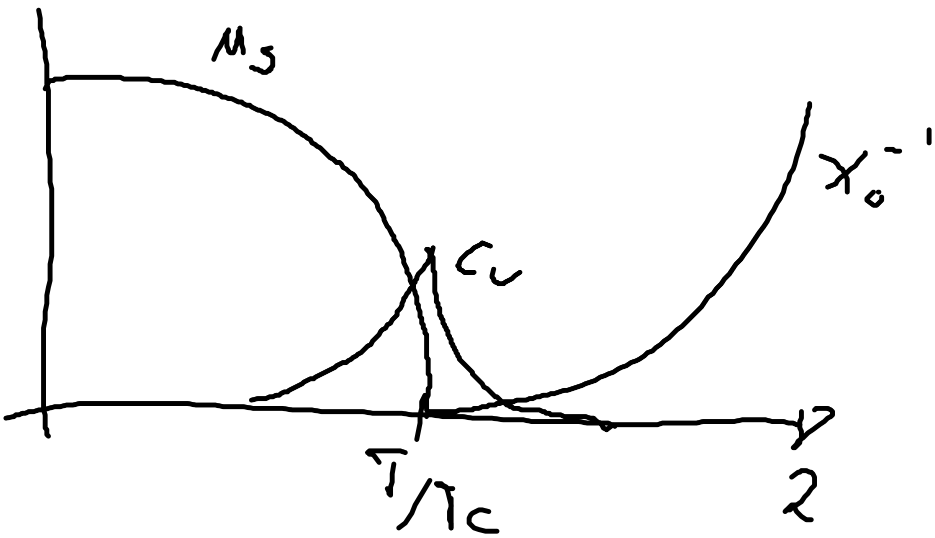
Magnetic order continued



$T < T_c$ $\quad$ M is finite at $T=0$

drops continuously $\to T_c$

$T \to T_c^-$ $\quad$ $M_S(T) \sim (T_c - T)^{1/3}$

$\frac{1}{3} = \beta$

$T \to T_c^+$ $\quad$ M has vanished

ferromagnetism has been lost

$\Rightarrow$ regular (linear response) definition can be used

$$\chi(T)\big|_{B=0} \sim (T-T_c)^{-\gamma} \qquad \gamma \approx \frac{4}{3}$$

$$C_V(T)\big|_{B=0} \sim (T-T_c)^{-\alpha} \qquad \alpha \approx 0.1$$

$\Rightarrow$ both diverge T_c
loss of long-range order

α, β, γ : critical exponents
- subject to a lot of statistical mechanics
- today: most accurate predictions from Quantum Monte Carlo simulations (but what to simulate?)

for $T \gg T_c$ behavior of system is more „normal"
i.e. paramagnetic

$$\chi(T) \sim (T-\Theta_c)^{-1}$$

„Curie-Weiss" law

Θ_c Curie-Weiss temp.

$\Theta_c \neq T_c$

	$\bar{m}_S\,[\mu_B]$	$m_{atom}\,[\mu_B]$	$T_c\,[K]$	$\Theta_c\,[K]$
Fe	2.2	6 (4)	1043	1100
Co	1.7	6 (3)	1394	1415
Ni	0.6	5 (2)	628	650

Eu	7.1	7	289	108
Gd	8.0	8	302	289
Dy	10.6	10	85	157

numbers in brackets are for quenched orb. momentum ($l=0 \Leftrightarrow J=S$)

- RE metals exhibit „atomic" magnetism
- TM not the case
  - ↳ no simple coupling between mag. moments
  - $\Rightarrow$ itinerant ferromagnetism

Ferromagnetism
- less well developed fundamental theory
  - ↳ mixing of single particle and many-body effects
  - strong collective effects and local coupling

mean-field theory
- without knowing anything about microscopic interaction we assume each spin feels an effective field:

$$\vec{H}_{eff} = \underbrace{\vec{H}}_{\text{external field}} + \underbrace{\lambda}_{\text{field constant}} \vec{M} \quad \leftarrow \text{effective internal field}$$

paramagnetic spins but all spins to be up

$$M_0(T) = \frac{g(J\,L\,S)\,\mu_B\,J}{V}\,B_J(\eta) \quad \eta \sim \frac{H}{T}$$

i.e.

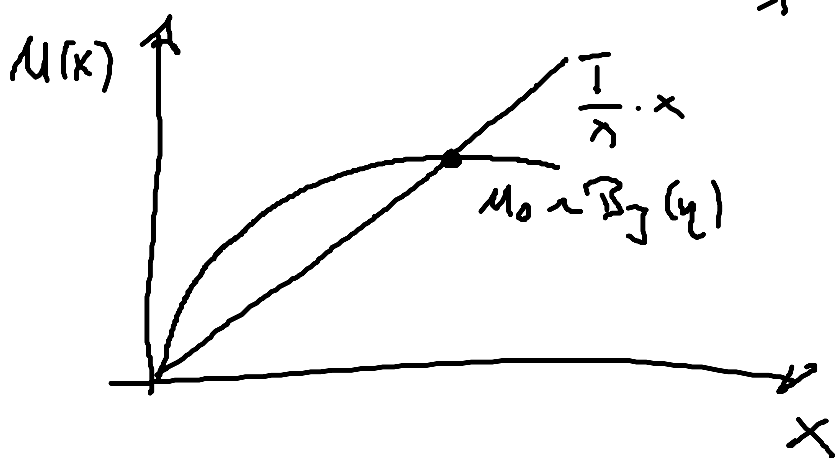
$$M(T) = M_0\left(\frac{H_{eff}}{T}\right) \xrightarrow{H\to 0} M_0\left(\frac{\lambda M}{T}\right)$$

Can such a solution exist?

attempt a graphical sol.

$$x = \frac{\lambda}{T} M(T) \quad \Rightarrow M(T) = M_0(x)$$

$$\to \frac{T}{\lambda} x = M_0(x)$$



ferromagn sol exists if $\underset{\text{slope}}{M_0'(0)} > \frac{T}{\lambda}$

condition for ferromag., but no microscopic insight into λ

Susceptibility: $M(T) = M_0\left(\frac{H_{eff}}{T}\right)$

$$\chi = \frac{\partial M}{\partial H} = \frac{\partial M_0}{\partial H_{eff}} \frac{\partial H_{eff}}{\partial H} = \frac{C}{T}\frac{\partial H_{eff}}{\partial H}$$

for paramag at $H = H_{eff}$ Curie's law $\chi_0 = \frac{C}{T}$

$$= \frac{C}{T}\frac{\partial}{\partial H}(H + \lambda M)$$

$$= \frac{C}{T}(1 + \lambda\chi)$$

$$\Rightarrow \quad \chi = \frac{C}{(T - \lambda C)} \sim (T - \Theta_c)^{-1}$$

Curie-Weiss law with $\Theta_c = \lambda C$

- CW law follows without microscopic model
- mean-field, i.e. spin in effective field

but
- $\Theta_c = T_c$ not observed experimentally
- $\gamma = 1$ and not $\gamma = \frac{4}{3}$ as in experiment

so we need better theory

nonetheless: order of magnitude estimate

$$C = \frac{N\mu_0\mu_B^2 g(JLS)^2 J(J+1)}{3k_B V} \approx J^2$$

$$\approx \left(\frac{N}{V}\right) \frac{\mu_0 m_{atom}^2}{3 k_B}$$

internal field is M_S at 0K

$$B^{int}(0K) = \mu_0 \underbrace{\lambda}_{\frac{\Theta_c}{C}} \underbrace{M_s(0K)}_{\frac{N}{V}\bar{m}_S} = \mu_0 \frac{\Theta_c}{C}\left(\frac{N}{V}\bar{m}_S\right)$$

$$\approx \frac{3 k_B \Theta_c \bar{m}_S}{m_{atom}^{3}}$$

with $m_{atom} \approx \bar{m}_S$

$$B^{int} \approx \frac{[5\,\Theta_c \text{ in K}]}{[m_{atom} \text{ in } \mu_B]} \text{ Tesla} \approx 10^3 \text{ Tesla !?!}$$

much larger than lab fields

$\Rightarrow$ magnetic interactions must be „strong"

temperature dep. of zero field mag.

$$M_S(T) = \frac{g(JLS)\mu_B J}{V} B_J(\eta)$$

$$= M(0K)\, B_J\left(\frac{g(JLS)\mu_0 \mu_B H_{eff}}{k_B T}\right)$$

(see Ashcroft)

$$M_S(T \to T_c^-) \sim (T_c - T)^{1/2}$$ at variance with exp $\beta = 1/3$

$$M_S(T \to 0) \sim e^{-\text{const}\, T}$$ and not $T^{3/2}$ (Bloch's law)

Heisenberg model

so far: mean field - no assumption on interaction (except large effective field λM) and paramagnetic spins

now: postulate the shape of an interaction

$$H_{ij}^{\text{coupling}} = -\frac{J_{ij}}{\mu_B^2} \vec{m}_i \vec{m}_j$$

$-\frac{J_{ij}}{\mu_B^2} m_i m_j$ FM parallel alignment

⋮ anything in between

$\frac{J_{ij}}{\mu_B^2} m_i m_j$ antiparallel alignment AFM

spins on a lattice

Heisenberg Hamiltonian

$$H^{\text{Heisenberg}} = \sum_{ij} H_{ij}^{\text{coupling}} = -\sum_{ij} \frac{J_{ij}}{\mu_B^2} \vec{m}_i \vec{m}_j$$

for this we need:

a) a lattice (real space is „gone")

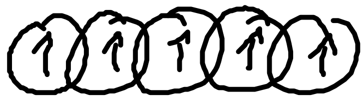
should be possible

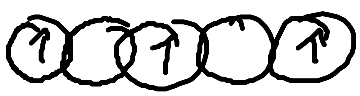
b) a model for the interaction (or at least values)

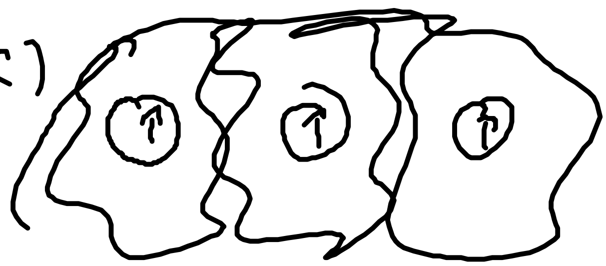
in practice : - model

: fit to experiment or DFT

possible coupling models :

a)  direct exchange between neighboring atoms

b)  super exchange, mediated by non-magnetic atoms

c)  indirect exchange, mediated by conduction electrons

solution strategies :

a) analytic : (in the past, but still today)

- full Heisenberg H has no analytic sol

↓

simplifications

- 1D, 2D

- restrict interactions, e.g. nearest-neighbors
  ↳ Ising model

$$H^{\text{Ising}} = - \underbrace{\sum_{ij}}_{\substack{\text{nearest}\\ \text{neighb.}}} \frac{J_{ij}}{\mu_B^2} \underbrace{\vec{m}_{i,z}\, \vec{m}_{j,z}}_{\pm 1 \text{ only}}$$

- approximations
  - mean-field
  - random-phase approx.
  - renormalization groups

  } wide field of statistical physics
  get restricted to inherent simplifications in Heisenberg Hamiltonian

b) numerically: mostly done with Monte Carlo

- obtain suitable J_{ij} parameters
- map out lattice
- randomize starting configuration
- choose spins: determine energy of new configuration E_{flip}

$\bar{E}_{flip} < 0$ accept

$\bar{E}_{flip} > 0$ accept randomly with probability $e^{-E_{flip}/k_B T}$

- repeat many times to get average energy $\bar{E}(T)$

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return to Ising model in magnetic field

$$H^{Ising} = -\sum_{\langle ij \rangle} J_{ij} \sigma_i \sigma_j - \sum_j h_j \sigma_j$$

$\langle ij \rangle$: only nn

h_j: magnetic field at site j

$$\sigma_i = \pm 1$$

even then:

- no analytic solution in 3D
- 2D: exact solution for $H=0$
  Lars Onsager 1944
- 1D exact sol:

further simplification: $J_{i,i+1} = J \quad h_i = h$

$$H = -J \sum_{i=1}^{N} \sigma_i \sigma_{i+1} - h \sum_{i=1}^{N} \sigma_i$$

periodic b.c. $\sigma_{N+1} = \sigma_1$

partition function

$$\frac{1}{k_B T}$$

$$Z(N,h,T) = \sum_{\sigma_1} \dots \sum_{\sigma_N} e^{\beta\left[J \sum_i \sigma_i \sigma_{i+1} + \frac{1}{2} \sum_i (\sigma_i + \sigma_{i+1})\right]}$$

define transfer matrix P:

$$\langle \sigma | P | \sigma' \rangle = e^{\beta\left[J\sigma\sigma' + \frac{h}{2}(\sigma + \sigma')\right]}$$

$$\langle 1 | P | 1 \rangle = e^{\beta[J+h]}$$

$$\langle -1 | P | -1 \rangle = e^{\beta[J-h]}$$

$$\langle -1 | P | 1 \rangle = \langle 1 | P | -1 \rangle = e^{-\beta J}$$

$$P = \begin{pmatrix} e^{\beta(J+h)} & e^{-\beta J} \\ e^{-\beta J} & e^{\beta(J-h)} \end{pmatrix}$$

$\Rightarrow$

$$Z = \sum_{\sigma_1} \dots \sum_{\sigma_N} \langle \sigma_1 | P | \sigma_2 \rangle \langle \sigma_2 | P | \sigma_3 \rangle \dots \langle \sigma_N | P | \sigma_1 \rangle$$

$$= \sum_{\sigma_1} \langle \sigma_1 | P^N | \sigma_1 \rangle = \mathrm{Tr}(P^N)$$

diagonalize P:

$$\lambda_\pm = e^{\beta J}\left[\cosh(\beta h) \pm \sqrt{\sinh^2(\beta h) + e^{-4\beta J}}\right.$$

$$\mathrm{Tr}(P^N) = \lambda_+^N + \lambda_-^N$$

thermodynamic limit $N \to \infty$ $\quad \lambda_+ > \lambda_-$ for any h

λ_+ will dominate over λ_-

$$\Rightarrow \quad Z(N,h,T) = \lambda_+^N$$

free energy per spin:

$$F(h,T) = -\frac{1}{\beta}\ln \lambda_+$$
$$= -J - \frac{1}{\beta}\ln\left[\cos(\beta h) + \sqrt{\sinh(\beta h) + e^{-4\beta J}}\right]$$

magnetization:

$$M = -\frac{\partial F}{\partial h} = \frac{\sinh(\beta h) + \dfrac{\sinh(\beta h)\cosh(\beta h)}{\sqrt{\sinh^2(\beta h) + e^{-4\beta J}}}}{\cosh(\beta h) + \sqrt{\sinh^2(\beta h) + e^{-4\beta J}}}$$