

Technische Universität Graz

Institute of Solid State Physics

Ferromagnetism



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Ferromagnetism

Below a critical temperature (called the Curie temperature) a magnetization spontaneously appears in a ferromagnet even in the absence of a magnetic field.

Iron, nickel, and cobalt are ferromagnetic.

Ferromagnetism overcomes the magnetic dipole-dipole interactions. It arises from the Coulomb interactions of the electrons. The energy that is gained when the spins align is called the exchange energy.

Schrödinger equation for two particles

$$-\frac{\hbar^2}{2m} \left(\nabla_1^2 + \nabla_2^2\right) \psi + V_1(\vec{r_1}) \psi + V_2(\vec{r_2}) \psi + V_{1,2}(\vec{r_1}, \vec{r_2}) \psi = E \psi$$

 $\psi(\vec{r_1}, \vec{r_2}) = \psi_1(\vec{r_1})\psi_2(\vec{r_2})$ is a solution to the noninteracting Hamiltonian, $V_{1,2} = 0$

$$\psi_{A}\left(\vec{r}_{1},\vec{r}_{2}\right) = \frac{1}{\sqrt{2}}\left(\psi_{1}\left(\vec{r}_{1}\right)\psi_{2}\left(\vec{r}_{2}\right) - \psi_{1}\left(\vec{r}_{2}\right)\psi_{2}\left(\vec{r}_{1}\right)\right)\left(\frac{1}{\sqrt{2}}\left(\uparrow\downarrow+\downarrow\uparrow\right)\right)\left(\downarrow\downarrow\right)\right)$$

$$\psi_{s}\left(\vec{r}_{1},\vec{r}_{2}\right) = \frac{1}{\sqrt{2}} \left(\psi_{1}(\vec{r}_{1})\psi_{2}(\vec{r}_{2}) + \psi_{1}(\vec{r}_{2})\psi_{2}(\vec{r}_{1})\right) \frac{1}{\sqrt{2}} \left(\uparrow\left(\vec{r}_{1}\right) \downarrow\left(\vec{r}_{2}\right) - \downarrow\left(\vec{r}_{1}\right) \uparrow\left(\vec{r}_{2}\right)\right)$$

Exchange (Austauschwechselwirking)

$$\psi_{A}(\vec{r}_{1},\vec{r}_{2}) = \frac{1}{\sqrt{2}} (\psi_{1}(\vec{r}_{1})\psi_{2}(\vec{r}_{2}) - \psi_{1}(\vec{r}_{2})\psi_{2}(\vec{r}_{1}))$$

 $\left\langle \psi_{A} \left| H \left| \psi_{A} \right\rangle = \frac{1}{2} \left[\left\langle \psi_{1}(\vec{r_{1}}) \psi_{2}(\vec{r_{2}}) \right| H \left| \psi_{1}(\vec{r_{1}}) \psi_{2}(\vec{r_{2}}) \right\rangle - \left\langle \psi_{1}(\vec{r_{1}}) \psi_{2}(\vec{r_{2}}) \right| H \left| \psi_{1}(\vec{r_{2}}) \psi_{2}(\vec{r_{1}}) \right\rangle - \left\langle \psi_{1}(\vec{r_{2}}) \psi_{2}(\vec{r_{1}}) \right| H \left| \psi_{1}(\vec{r_{1}}) \psi_{2}(\vec{r_{2}}) \right\rangle + \left\langle \psi_{1}(\vec{r_{2}}) \psi_{2}(\vec{r_{1}}) \right| H \left| \psi_{1}(\vec{r_{2}}) \psi_{2}(\vec{r_{1}}) \right\rangle \right]$

$$\psi_{S}(\vec{r}_{1},\vec{r}_{2}) = \frac{1}{\sqrt{2}} (\psi_{1}(\vec{r}_{1})\psi_{2}(\vec{r}_{2}) + \psi_{1}(\vec{r}_{2})\psi_{2}(\vec{r}_{1}))$$

 $\left\langle \psi_{s} \left| H \left| \psi_{s} \right\rangle = \frac{1}{2} \left[\left\langle \psi_{1}(\vec{r}_{1})\psi_{2}(\vec{r}_{2}) \right| H \left| \psi_{1}(\vec{r}_{1})\psi_{2}(\vec{r}_{2}) \right\rangle + \left\langle \psi_{1}(\vec{r}_{1})\psi_{2}(\vec{r}_{2}) \right| H \left| \psi_{1}(\vec{r}_{2})\psi_{2}(\vec{r}_{1}) \right\rangle + \left\langle \psi_{1}(\vec{r}_{2})\psi_{2}(\vec{r}_{1}) \right| H \left| \psi_{1}(\vec{r}_{1})\psi_{2}(\vec{r}_{2}) \right\rangle + \left\langle \psi_{1}(\vec{r}_{2})\psi_{2}(\vec{r}_{1}) \right| H \left| \psi_{1}(\vec{r}_{2})\psi_{2}(\vec{r}_{1}) \right\rangle \right]$

The difference in energy between the ψ_A and ψ_S is twice the **exchange energy**.

Exchange

The exchange energy can only be defined when you speak of multielectron wavefunctions. It is the difference in energy between the symmetric solution and the antisymmetric solution. There is only a difference when the electron-electron term is included. Coulomb repulsion determines the exchange energy.

In ferromagnets, the antisymmetric state has a lower energy. Thus the state with parallel spins has lower energy.

In antiferromagnets, the symmetric state has a lower energy. Neighboring spins are antiparallel.

Ordered states have a lower entropy than free electrons.

Mean field theory (Molekularfeldtheorie)

Heisenberg Hamiltonian
$$H = -\sum_{i,j} J_{i,j} \vec{S}_i \cdot \vec{S}_j - g \mu_B \vec{B} \cdot \sum_i \vec{S}_i$$

Mean field approximation
 $H_{MF} = \sum_i \vec{S}_i \cdot \left(\sum_{\delta} J_{i,\delta} \langle \vec{S} \rangle + g \mu_B \vec{B} \right)$
 δ sums over the neighbors of spin *i*
 $\vec{B}_{MF} = \frac{1}{g \mu_B} \sum_{\delta} J_{i,\delta} \langle \vec{S} \rangle$
magnetization $\vec{M} = g \mu_B \frac{N}{V} \langle \vec{S} \rangle$

eliminate <*S*>

Mean field theory

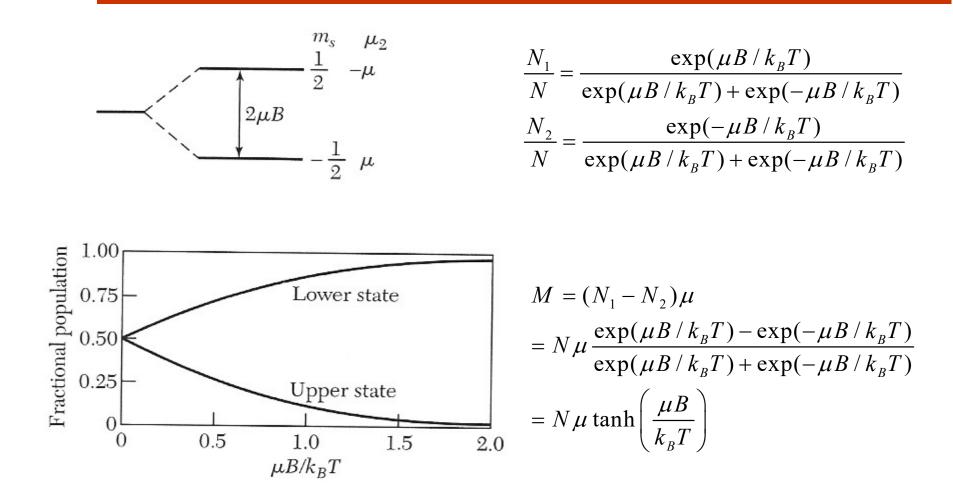
$$\vec{B}_{MF} = \frac{V}{Ng^2 \mu_B^2} z J \vec{M}$$

z is the number of nearest neighbors In mean field, the energy of the spins is

$$E = \pm \frac{1}{2} g \mu_B (B_{MF} + B_a)$$

We calculated the populations of the spins in the paramagnetism section

Spin populations



Mean field theory

$$M = \frac{1}{2}g\mu_B \frac{N}{V} \tanh\left(\frac{g\mu_B \left(B_{MF} + B_a\right)}{2k_B T}\right)$$

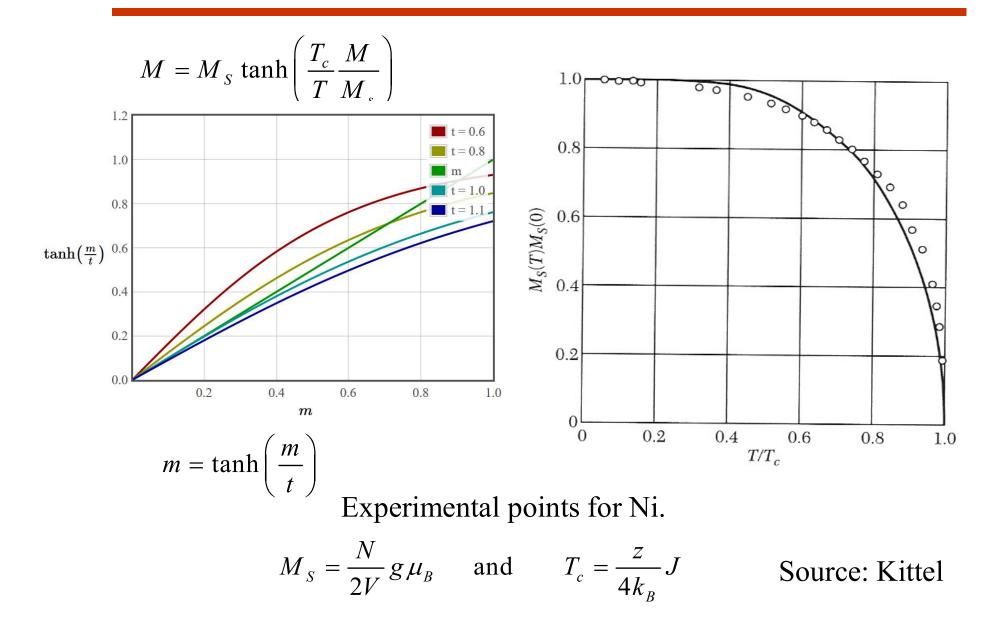
For zero applied field

$$M = M_s \tanh\left(\frac{T_c}{T}\frac{M}{M_s}\right)$$

$$M_{S} = \frac{N}{2V} g \mu_{B}$$
 and $T_{c} = \frac{z}{4k_{B}} J$

 M_s = saturation magnetization T_c = Curie temperature

Mean field theory



Ferromagnetism

Material Curie temp. (K)	
Со	1388
Fe	1043
FeOFe ₂ O ₃	858
NiOFe ₂ O ₃	858
$CuOFe_2O_3$	728
$MgOFe_2O_3$	713
MnBi	630
Ni	627
MnSb	587
MnOFe ₂ O ₃	573
$Y_3Fe_5O_{12}$	560
CrO ₂	386
MnĀs	318
Gd	292
Dy	88
EuO	69
Nd ₂ Fe ₁₄ B	353
Sm_2Co_{17}	700

$$M_{S} = \frac{N}{2V} g \mu_{B}$$

$$T_c = \frac{Z}{4k_B}J$$

Electrical insulator $M_s = 10 M_s$ (Fe) rare earth magnets

Curie - Weiss law

$$M = \frac{1}{2}g\mu_B \frac{N}{V} \tanh\left(\frac{g\mu_B \left(B_{MF} + B_a\right)}{2k_B T}\right)$$

$$\vec{B}_{MF} = \frac{V}{Ng^2 \mu_B^2} z J \vec{M}$$

Above T_c we can expand the hyperbolic tangent $tanh(x) \approx x$ for

x << 1

$$M \approx \frac{1}{4} g^2 \mu_B^2 \frac{N}{V k_B T} \left(\frac{V}{N g^2 \mu_B^2} z J M + B_a \right)$$

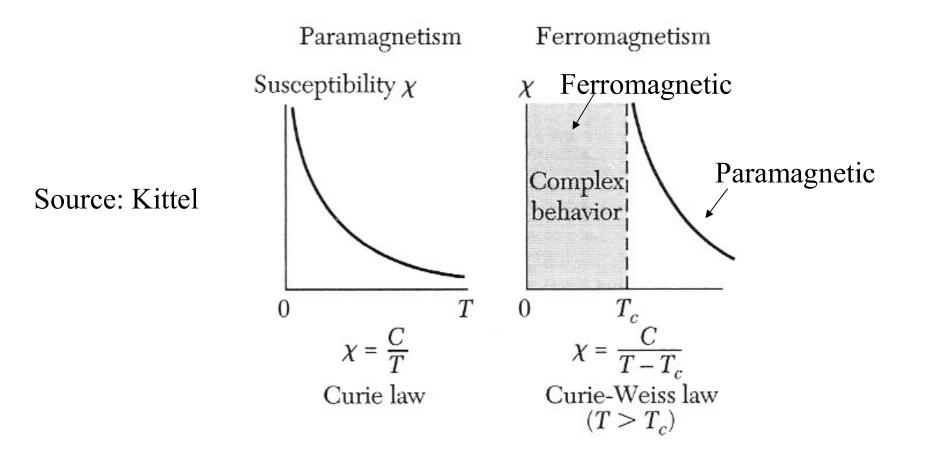
Solve for *M*

$$M \approx \frac{g^2 \mu_B^2 N}{4V k_B} \frac{B_a}{T - T_c} \qquad T_c = \frac{z}{4k_B} J$$

Curie Weiss Law $\chi = \frac{dM}{dH} \approx \frac{C}{T - T_a}$

Critical fluctuations near T_c

Ferromagnets are paramagnetic above T_c



Critical fluctuations near T_c .

Magnetization of a Magnetite Single Crystal Near the Curie Point*

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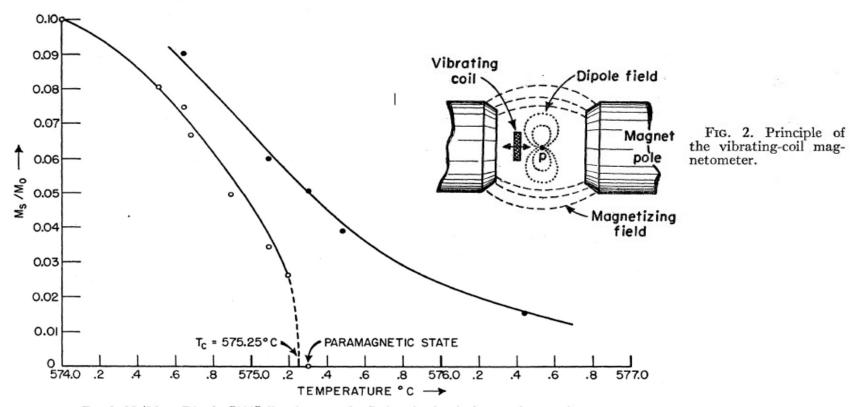


FIG. 9. M_s/M_0 vs T in the [111] direction near the Curie point for single-crystal magnetite.

Magnetic ordering

 $\varphi_2 = 2\varphi_1$

φ1

