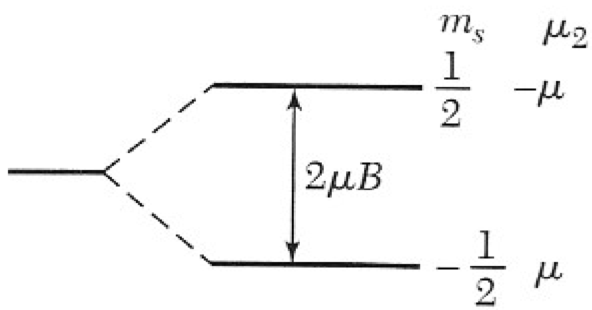
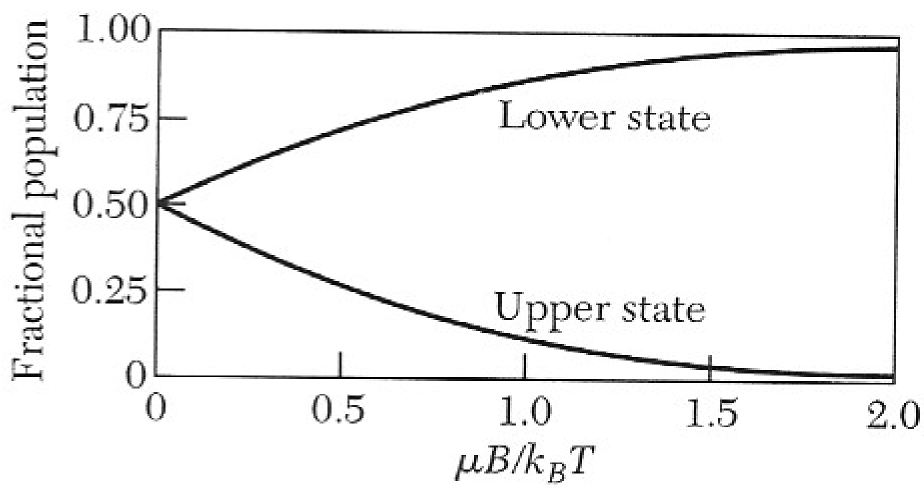
Paramagnetism, spin 1/2

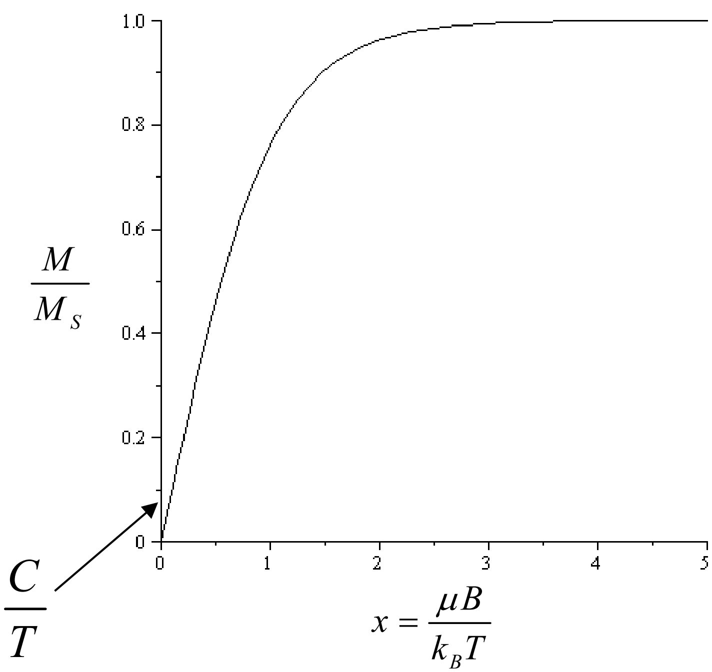


$$M = N\mu \tanh\left(\frac{\mu B}{k_B T}\right) \approx \frac{N\mu^2 B}{k_B T} = \frac{CB}{T}$$

for $\mu B << k_B T$

Curie law





$\chi \approx \frac{C}{T}$

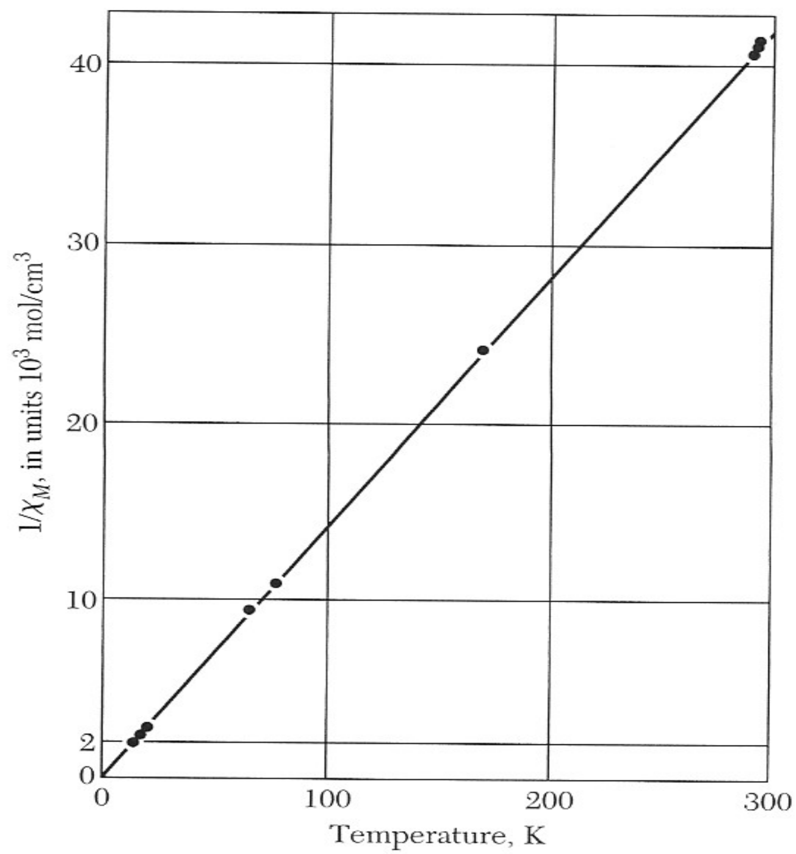
Curie law

for $\quad \mu B << k_B T \quad M = CB/T$

$$\chi \propto \left.\frac{dM}{dB}\right|_{B=0} = \frac{C}{T}$$

C is the Curie constant

$Gd(C_2H_3SO_4)_3 9H_2O$



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. Is 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

$$-\frac{\hbar^2}{2m}\left(\frac{\partial^2}{\partial x_1^2}+\frac{\partial^2}{\partial y_1^2}+\frac{\partial^2}{\partial z_1^2}+\frac{\partial^2}{\partial x_2^2}+\frac{\partial^2}{\partial y_2^2}+\frac{\partial^2}{\partial z_2^2}\right)\psi + V_1(\vec{r}_1)\psi + V_2(\vec{r}_2)\psi + V_{1,2}(\vec{r}_1,\vec{r}_2)\psi = E\psi$$

$\psi(\vec{r}_1,\vec{r}_2)=\psi_1(\vec{r}_1)\psi_2(\vec{r}_2)$ is a solution to the noninteracting Hamiltonian, $V_{1,2}=0$

$$\psi_A(\vec{r}_1,\vec{r}_2)=\frac{1}{\sqrt{2}}\left(\psi_1(\vec{r}_1)\psi_2(\vec{r}_2)-\psi_1(\vec{r}_2)\psi_2(\vec{r}_1)\right)\begin{pmatrix}\uparrow\uparrow\\ \frac{1}{\sqrt{2}}\left(\uparrow\downarrow+\downarrow\uparrow\right)\\ \downarrow\downarrow\end{pmatrix}$$

$$\psi_S(\vec{r}_1,\vec{r}_2)=\frac{1}{\sqrt{2}}\left(\psi_1(\vec{r}_1)\psi_2(\vec{r}_2)+\psi_1(\vec{r}_2)\psi_2(\vec{r}_1)\right)\frac{1}{\sqrt{2}}\left(\uparrow\downarrow-\downarrow\uparrow\right)$$

Exchange (Austauschwechselwirking)

$$\psi_A(\vec{r}_1,\vec{r}_2) = \frac{1}{\sqrt{2}}\left(\psi_1(\vec{r}_1)\psi_2(\vec{r}_2) - \psi_1(\vec{r}_2)\psi_2(\vec{r}_1)\right)$$

$$\left\langle \psi_A \middle| H \middle| \psi_A \right\rangle = \frac{1}{2}[\left\langle \psi_1(\vec{r}_1)\psi_2(\vec{r}_2) \middle| H \middle| \psi_1(\vec{r}_1)\psi_2(\vec{r}_2) \right\rangle - \left\langle \psi_1(\vec{r}_1)\psi_2(\vec{r}_2) \middle| H \middle| \psi_1(\vec{r}_2)\psi_2(\vec{r}_1) \right\rangle$$
$$- \left\langle \psi_1(\vec{r}_2)\psi_2(\vec{r}_1) \middle| H \middle| \psi_1(\vec{r}_1)\psi_2(\vec{r}_2) \right\rangle + \left\langle \psi_1(\vec{r}_2)\psi_2(\vec{r}_1) \middle| H \middle| \psi_1(\vec{r}_2)\psi_2(\vec{r}_1) \right\rangle]$$

$$\psi_S(\vec{r}_1,\vec{r}_2) = \frac{1}{\sqrt{2}}\left(\psi_1(\vec{r}_1)\psi_2(\vec{r}_2) + \psi_1(\vec{r}_2)\psi_2(\vec{r}_1)\right)$$

$$\left\langle \psi_S \middle| H \middle| \psi_S \right\rangle = \frac{1}{2}[\left\langle \psi_1(\vec{r}_1)\psi_2(\vec{r}_2) \middle| H \middle| \psi_1(\vec{r}_1)\psi_2(\vec{r}_2) \right\rangle + \left\langle \psi_1(\vec{r}_1)\psi_2(\vec{r}_2) \middle| H \middle| \psi_1(\vec{r}_2)\psi_2(\vec{r}_1) \right\rangle$$
$$+ \left\langle \psi_1(\vec{r}_2)\psi_2(\vec{r}_1) \middle| H \middle| \psi_1(\vec{r}_1)\psi_2(\vec{r}_2) \right\rangle + \left\langle \psi_1(\vec{r}_2)\psi_2(\vec{r}_1) \middle| H \middle| \psi_1(\vec{r}_2)\psi_2(\vec{r}_1) \right\rangle]$$

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 multi-electron 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.

Mean field theory (Molekularfeldtheorie)

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

Exchange energy

Mean field approximation

$$H_{MF} = \sum_i \vec{S}_i \cdot \left(\sum_\delta J_{i,\delta} \left\langle \vec{S} \right\rangle + g\mu_B \vec{B} \right)$$

Looks like a magnetic field B_{MF}

δ sums over the neighbors of spin *i*

$$\vec{B}_{MF} = \frac{1}{g\mu_B} \sum_\delta J_{i,\delta} \left\langle \vec{S} \right\rangle$$

magnetization → $$\vec{M} = g\mu_B \frac{N}{V} \left\langle \vec{S} \right\rangle$$

eliminate <*S*>

Mean field theory

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

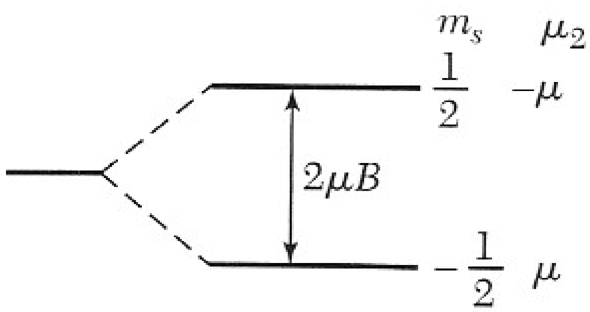
z is the number of nearest neighbors

In mean field, the energy of the spins is

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

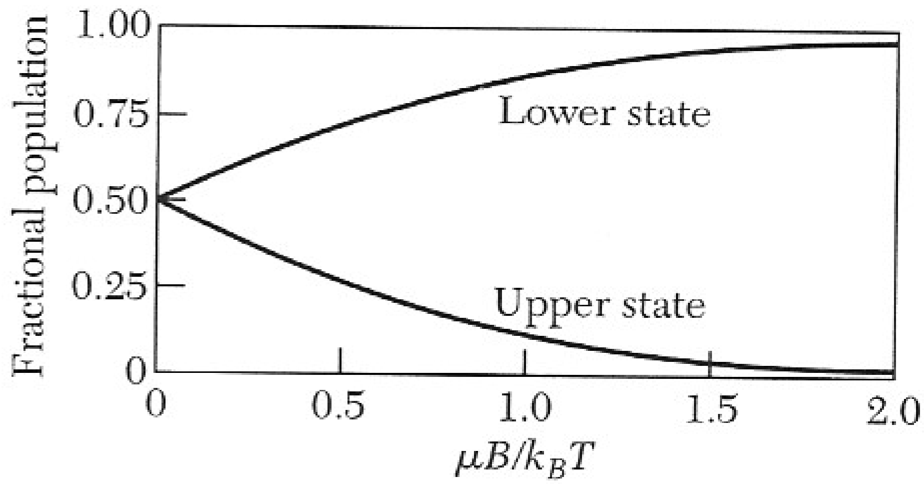
We calculated the populations of the spins in the paramagnetism section

Spin populations



$$\frac{N_1}{N} = \frac{\exp(\mu B / k_B T)}{\exp(\mu B / k_B T) + \exp(-\mu B / k_B T)}$$

$$\frac{N_2}{N} = \frac{\exp(-\mu B / k_B T)}{\exp(\mu B / k_B T) + \exp(-\mu B / k_B T)}$$



$$M = (N_1 - N_2)\mu$$

$$= N\mu \frac{\exp(\mu B / k_B T) - \exp(-\mu B / k_B T)}{\exp(\mu B / k_B T) + \exp(-\mu B / k_B T)}$$

$$= N\mu \tanh\left(\frac{\mu B}{k_B T}\right)$$

Mean field theory

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

For zero applied field

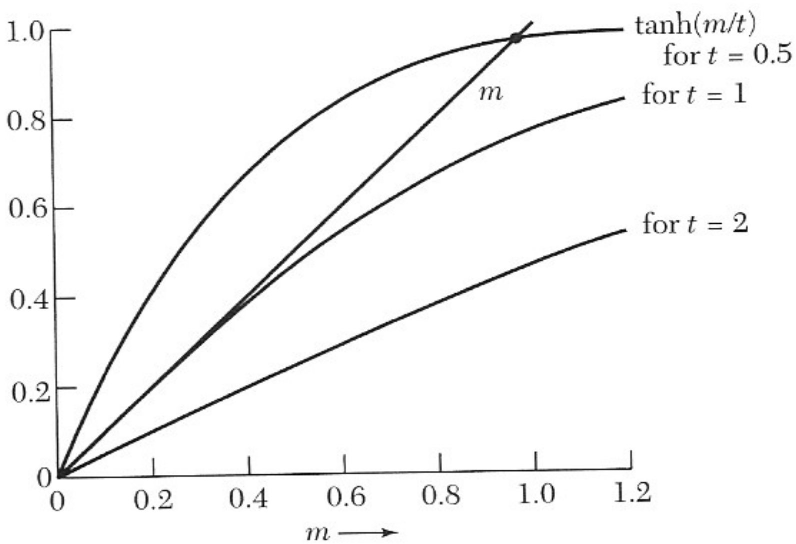
$$M = M_S \tanh\left(\frac{T_c}{T} \frac{M}{M_s} \right)$$

$$M_S = \frac{N}{2V} g \mu_B \quad \text{and} \quad T_c = \frac{z}{4 k_B} J$$

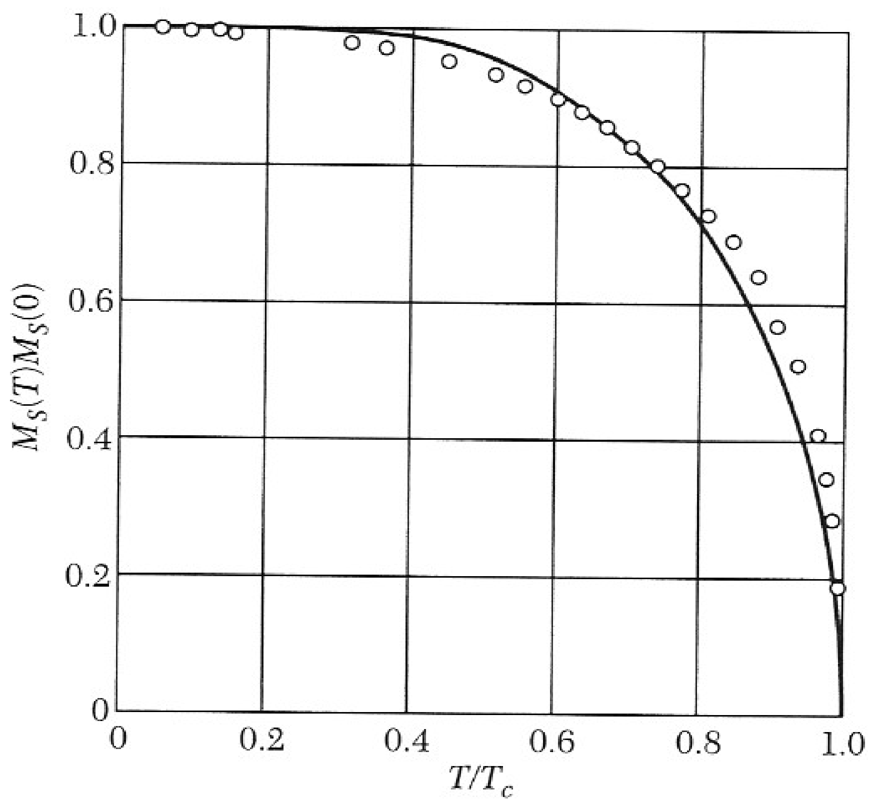
M_s = saturation magnetization $\qquad$ T_c = Curie temperature

Mean field theory

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



$$m = \tanh\left(\frac{m}{t}\right)$$



Experimental points for Ni.

Ferromagnetism

Material	Curie temp. (K)	
Co	1388	
Fe	1043	
$FeOFe_2O_3$	858	
$NiOFe_2O_3$	858	
$CuOFe_2O_3$	728	
$MgOFe_2O_3$	713	
MnBi	630	
Ni	627	
MnSb	587	
$MnOFe_2O_3$	573	
$Y_3Fe_5O_{12}$	560	
CrO_2	386	
MnAs	318	
Gd	292	
Dy	88	
EuO	69	Electrical insulator
$Nd_2Fe_{14}B$	353	$M_s = 10\ M_s(\mathrm{Fe})$
Sm_2Co_{17}	700	rare earth magnets

Curie - Weiss law

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

Above T_c we can expand the hyperbolic tangent $\tanh(x) \approx x$ for $x << 1$

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

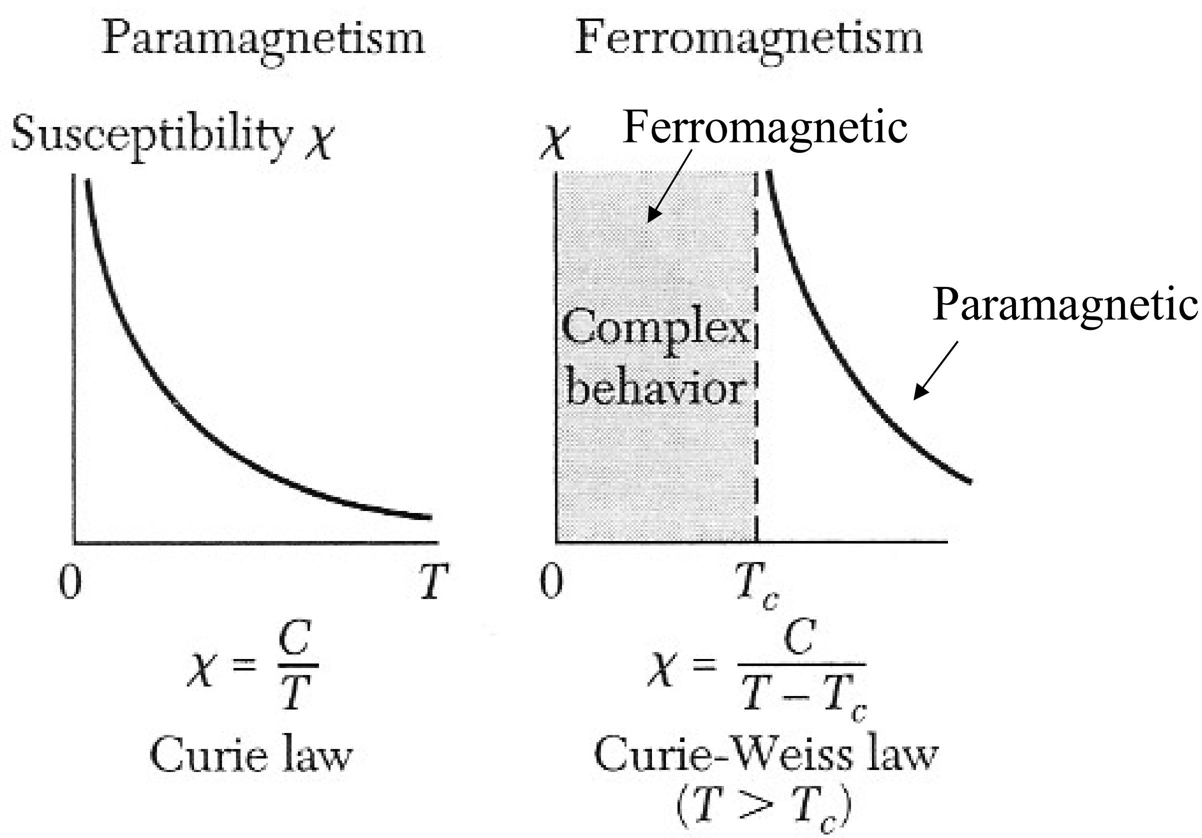
Solve for M

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

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

Critical fluctuations near T_c

Ferromagnets are paramagnetic above T_c



Critical fluctuations near T_c.