6. Magnetism

Hamilton for single atom in magnetic field

$\hat{H} = \frac{(\vec{p}+e\vec{A})^2}{2m}$, with: $\vec{B} = \mu_0 \vec{H} = \nabla \times \vec{A}$ and $\nabla \cdot \vec{A} = 0$

$$\hat{H} = \frac{\vec{p}^2}{2m} + \frac{e}{m}\vec{A}\vec{p} + \frac{e^2\vec{A}^2}{2m}$$

$$B = (0, 0, B_0) = const., \ \vec{A} = -\frac{1}{2}(\vec{r} \times \vec{B_0})$$

$$\hat{H} = \frac{\vec{p}^2}{2m} - \frac{e}{2m}(\vec{r} \times \vec{B_0})\vec{p} + \frac{e^2(\vec{r}\times\vec{B_0})^2}{8m}$$

$$\hat{H} = \frac{\vec{p}^2}{2m} + \frac{e}{2m}(\vec{r} \times \vec{p})\vec{B_0} + \frac{e^2}{8m}(x^2+y^2)\vec{B_0}^2$$

$$\hat{H} = \frac{\vec{p}^2}{2m} + \underbrace{\frac{e}{2m}L_z B_0}_{\text{paramagnetism}} + \underbrace{\frac{e^2}{8m}(x^2+y^2)\vec{B_0}^2}_{\text{diamagnetism}}$$

6. Magnetism

magnetic moment $\vec{m} = \frac{\partial \hat{H}}{\partial \vec{B_0}}$

$$\vec{m} = -[\underbrace{\frac{e}{2m}\langle L_z \rangle}_{\text{paramagnetism}} + \underbrace{\frac{e^2 B_0}{4m}\langle x^2+y^2 \rangle}_{\text{diamagnetism}}], \ e < 0$$

Magnetization $\vec{M} = N \cdot \vec{m} = \chi \cdot \vec{H} = \chi \cdot \frac{\vec{B}}{\mu_0}$

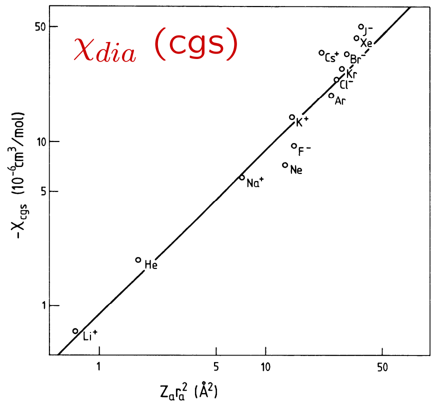
6.1 (Langevin) diamagnegtism

Diamagnetism arises from a change of orbital momentum by an applied external magnetic field H (<u>Lenz's law</u>).

Diamagnetic susceptibility

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

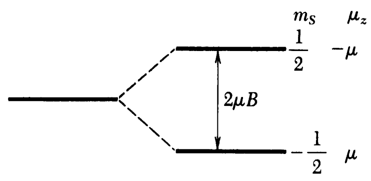
$$\chi_{dia} \simeq -10^{-4} \ll 1$$



6.2 Paramagnetism

Energy $U = -\vec{m}\vec{B} = g\mu_B \cdot m_j B$

$\vec{m} = -g\mu_B \cdot \vec{J}, m_j = -j, \ldots, j$

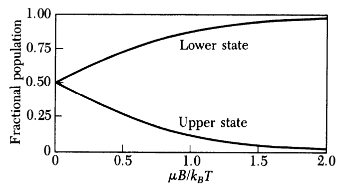


Bohr magneton

$\mu_B = \frac{|e|\hbar}{2m} = 0.579 \cdot 10^{-4}$ eV/Tesla

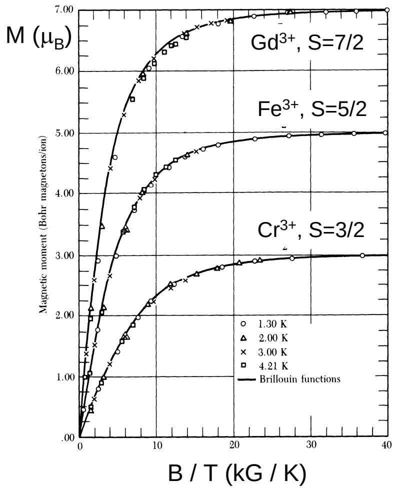
Spin $S_z = \pm 1/2$

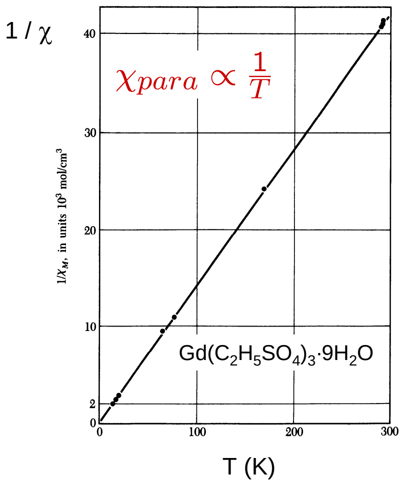
$$\frac{N_{1,2}}{N} = \frac{e^{\pm U/k_B T}}{e^{U/k_B T} + e^{-U/k_B T}}$$



$$\boxed{\vec{M} = N \cdot \vec{m}(N_1 - N_2) = N\vec{m}\tanh(U/k_B T) \simeq N\vec{m}\frac{U}{k_B T}}$$

6.2 Paramagnetism





6.2 Paramagnetism

Spin: $J_z = m_j,\ m_j = -j, \ldots, j$

$$\boxed{\text{Magnetization: } M(B,T) = NgJ_B B_J(x)}$$

with Brillouin function

$B_J(x) = \frac{2J+1}{2J}\coth(\frac{(2J+1)x}{2J}) - \frac{1}{2J}\coth(\frac{x}{2J}), x = gJ\mu_B B/k_B T$

for $x \ll 1$:

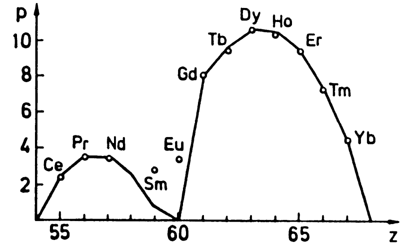
$$\boxed{\text{Curie law: } \chi_{para} = \frac{C}{T}}$$

6.2 Paramagnetic ions, 4f-electrons

Hund´s rules:

1) S is maximal
2) L is maximal (consistent with S)
3) J=|L-S| if shell is less than half filled
   J=|L+S| if shell is more than half filled
   J = S if shell is half filled

Trivalent 4f - ions:



6.2 Paramagnetic ions, 3d-electrons

Table 2 Effective magneton numbers for iron group ions

Ion	Configuration	Basic level	p(calc) = $g[J(J+1)]^{1/2}$	p(calc) = $2[S(S+1)]^{1/2}$	p(exp)[a]
Ti^{3+}, V^{4+}	$3d^1$	$^2D_{3/2}$	1.55	1.73	1.8
V^{3+}	$3d^2$	$^3F_2$	1.63	2.83	2.8
Cr^{3+}, V^{2+}	$3d^3$	$^4F_{3/2}$	0.77	3.87	3.8
Mn^{3+}, Cr^{2+}	$3d^4$	$^5D_0$	0	4.90	4.9
Fe^{3+}, Mn^{2+}	$3d^5$	$^6S_{5/2}$	5.92	5.92	5.9
Fe^{2+}	$3d^6$	$^5D_4$	6.70	4.90	5.4
Co^{2+}	$3d^7$	$^4F_{9/2}$	6.63	3.87	4.8
Ni^{2+}	$3d^8$	$^3F_4$	5.59	2.83	3.2
Cu^{2+}	$3d^9$	$^2D_{5/2}$	3.55	1.73	1.9

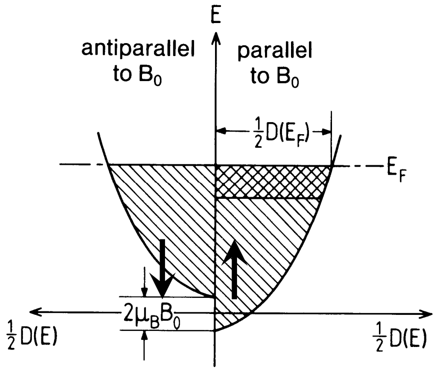
[a]Representative values.

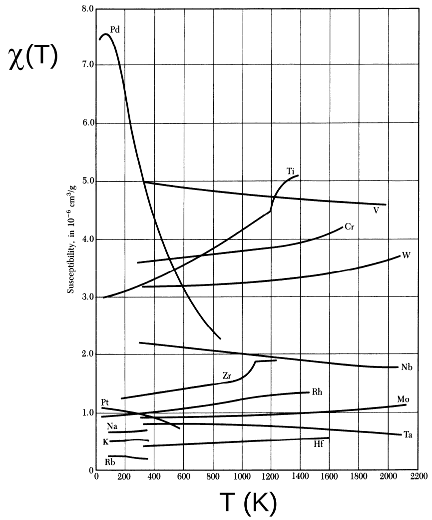
for d-electrons quenching of orbital moments in cubic symmetry

6.2 Pauli paramagnetism of conduction electrons

$$M = \mu_B(N_\uparrow - N_\downarrow) = \mu_B^2 D(E_F) B$$

$$\chi = \mu_0 \mu_B^2 D(E_F)$$

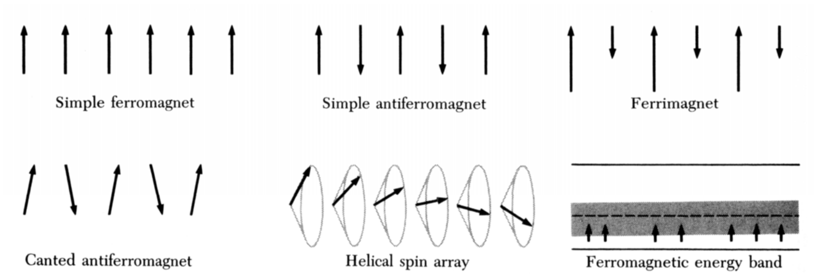




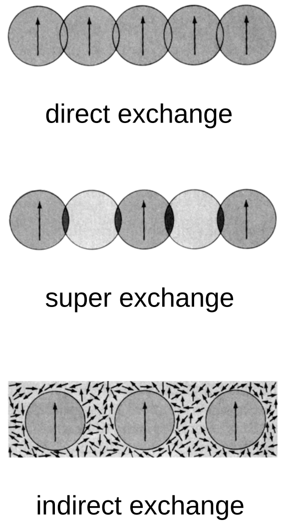
6.3. Exchange coupling

⇒ ordering of magnetic moments in absence of external B

⇒ spontaneous magnetization below the Curie temperature T_C
above T_C: paramagnetic behavior

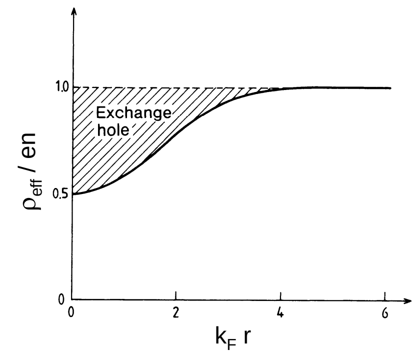


6.3. Exchange interaction

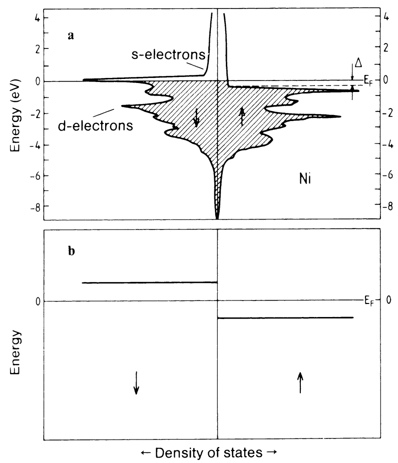


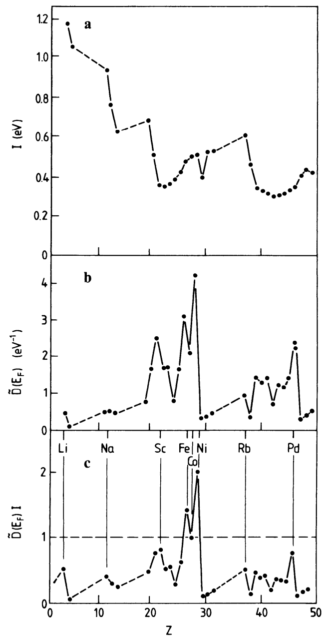
For free electrons:
exchange hole = effective charge density seen by a single electron

$$\rho_{eff} = \frac{e \cdot n}{2}\left[1 - 9\frac{(\sin k_F r - k_F r \cos k_F r)^2}{(k_F r)^6}\right]$$



6.4. Stoner-Wohlfarth model

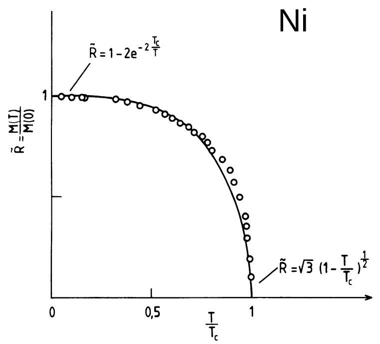


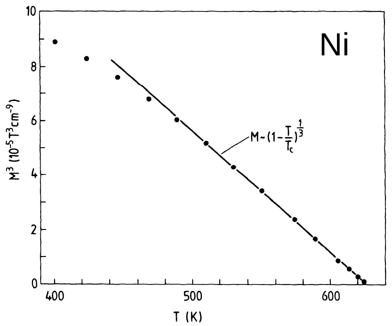


$$I \frac{D(E_F)}{2n} = I \tilde{D}(E_F) > 1$$

6.5. Tempeature dependence of ferromagnetism

T < T_C: ferromagnetic behavior





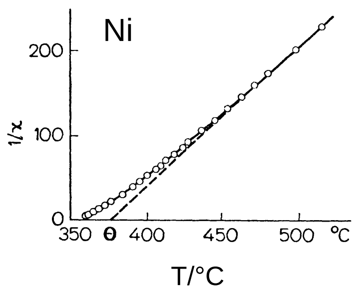
Mean field theory: $M(T) = \sqrt{3}(1 - \frac{T}{T_C})^{1/2}$

6.5. Temperature dependence

T > T_C: paramagnetic behavior

magnetic susceptibility diverges according to Curie-Weiss law:

$$\boxed{\chi(T) = \frac{C}{T - T_C}, \ T_C = \lambda C}$$



As $T \to T_c$ from above, the susceptibility χ becomes proportional to $(T - T_c)^{-\gamma}$; as $T \to T_c$ from below, the magnetization M_s becomes proportional to $(T_c - T)^{\beta}$. In the mean field approximation, $\gamma = 1$ and $\beta = \frac{1}{2}$.

	γ	β	T_c, in K
Fe	1.33 ± 0.015	0.34 ± 0.04	1043
Co	1.21 ± 0.04	—	1388
Ni	1.35 ± 0.02	0.42 ± 0.07	627.2
Gd	1.3 ± 0.1	—	292.5
CrO_2	1.63 ± 0.02	—	386.5
$CrBr_3$	1.215 ± 0.02	0.368 ± 0.005	32.56
EuS	—	0.33 ± 0.015	16.50

6.5. Temperature dependence of ferromagnetism

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EuS	—	0.33 ± 0.015	16.50

spin waves

6.6. Mean field theory

$$\boxed{B_{eff} = B_{int} + B_{ext} = \lambda\mu_0 M + B_{ext}}$$

$T > T_C$:

$$\mu_0 \cdot M = \chi_{para}(B_{int} + B_{ext}) = \frac{C}{T}(\lambda\mu_0 M + B_{ext})$$

$$\boxed{\chi = \frac{M}{\mu_0 B_{ext}} = [(1 - \frac{C}{T}\lambda)]^{-1} = \frac{T}{T - C\lambda} = \frac{T}{T - T_C}}$$

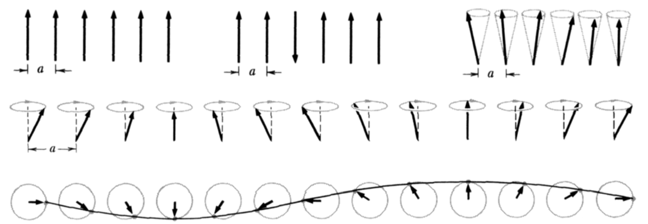
$T < T_C$, Spin 1/2 :

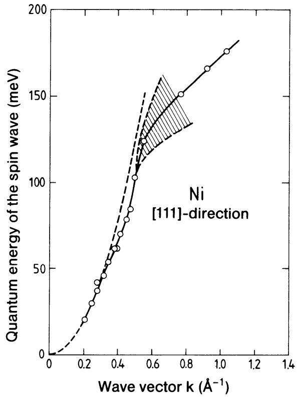
$$\vec{M} = N\vec{m}\tanh(\vec{m}\cdot(\mu_0\lambda\vec{M} + \vec{B}_{ext})/k_B T)$$
$$\simeq N\vec{m}\tanh(\vec{m}\cdot\mu_0\lambda\vec{M}/k_B T)$$

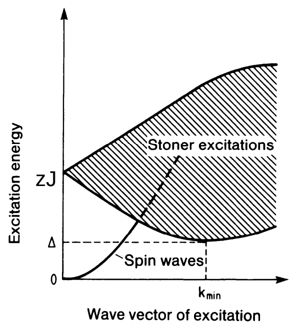
$\tanh(x) \simeq x - x^3/3$

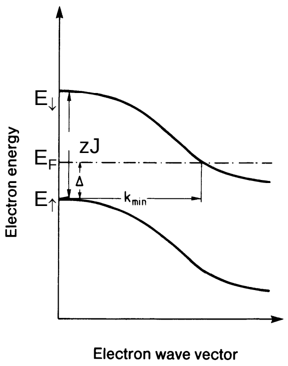
$$\boxed{\Rightarrow M(T) = \sqrt{3}(1 - \frac{T}{T_C})^{1/2}}$$

6.7. Spin waves - magnons

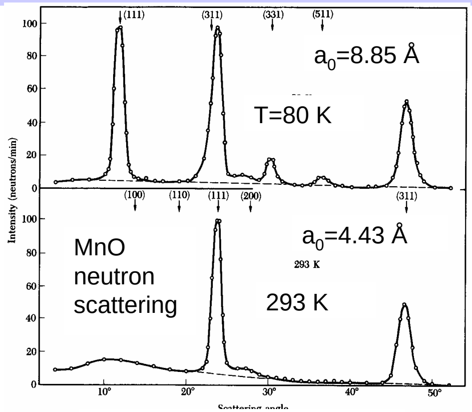




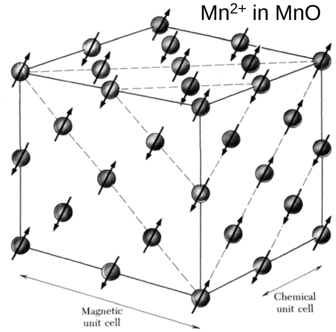


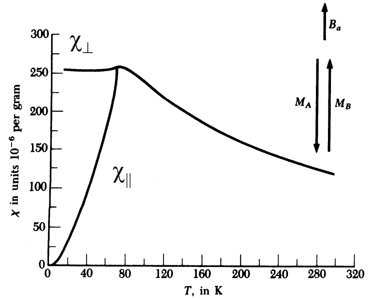


6.8. Antiferromagnetic order



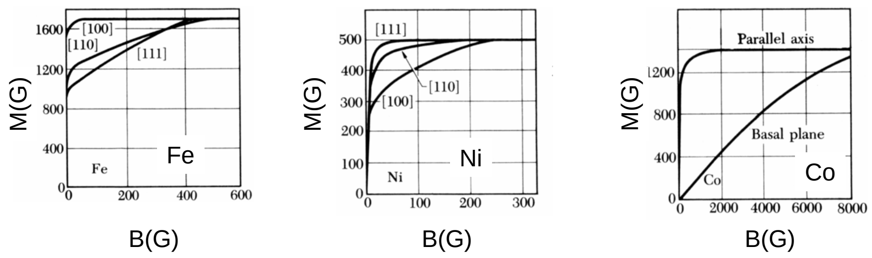
Substance	Paramagnetic ion lattice	Transition temperature, T_N, in K
MnO	fcc	116
MnS	fcc	160
MnTe	hex. layer	307
MnF_2	bc tetr	67
FeF_2	bc tetr	79
$FeCl_2$	hex. layer	24
FeO	fcc	198
$CoCl_2$	hex. layer	25





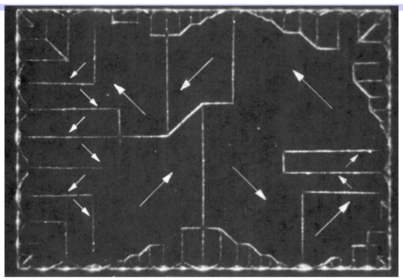
6.9. Magnetic anisotropy

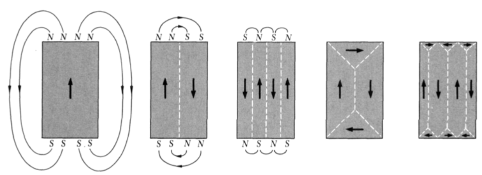
Magnetization M depends not only on external field B
but also on crystal orientation

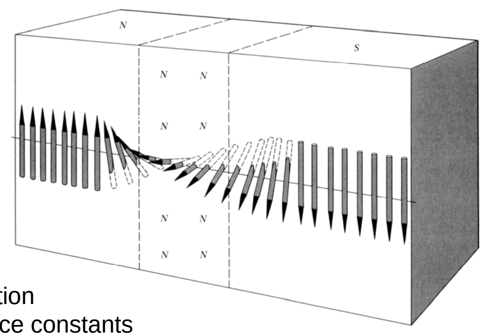


- crystalline anisotropy (L-S coupling)
- shape anisotropy (dipolar interaction, stray fields)
- interface anisotropy

6.9. Domains







Reduction of magnetic stray field
⇒ magnetic domains
⇒ reduction of the total energy

Domain distribution determined by
microscopic and macroscopic properties
(shape, anisotropy, exchange interaction)

Domain boundaries: continuous spin rotation
Width of domain wall in bulk: few 100 lattice constants