac{3}{2} \rightarrow 3\mu_B$

$L = +3 \rightarrow 3\mu_B$

$\mu = (2S + L)\mu_B$

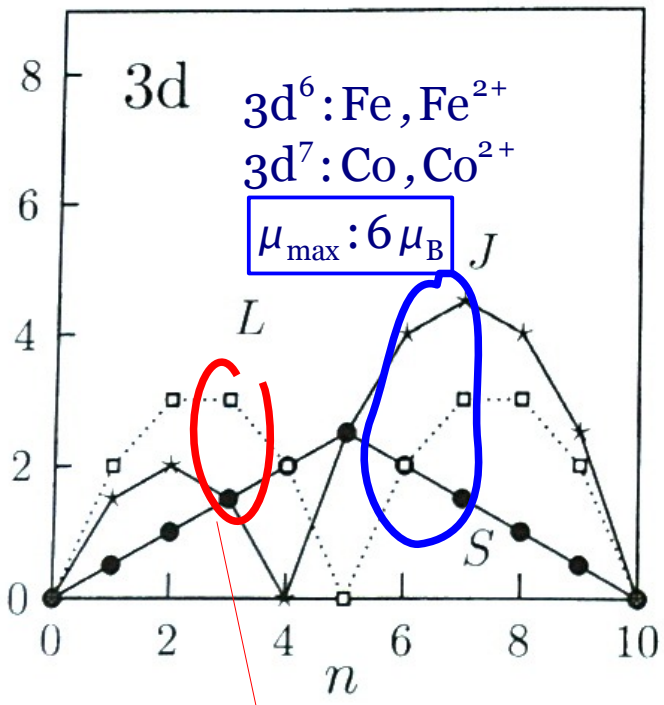
$J = +\frac{9}{2}$ and $g = +\frac{4}{3} \rightarrow \mu = g_J J \mu_B$

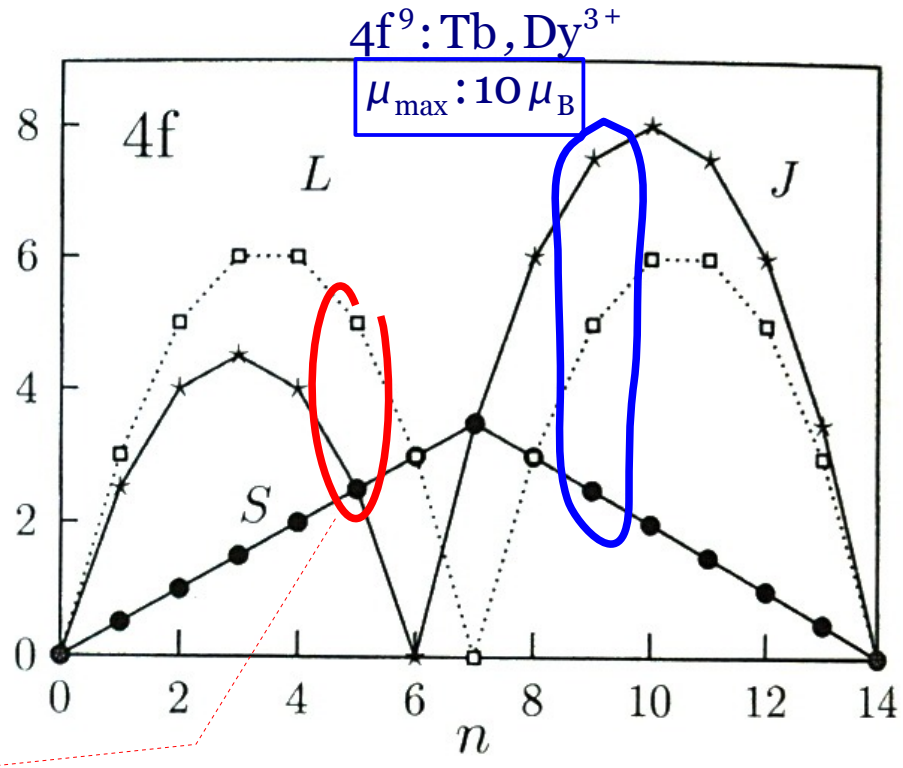
$\mu = 6\mu_B$

Appendix

$$g = \frac{3}{2} + [S(S+1) - L(L+1)]/2J(J+1)$$
$$= \frac{3}{2} + \left(\frac{3}{2}\frac{5}{2} - 3\times 4\right)/\left(2\frac{9}{2}\frac{11}{2}\right)$$
$$= \frac{3}{2} - \frac{33}{4}\frac{2}{99} = \frac{4}{3}$$

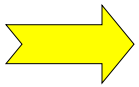
Hund's rules for the 3d and 4f series





$\mu = 0\ \mu_B$

From: Blundell's



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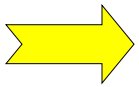

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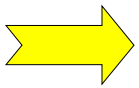

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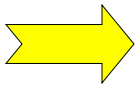

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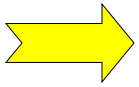

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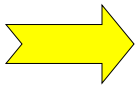


6. Magnetic anisotropy

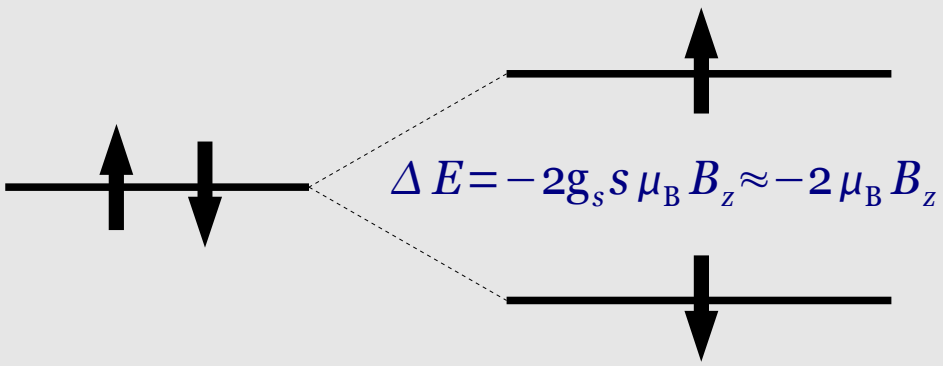
Energetics

For both classical physics and quantum mechanics:

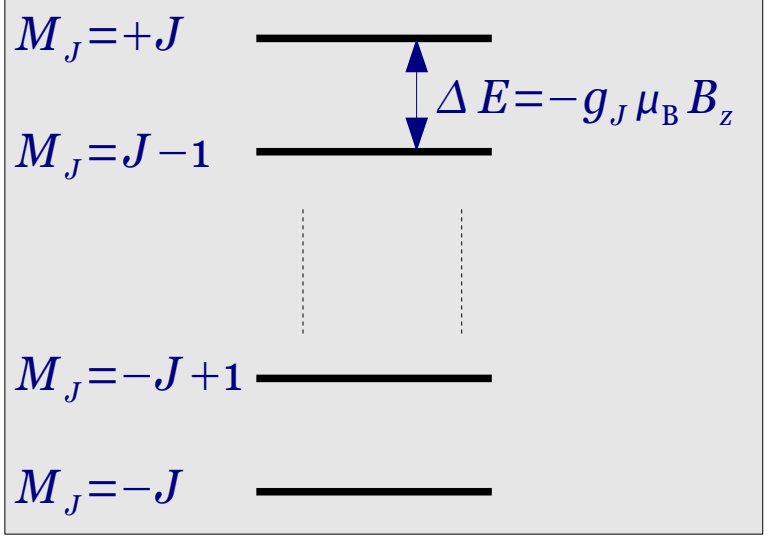
$$E = -\boldsymbol{\mu}.\mathbf{B} = -\mu_0 \boldsymbol{\mu}.\mathbf{H}$$

$\boldsymbol{\mu}$ Magnetic moment
$\mathbf{H}$ Magnetic field
$\mathbf{B}$ Magnetic induction

Spin moment 1/2



Quantum momentum J



Consequences

- Polarizability
- Oscillations
- Spectroscopy
- Resonances etc.

Classical physics

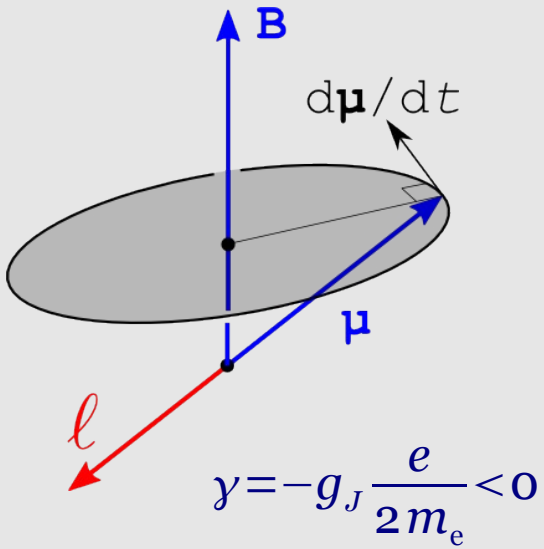
$$E = -\boldsymbol{\mu}.\mathbf{B} = -\mu B \cos\theta$$

Larmor precession

Field H creates a torque on ℓ

$$\Rightarrow \frac{d\boldsymbol{\ell}}{dt} = \boldsymbol{\Gamma} = \mu_0 \boldsymbol{\mu} \times \mathbf{H} = \mu_0 \gamma \boldsymbol{\ell} \times \mathbf{H}$$

$$\Rightarrow \frac{d\boldsymbol{\mu}}{dt} = \mu_0 \gamma \boldsymbol{\mu} \times \mathbf{H}$$



Figures

$\gamma/2\pi$ has meaning Hz/T

For spin angular momentum $\gamma_s \approx -\frac{e}{m_e}$

$\Rightarrow \gamma_s/2\pi \approx 28$ GHz/T

$\gamma_{orb}/2\pi \approx 14$ GHz/T

Application

Landau-Lifshitz-Gilbert equation
for precessional dynamics of magnetization

$$\dot{m} = \mu_0 \gamma \mathbf{m} \times \mathbf{H} + \alpha \mathbf{m} \times \dot{\mathbf{m}}$$

- Ferromagnetic resonance (FMR): yields γ and μ
- Spin waves, precessional switching, spin torque etc.

Semi-classical view

Maxwell equation $\nabla \times \mathbf{E} = -\frac{\partial \mathbf{B}}{\partial t}$

➡ Lenz law with $E_\theta(r) = -\frac{r}{2}\frac{\partial B_z}{\partial t}$

Work provided to the electron, which changes its energy, thus its orbit and angular momentum, even for full shells

Quantum mechanics

Introduce vector potential **A** in Hamiltonian

$\mathbf{p} \rightarrow \mathbf{p} + e\mathbf{A}$

➡ $\chi = \mu_0 M_s / B$ Dimensionless susceptibility

$= -n\mu_0 e^2 \langle r^2 \rangle / 6m_e$

n Volumic density of electrons

Figures

$r = n^2 a_0 / Z$ $\quad a_0 = \frac{4\pi\epsilon_0\hbar^2}{m_e e^2}$

$n \approx 6 \times 10^{28}$ atoms/m^3

➡ $\chi \approx -10^{-5}$

Diamagnetism is weak and essentially temperature-independent

➡ χ may be enhanced in the following cases:

⇨ Large n, large a, low *Z*
(ex: aromatic materials)

⇨ Low effective mass
(see later on: metals)

(Weak electron binding)

Calculation

Framework: localized moments $\mu_J = g_J J \mu_B$

Partition function: $Z = \sum_{M_J=-J}^{+J} \exp(-\beta E)$ with: $E = -\mu_0 \mu_z H$

$$\Rightarrow \langle \mu_z \rangle = \frac{1}{\beta \mu_0 Z} \frac{\partial Z}{\partial H}$$

Results

$$\langle \mu_z \rangle = \mu_J \mathcal{B}_J(x) \quad \text{with:} \quad x = \beta \mu_0 g_J J \mu_B H$$

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

⇒ Case spin 1/2

$\mathcal{B}_{1/2}(x) = \tanh(x)$ $\qquad$ $\mathcal{B}_{1/2}(x) \sim x$

⇒ Case spin → ∞ (Langevin)

$\mathcal{B}_{\infty}(x) = \mathcal{L}(x)$ $\qquad$ $\mathcal{L}(x) \sim x/3$

Expansions

Curie law (low-field expansion):

$$\chi = n \langle \mu_J \rangle / H = C/T$$

Figures

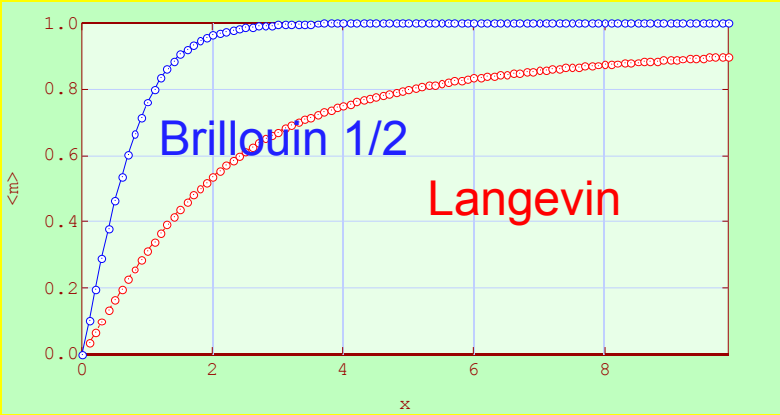
$$C = \frac{\mu_0 n m_{\text{eff}}^2}{3 k_B}$$

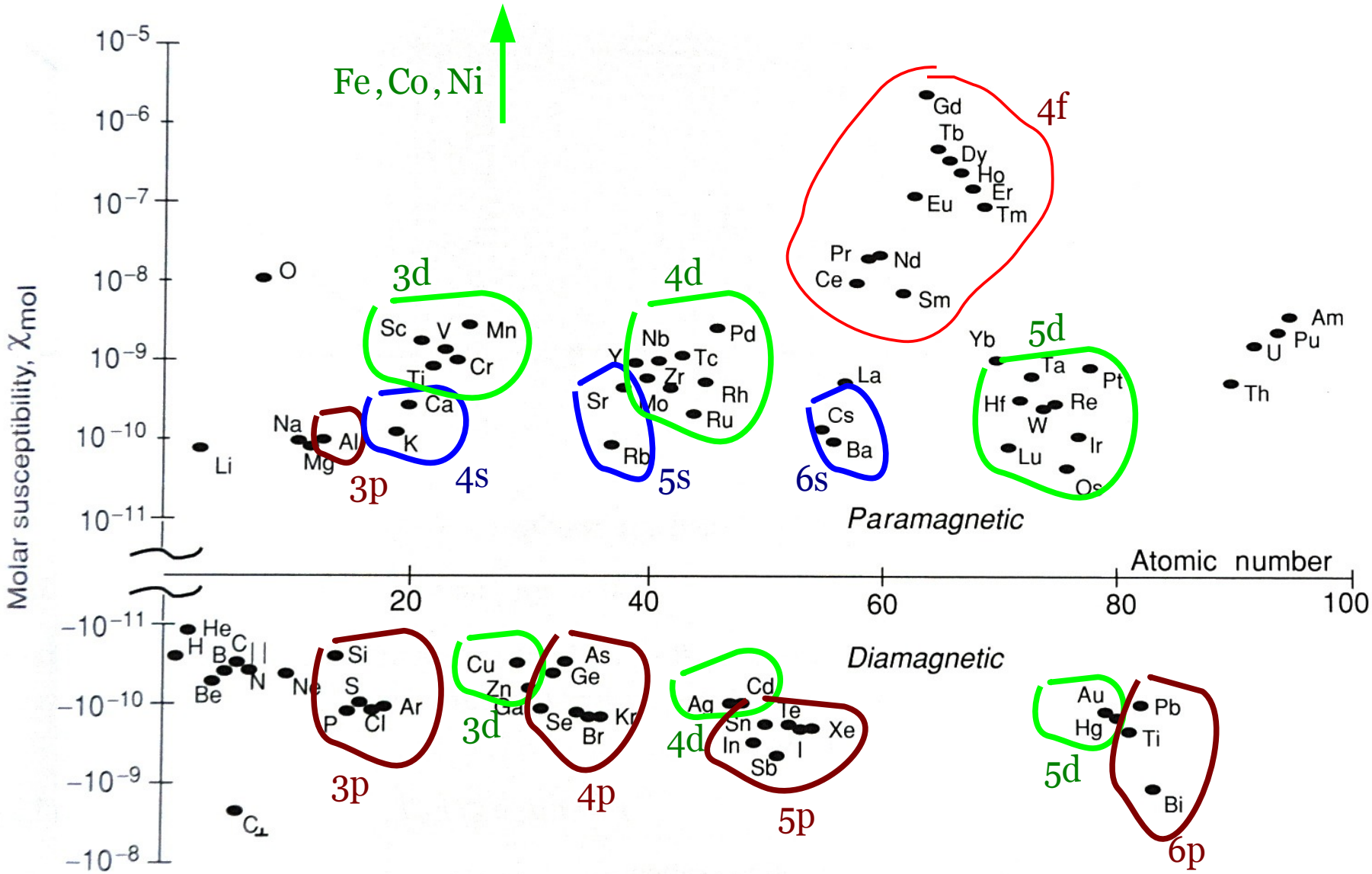
with: $m_{\text{eff}} = g_J \mu_B \sqrt{J(J+1)}$

$$x \approx \frac{\mu_B B}{k_B T} = \frac{9.274 \times 10^{-24}}{1.38 \times 10^{-23}} \frac{B}{T}$$

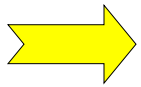
Rule of thumb:

μ_B gets polarized at 1K under 1T

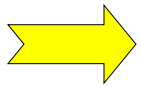



Fe, Co, Ni
Molar susceptibility, χ_{mol}
10^{-5}
10^{-6}
10^{-7}
10^{-8}
10^{-9}
10^{-10}
10^{-11}
-10^{-11}
-10^{-10}
-10^{-9}
-10^{-8}
Atomic number
20
40
60
80
100
Paramagnetic
Diamagnetic
4f
Gd
Tb
Dy
Ho
Er
Tm
Eu
Pr
Nd
Ce
Sm
3d
Sc
V
Mn
Cr
Ti
Ca
K
4s
3p
Na
Al
Mg
Li
O
4d
Nb
Pd
Y
Tc
Zr
Rh
Mo
Ru
Sr
Rb
5s
6s
La
Cs
Ba
5d
Yb
Ta
Pt
Hf
Re
W
Ir
Lu
Os
Am
Pu
U
Th
He
H
B
C
N
Be
Ne
Si
S
Ar
P
Cl
3p
Cu
Zn
Ga
As
Ge
Se
Br
Kr
3d
4p
Ag
Cd
Sn
In
Te
I
Xe
Sb
4d
5p
Au
Hg
Pb
Ti
Bi
5d
6p

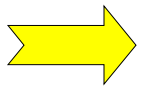
From: Coey



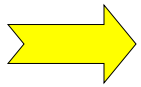
1. Magnetic moments



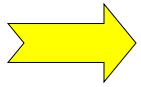
2. Magnetism of single atoms



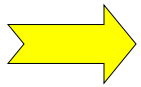
3. Moments in fields



4. Magnetic ordering



5. Magnetism in metals



6. Magnetic anisotropy

Reminder: Curie law for paramagnetism

$\langle \mu_z \rangle = \mu_J \mathcal{B}_J(x)$ with: $x = \beta \mu_0 \mu_J H$

⇨ No magnetization at zero field

⇨ $1\mu_B$ gets polarized at 1K under 1T

⇨ Postulate of molecular field to explain magnetic ordering

Mean-field equations

Internal field: $\mathbf{H_i} = n_W \mathbf{M_s} + \mathbf{H}$

$n_W \mathbf{M_s}$ → Molecular field

⇨ $M_s = M_0 \mathcal{B}_J(x_0)$ with: $M_0 = n\mu_J$, $x_0 = x(H=0)$

Can be rewritten:

$$\frac{M_s}{M_0} = \mathcal{B}_J(x_0) = \left(\frac{1}{3} \frac{T}{n_W C} \frac{J+1}{J} \right) x_0$$

Reminder: notations

$\mu_J = g_J \mu_B J$

$x_0 = \beta \mu_0 \mu_J n_W M_s$

$\chi = n\langle \mu_J \rangle / H = C/T$

$C = \frac{\mu_0 n m_{eff}^2}{3 k_B}$

$m_{eff} = g_J \mu_B \sqrt{J(J+1)}$

Reminder: self-consistent equation

$$\mathcal{B}_J(x_0) = \left(\frac{1}{3}\frac{T}{n_W C}\frac{J+1}{J}\right)x_0$$

Initial slope: $\frac{J+1}{3J}$

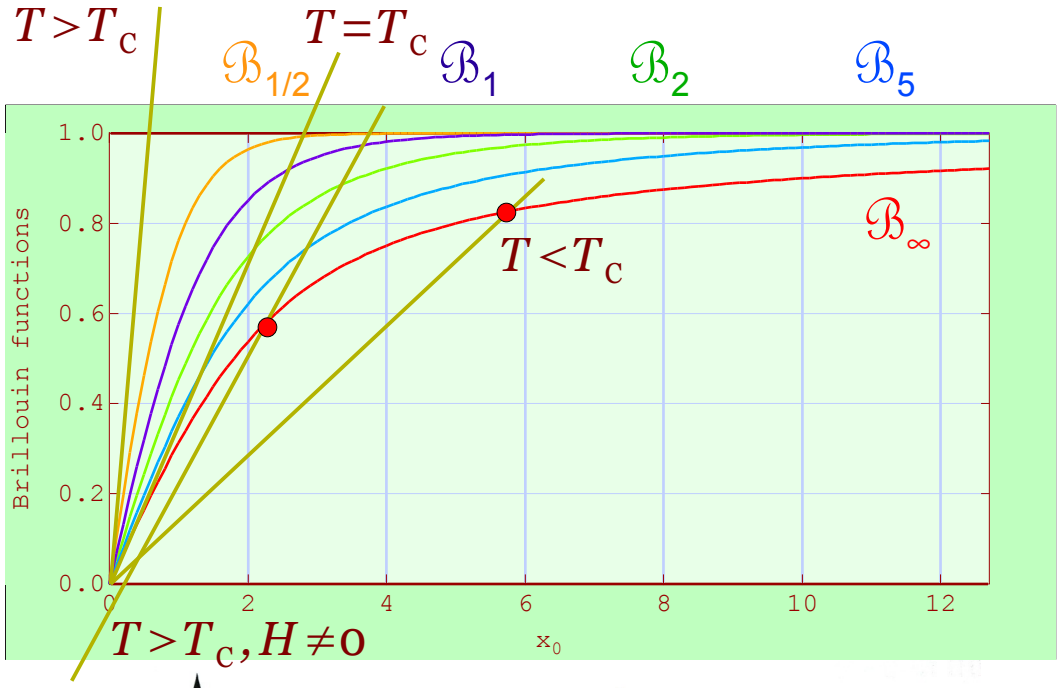
Some results

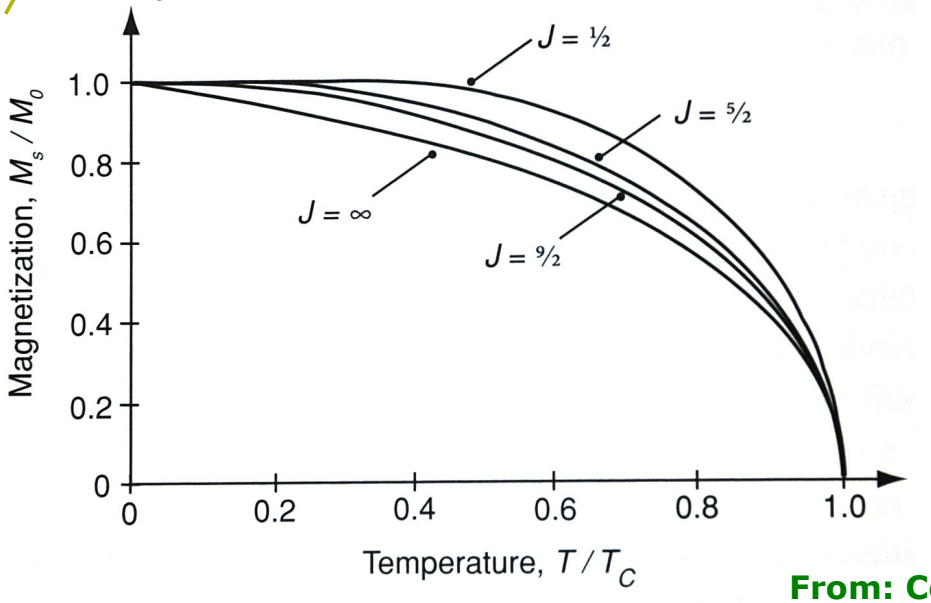
$$T_C = n_W C = \frac{\mu_0 n_W n g_J^2 \mu_B^2 J(J+1)}{3k_B}$$

For $T > T_C$: $\chi = \frac{C}{T - T_C}$

Notice

- Mean-field theory yields trends and orders of magnitude only
- Notice for low dimension: $T_C \sim n_W$





From: Coey

From Weiss field to Heisenberg Hamiltonian

Weiss molecular field $\mathbf{H_i} = n_W \mathbf{M_s} + \mathbf{H}$

Generalization $E_{i,j} = -2\sum_{i>j} J_{i,j}\mathbf{S_i}.\mathbf{S_j} = -2\left(\sum_j J_{i,j}\mathbf{S_j}\right).\mathbf{S_i}$ $\Big\}\ 2ZJ_{i,j} = \mu_0 n_W n g_S^2 \mu_B^2$

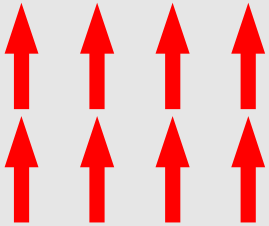
$\mathbf{S_i}$ → dimensionless spin

Z : number of nearest neighbors

Shift notation: *J* for exchange, *S* for atomic spin

Ferromagnet

$J_{i,j} > 0$



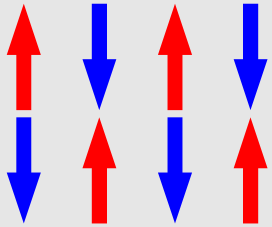
➡ Fe

$M_s = 1.73 \times 10^6$ A/m

$T_C = 1043$ K

Antiferromagnet

$J_{i,j} < 0$



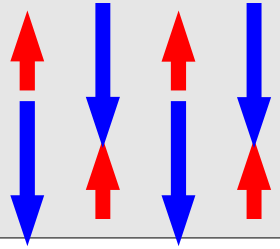
➡ CoO

$J = 3/2$

$T_N = 292$ K

Ferrimagnet

$J_{i,j} < 0$



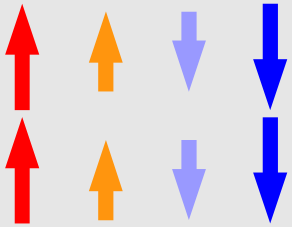
➡ Fe3O4

$M_s = 480$ kA/m

$T_C = 858$ K

Helical

$J_1, J_2 \ldots$



➡ Dy

$\mu = 10.4\,\mu_B$

$T \in 85 - 179$ K

Direct exchange

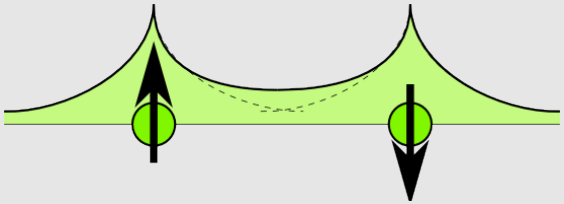
Interatomic principle of first Hund's rules

Fermions: antisymmetric wave function: $\psi(2,1) = -\psi(1,2)$

Space: $\phi_s = (1/\sqrt{2})(\psi_1 + \psi_2)$

Spin S=0

$$\phi_s = (1/\sqrt{2})\left[\left|\uparrow_1,\downarrow_2\right\rangle - \left|\uparrow_2,\downarrow_1\right\rangle\right]$$



Spin singlet state

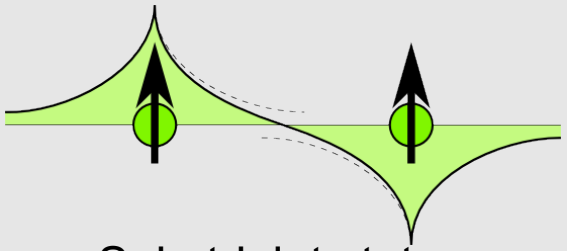
Space: $\phi_s = (1/\sqrt{2})(\psi_1 - \psi_2)$

Spin S=1

$$\phi_s = (1/\sqrt{2})\left|\uparrow_1,\uparrow_2\right\rangle$$

$$\phi_s = (1/\sqrt{2})\left[\left|\uparrow_1,\downarrow_2\right\rangle + \left|\uparrow_2,\downarrow_1\right\rangle\right]$$

$$\phi_s = (1/\sqrt{2})\left|\downarrow_1,\downarrow_2\right\rangle$$

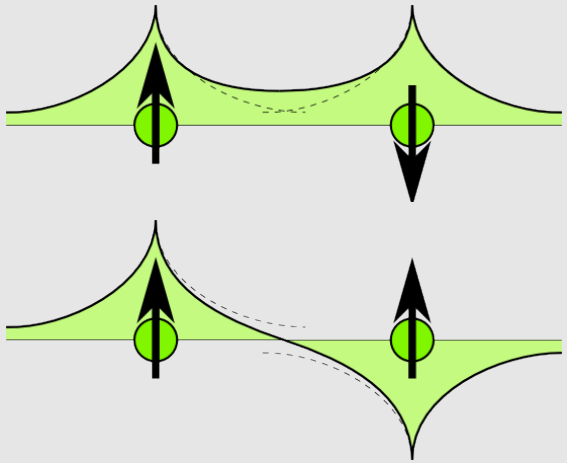


Spin triplet state

Hamiltonian: $\mathcal{H} = -2J_{1,2}\mathbf{S_1}.\mathbf{S_2}$

Exchange integral

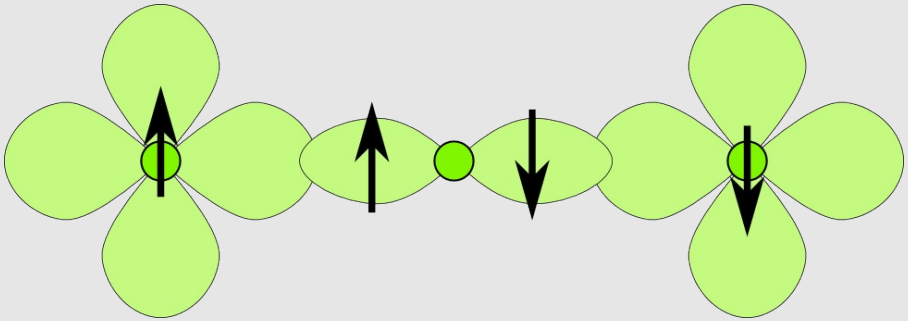
Direct exchange



Molecules → singlet

Metals → Ferro/Antiferro

Superexchange

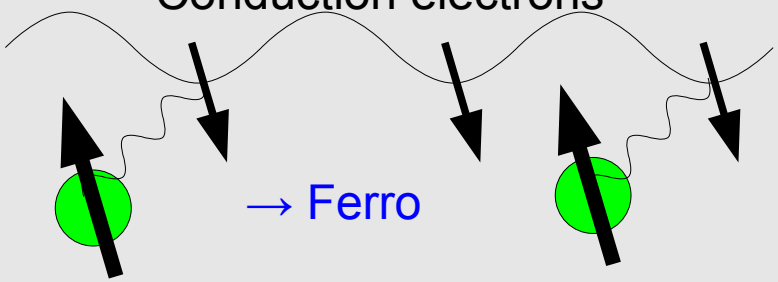


Bond length and orientation dependent

Often: π → Antiferro; π/2 → Ferro

Indirect exchange

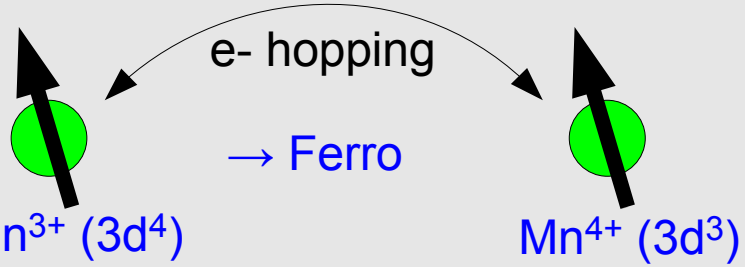
Conduction electrons



RKKY, Rare earth(4f), GaMnAs(3d)

Double exchange

Mixed-valence states



Ex: (La0.7Ca0.3)Mn03

- Often enhanced magnetic moments in metals because of band narrowing

- Decreased ordering temperature

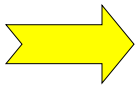
$$T_C = \frac{2 Z J_{i,j} S(S+1)}{3 k_B}$$

Lower number of neighbors → Tc reduced

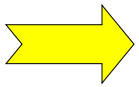
Thermal excitations in low dimension

→ Spin waves, Mermin-Wagner theorem (theoretically no order at finite temperature in 2D, no order in 1D)

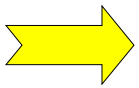
- Qualitative change of magnetic order (strain, structure, mixing – dead layers)
  - ⇨ fcc or fct Fe: mixed ferro/spiral antiferro
  - ⇨ 1ML Fe/W(001): Antiferromagnetic
  - ⇨ Small clusters may be ferromagnetic. Ex: Rh



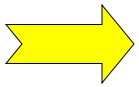
1. Magnetic moments



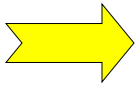
2. Magnetism of single atoms



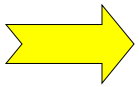
3. Moments in fields



4. Magnetic ordering

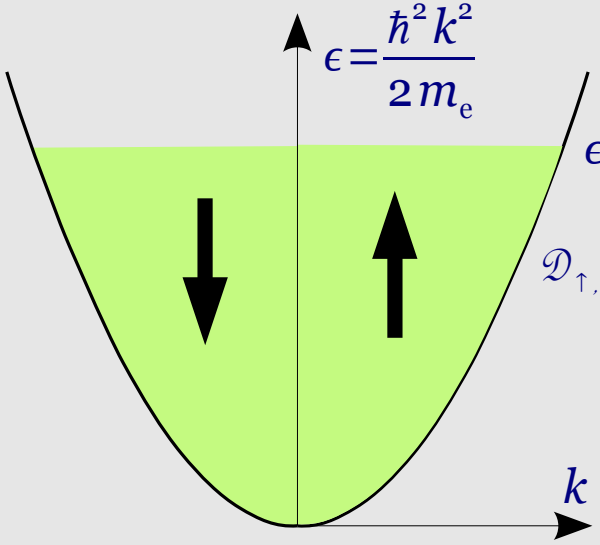


5. Magnetism in metals



6. Magnetic anisotropy

Free electron model



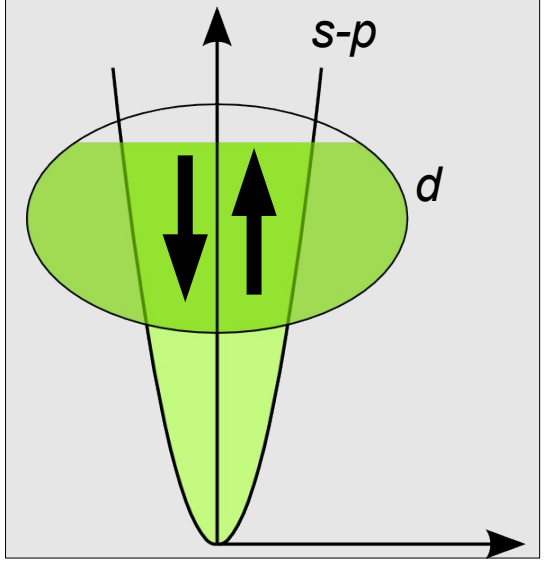
Density of states at the Fermi level

$$\mathcal{D}_{\uparrow,\downarrow}(\epsilon_F) = (1/4\pi^2)\left(2m_e/\hbar^2\right)^{3/2} \epsilon_F^{1/2} = \frac{3n}{4\epsilon_F}$$

$$k_B T_F = \epsilon_F$$

$$\mathcal{D}_{\uparrow,\downarrow}(\epsilon_F) = \frac{1}{2}\mathcal{D}(\epsilon_F)$$

Two-band model



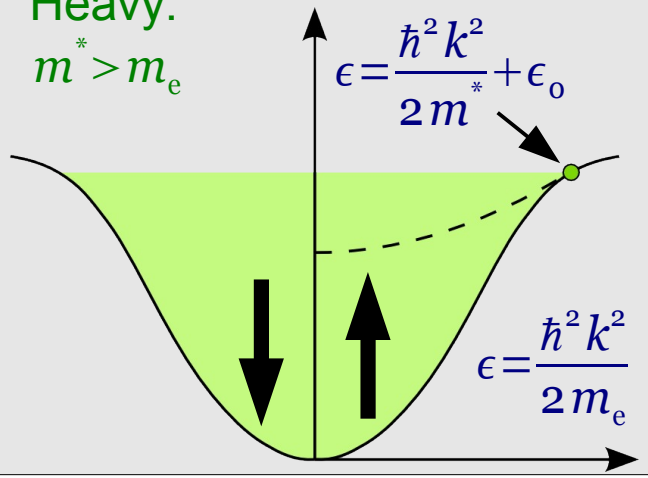
Effective mass etc.

Definitions

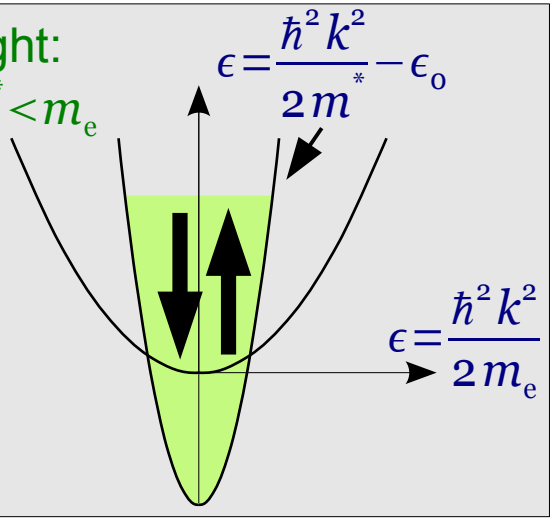
$$\frac{d\epsilon}{dk} = \frac{\hbar k}{m^*} = \hbar v_F$$

$$\Rightarrow m^* = \frac{\hbar k}{d\epsilon/dk}$$

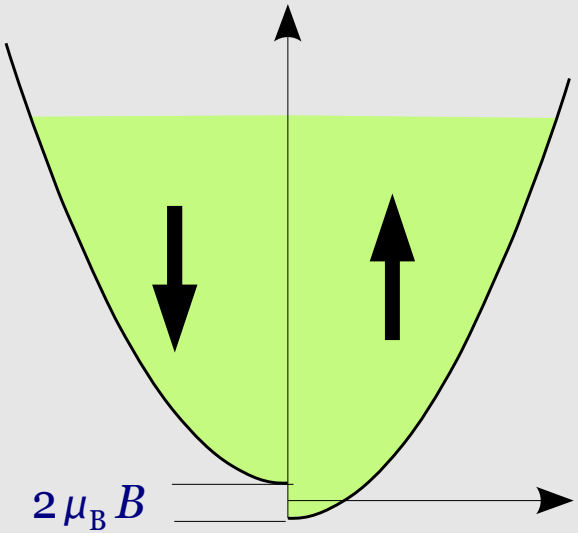
Heavy: $m^* > m_e$



Light: $m^* < m_e$



Pauli paramagnetism



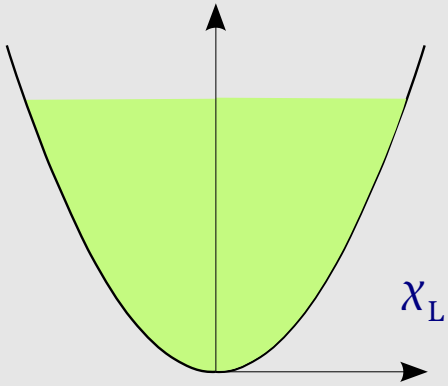
$$\chi_P = \frac{\mu_0 M_S}{B} = \mu_0 \mu_B^2 \mathcal{D}(\epsilon_F) = \frac{3\mu_0 n \mu_B^2}{2k_B T_F}$$

Reminder Curie law:

$$\chi_C = \frac{\mu_0 n m_{eff}^2}{3 k_B T}$$

- Temperature independent
- Proportional to $\mathcal{D}(\epsilon_F)$
- Weak as $T_F \gg 300$ K

Landau diamagnetism

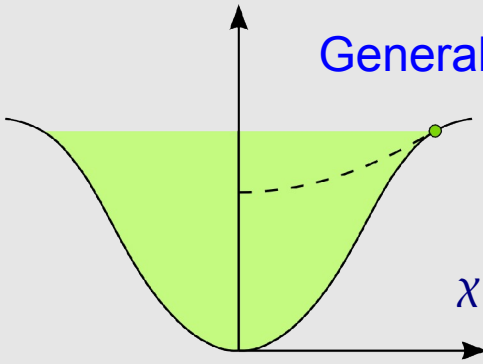


Free electrons

$$\chi_L = \frac{-\mu_0 n \mu_B^2}{2k_B T_F} = -\frac{1}{3}\chi_P$$

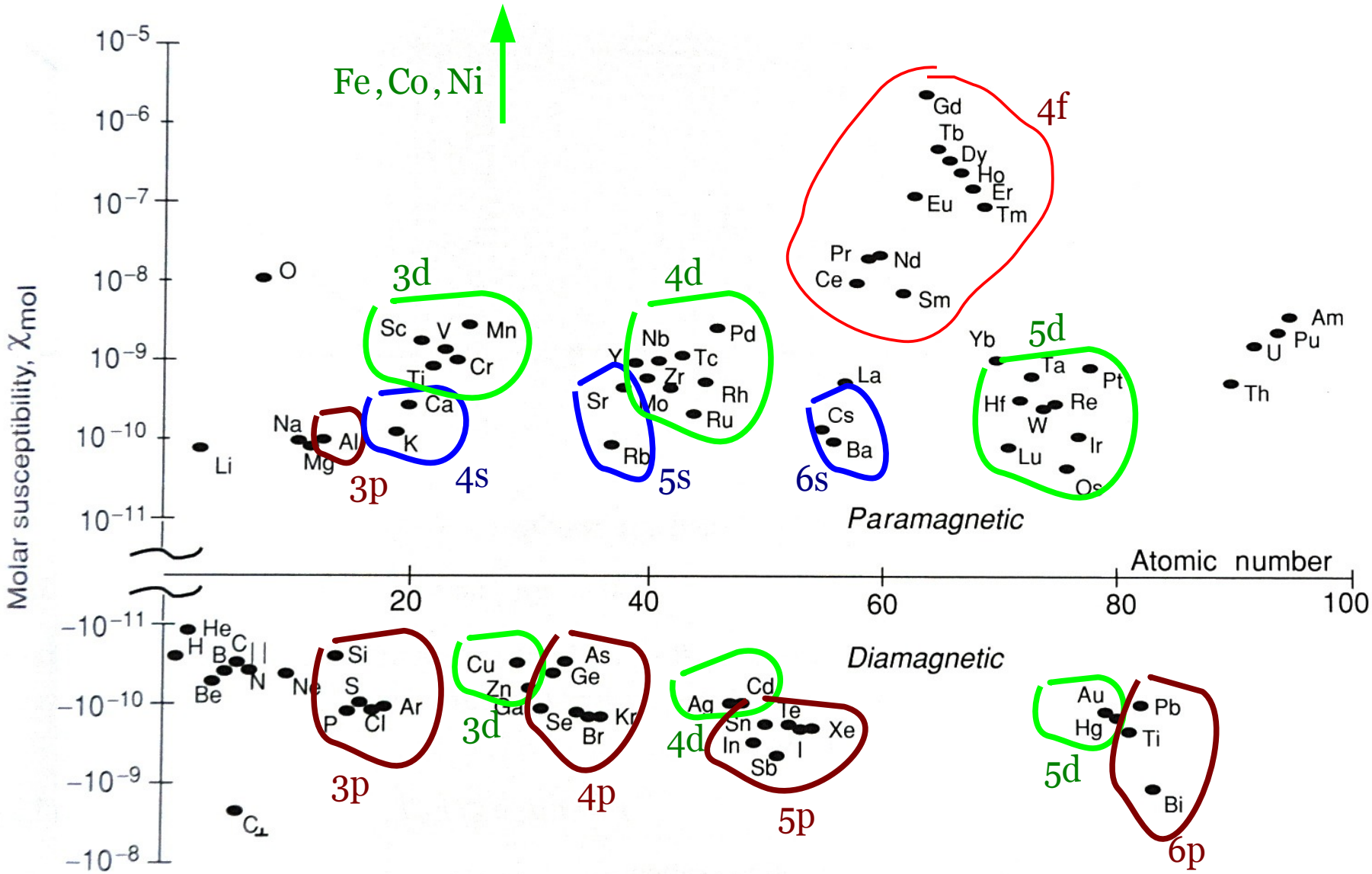
$\chi_L + \chi_P > 0$ ⇒ Paramagnetism expected

Generalization to bands



$$\chi_L = -\frac{1}{3}\left(\frac{m_e}{m^*}\right)^2 \chi_P$$

⇒ Diamagnetism may dominate even in metals


Fe, Co, Ni
Molar susceptibility, χ_{mol}
10^{-5}
10^{-6}
10^{-7}
10^{-8}
10^{-9}
10^{-10}
10^{-11}
-10^{-11}
-10^{-10}
-10^{-9}
-10^{-8}
Atomic number
20
40
60
80
100
Paramagnetic
Diamagnetic
3d
4s
3p
4d
5s
4f
5d
6s
3d
4p
3p
4d
5p
5d
6p
O
Li
Na
Mg
Al
Sc
V
Mn
Cr
Ti
Ca
K
Y
Nb
Pd
Tc
Zr
Rh
Mo
Ru
Sr
Rb
Gd
Tb
Dy
Ho
Er
Tm
Eu
Pr
Nd
Ce
Sm
La
Cs
Ba
Yb
Ta
Pt
Hf
Re
W
Ir
Lu
Os
Am
Pu
U
Th
He
H
B
C
N
Be
Ne
Si
S
P
Cl
Ar
Cu
Zn
Ga
Ge
As
Se
Br
Kr
Ag
Cd
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Te
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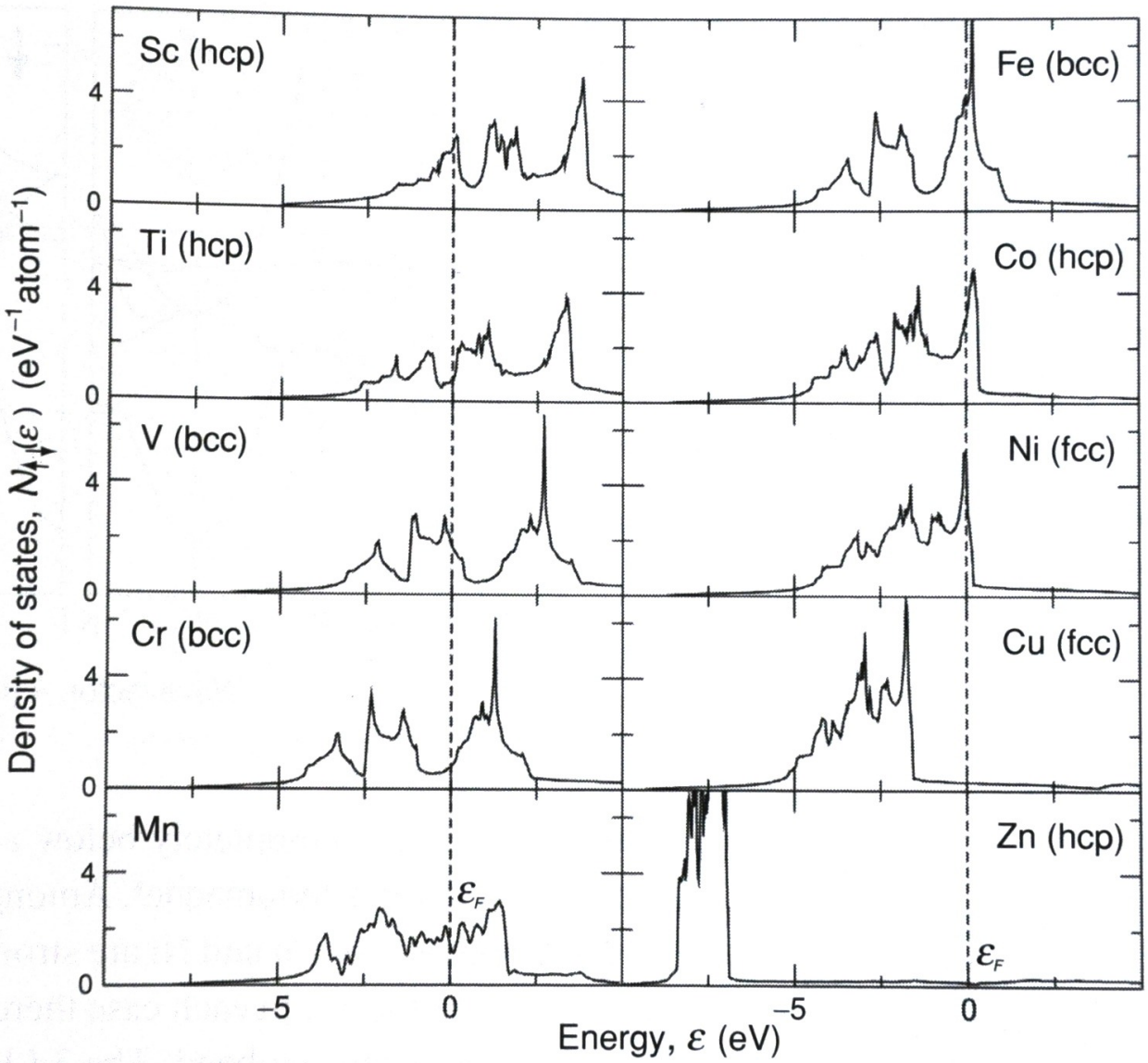
Xe
Au
Hg
Pb
Ti
Bi

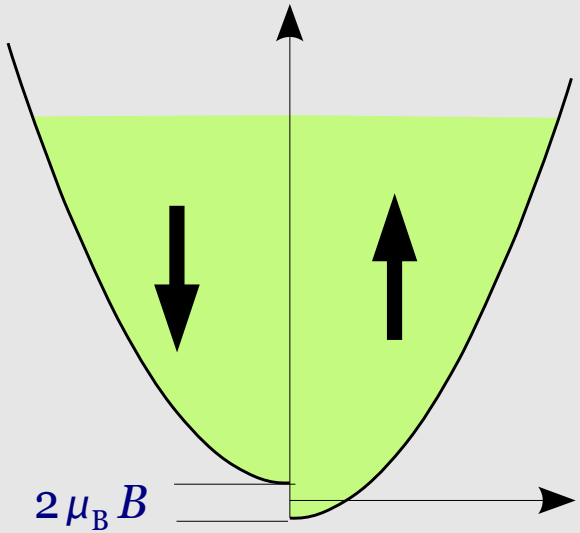
From: Coey

Band structure calculation of the 3d series (paramagnetic state)



From: Coey

Mean field for band magnetism



$$\mathbf{H_i} = n_S \mathbf{M} + \mathbf{H}$$

$$\chi_P = \mu_o \mu_B^2 \mathcal{D}(\epsilon_F)$$

Enhanced susceptibility:

$$\chi = \frac{M}{H} = \frac{\chi_P H_i}{H} = (n_S \chi + 1)\chi_P$$

$$\Rightarrow \quad \chi = \frac{\chi_P}{(1 - n_S \chi_P)}$$

Divergence → spontaneous moment

Stoner criterium

n_S can be related to the exchange energy

$$-(I/4)\left(\frac{n^{\uparrow} - n^{\downarrow}}{n}\right)^2$$ (Coulomb + Pauli)

Stoner criterium for ferromagnetism:

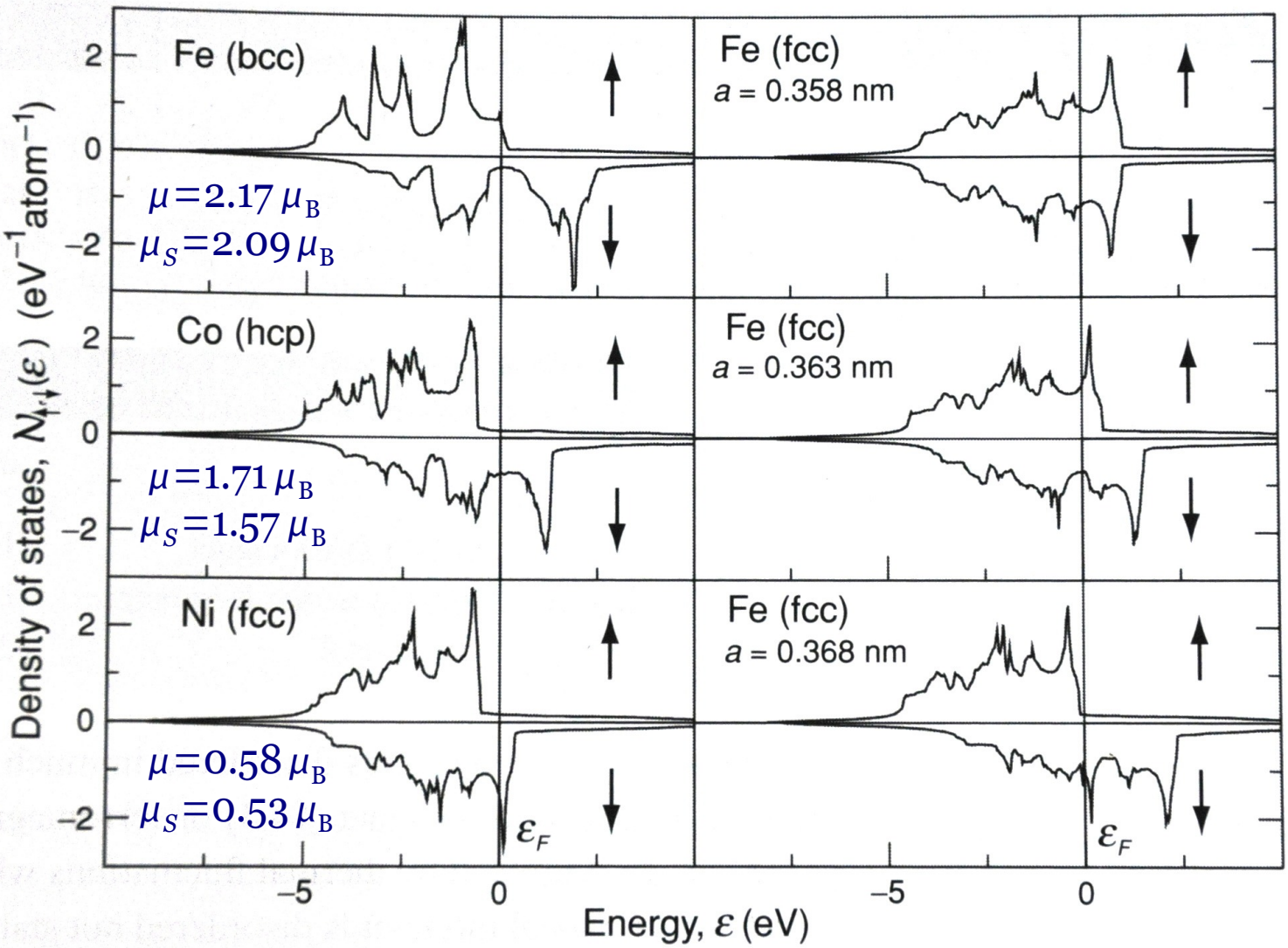
$$I\frac{\mathcal{D}_{\uparrow,\downarrow}(\epsilon_F)}{n} > 1$$

$$I\,\rho_{\uparrow,\downarrow}(\epsilon_F) > 1$$ (expressed for one atom)

Remember

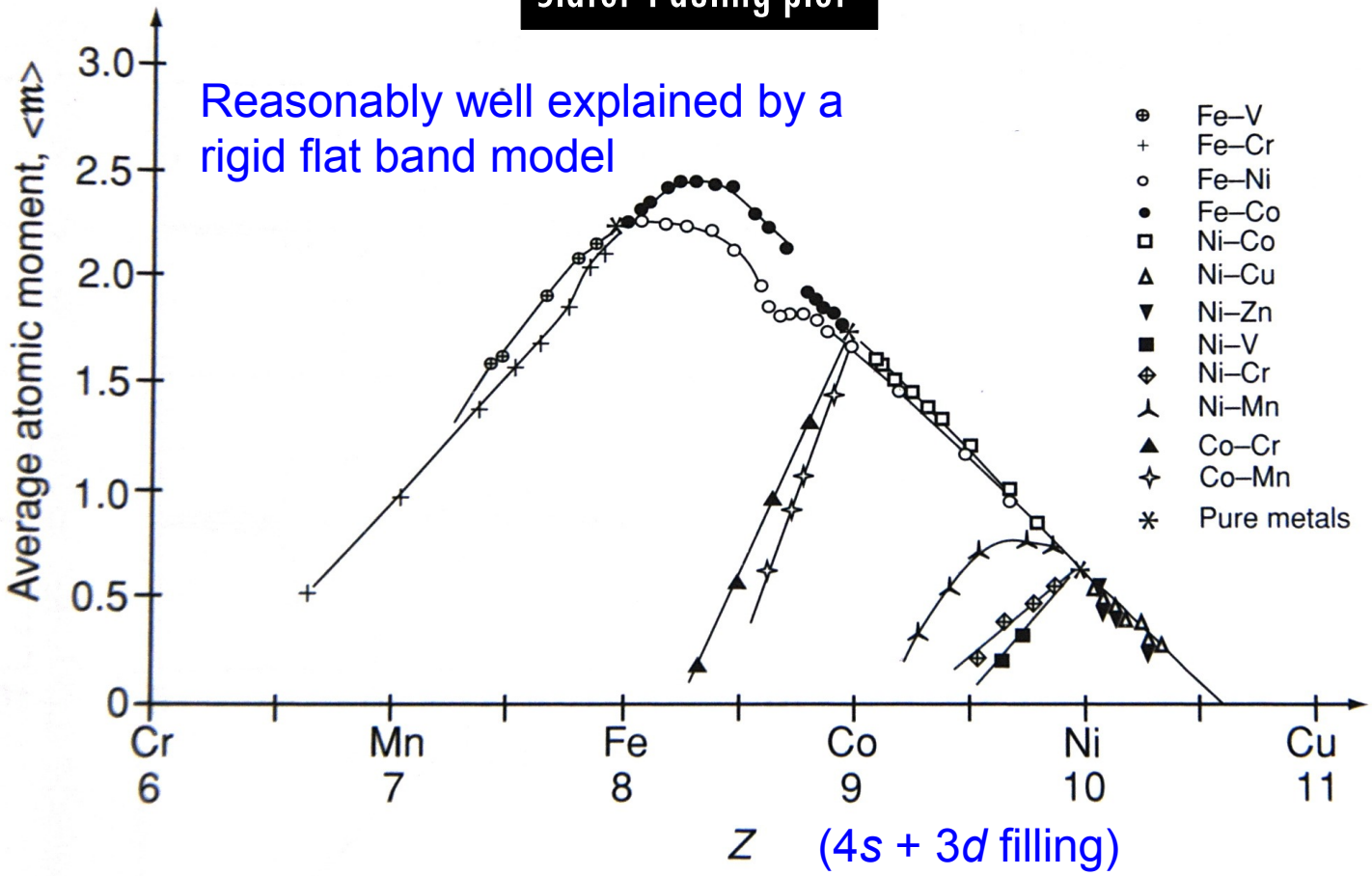
- Ordering for high DOS at Fermi energy
- Atomic moment may not be a multiple of μ_B

Band structure calculation of the 3d series (magnetic state)



From: Coey

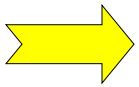
Slater-Pauling plot



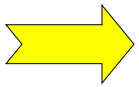
Notes

- Relevance for alloys
- Nano-alloys: enhanced moment and anisotropy of Co-Fe at interfaces

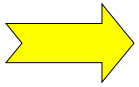
From: Coey



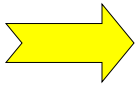
1. Magnetic moments



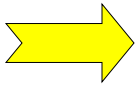
2. Magnetism of single atoms



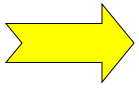
3. Moments in fields



4. Magnetic ordering



5. Magnetism in metals



6. Magnetic anisotropy

Physics at play

Crystal electric field: Coulomb interaction between electronic orbitals and the crystal environment

→ Hamiltonian $\mathcal{H}_{cf}$

Reminder: spin-orbit coupling S and L:

→ Hamiltonian $\mathcal{H}_{so}$

Figures

	$\mathcal{H}_{cf}$	$\mathcal{H}_{so}$
3d	1−10 eV	10−100 meV
4f	25 meV	100−500 meV

3d metals

Major effect: $\mathcal{H}_{cf}$

⇨ L is not a good quantum number

⇨ Quenching of orbital momentum
→ J~S and g~2

Perturbation: $\mathcal{H}_{so}$

⇨ Magnetic anisotropy (see next slide)

4f metals

Major effect: $\mathcal{H}_{so}$

⇨ L is a good quantum number

⇨ Moments close to atomic values

Perturbation: $\mathcal{H}_{cf}$

⇨ Magnetic anisotropy (see next slide)

Origin and formalism

Definition: angular dependance of the energy of a magnetic material (F, AF etc.)

Origin: crystal-field, assisted with spin-orbit in the 3*d* series.

Group theory is used to predict terms in expansions:

Cubic symmetry $E_{mc} = K_1\left(\alpha_1^2\alpha_2^2 + \alpha_2^2\alpha_3^2 + \alpha_3^2\alpha_1^2\right) + K_2\left(\alpha_1^2\alpha_2^2\alpha_3^2\right) + \ldots$

Hexagonal symmetry $E_{mc} = K_1\sin^2\theta + K_2\sin^4\theta + K_3\sin^6\theta + K_3'\sin^6\theta\sin^6\phi + \ldots$

Consequences and figures

- Anisotropy lies at the base of magnets and recording
- Low symmetry favors high anisotropy
- K range from <1 to 10^7 J/m^3 in known materials

Nano-alloys

- Alloys: allows low symmetry (distortions, interfaces, band filling etc.)
- Nano: changes lattice parameter and symmetry. Cf FeCo: low anisotropy in bulk, peak anisotropy at interfaces and steps.

Origin and formalism

Definition: dependence of magnetic anisotropy on strain

Origin: can be viewed as the strain-derive of magneto-crystalline anisotropy

Notice: mirror effect to magneto-striction

In principle a third-rank tensor is required:

→ Strain is a second-rank tensor

→ Magnetization is a vector

Simple example of a polycristalline sample under uniaxial strain:

$$E_{mel} = -\lambda_S \frac{E}{2}(3\cos^2\theta - 1)\epsilon + \frac{1}{2}E\epsilon^2 + \dots$$

E Young's modulus

Consequences and figures

- Order of magnitude of Lambda: 10^{-6}
- Limits coercivity in low-anisotropy materials
- Underpins effects such as invar
- Magneto-striction is used in actuators

Nano-alloys

- Alloys: composition changes Emel
- Nano: huge strain. Non-linear terms (largely unknown) play the leading role.