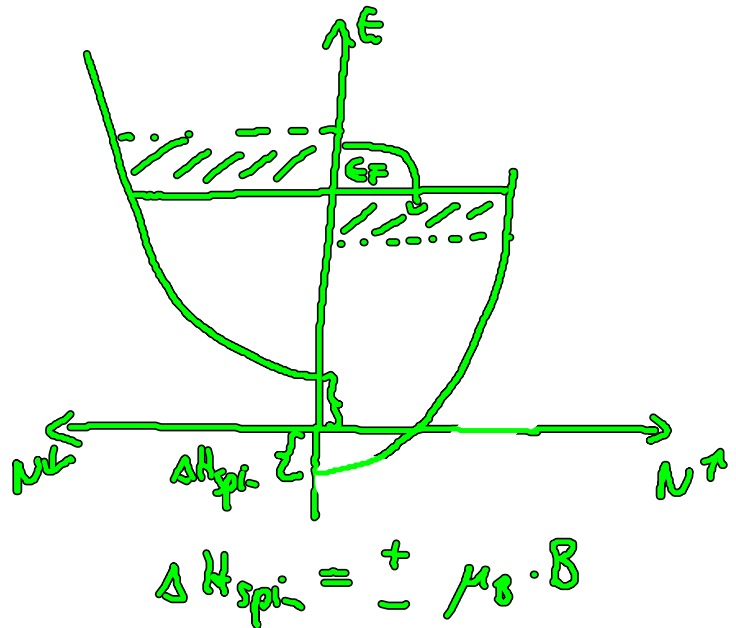
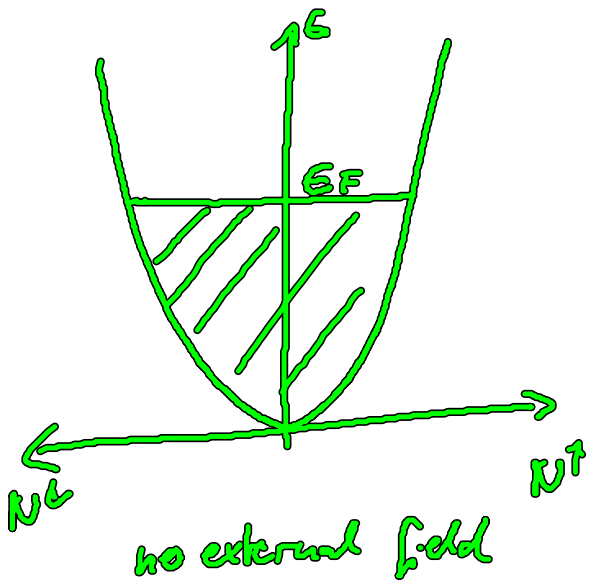


Recap: Atomic Magnetism

- $J \neq 0$: paramagnetism, $\chi \sim 10^{-2}$
most free atoms
- Larmor diamagnetism:
if closed shell \rightarrow only this survives
 $\chi \sim -10^{-6} - 10^{-4}$
- 2nd order: van Vleck \rightarrow quantitative agreement
also for $J=0$ atoms

Opposite case: Electron gas

Pauli part: response of electron spins



We know: Unpolarized e gas:

$$N(\epsilon) = \frac{1}{2\pi^2} \left(\frac{2m}{\hbar^2} \right)^{3/2} \sqrt{\epsilon}$$

$$\frac{N}{V} = \int d\epsilon N(\epsilon) \cdot f(\epsilon, T)$$

$$\rightarrow \epsilon_F = \frac{50.1 \text{ eV}}{\left(\frac{\hbar^2}{2m} \right)} \quad \text{at } T \approx 0$$

$$\rightarrow N(\epsilon_F) = \frac{1}{(20.7 \cdot \text{eV} \cdot \hbar^3)} \left(\frac{\hbar^2}{2m} \right)^{3/2}$$

Spin polarization: Response to external field B

$$N(\epsilon) \begin{cases} \rightarrow N^\uparrow(\epsilon) = \frac{1}{2} N(\epsilon - \mu_B \cdot B) \\ \rightarrow N^\downarrow(\epsilon) = \frac{1}{2} N(\epsilon + \mu_B \cdot B) \end{cases}$$

$$M = (N^\uparrow - N^\downarrow) \mu_B = N(\epsilon_F) \cdot \mu_B^2 \cdot B$$

NB: $\mu_B B \sim 10^{-9} \text{ eV}$

→ "missing" part in DOS near Fermi level
approximately rectangular: $N(\epsilon_F) \cdot \mu_B \cdot B$

$$\Rightarrow \chi_{\text{mag, Pauli}} = \mu_0 \mu_B^2 \cdot N(\epsilon_F) \sim 10^{-6} \cdot \left(\frac{2.57}{\frac{\hbar^2}{2m}} \right)$$

small

$$\chi_{\text{mag, Pauli}} \ll \chi_{\text{mag, atom}}$$

For completeness:

Diamagnetic response (Landau; "screening currents" due to equal momenta)

$$\chi_{\text{mag, Landau}} = -\frac{1}{3} \chi_{\text{mag, Pauli}}$$

also small

Atomic Magnetism in Solids

	Paramagnetism	Diamagnetism
Atoms	$\sim \frac{1}{7} 10^{-2}$	const. $\sim 10^{-4}$
e gas	$\sim 10^{-6}$	$\sim 10^{-6}$

Weak coupling: expect superposition

- Insulators ("simple" elements) noble gas solids
ionic solids (NaCl)
molecular solids (ice)
However: not TM ions
RE ions
→ essentially closed shell "atomic" entities
→ diamagnetic response

- RE/TM ionic materials (insulators)

Usually, not closed shell → paramagnets in simplest case

RE elements: f shells → atomic like magnetism is a good approximation

TM elements: d shells involved in bonding
"see" the crystal environment

→ "crystal field splitting"

Still, Curie's law → different effective μ_{eff} in solid

- Semiconductors → Covalent → "closed-shell" like
→ diamagnetism

• metals:
• Closed-shell like ion cores
• e gas

Simple metals (Na, Li, Al) = paramagnetic

BUT - that's not all.

Magnetic Order

TM, RE elements:

not just superposition of atom, electron gas cores!

Rather:
• Permanent magnetism
• Magnetic phase transitions
• ...

Reason: Correlation (Pauli → "exchange"
or "beyond")

Phenomenology

Textbook magnetic order: Based on a "discrete local moment" idea

- Ferromagnetism $\uparrow\uparrow\uparrow\uparrow\uparrow$ "spontaneous magnetization"
- Antiferromagnetism $\uparrow\downarrow\uparrow\downarrow\uparrow$
- Ferrimagnetism $\uparrow\downarrow\uparrow\downarrow$

• ... but that's not all!

e.g. Spin density wave in Cr:

$$\text{Periodicity: } \underline{Q} = (0, 0, 1 \pm \delta)$$

$$\delta \approx 0.05$$

and two magnetic transitions

$$T_N \sim 310 \text{ K}$$

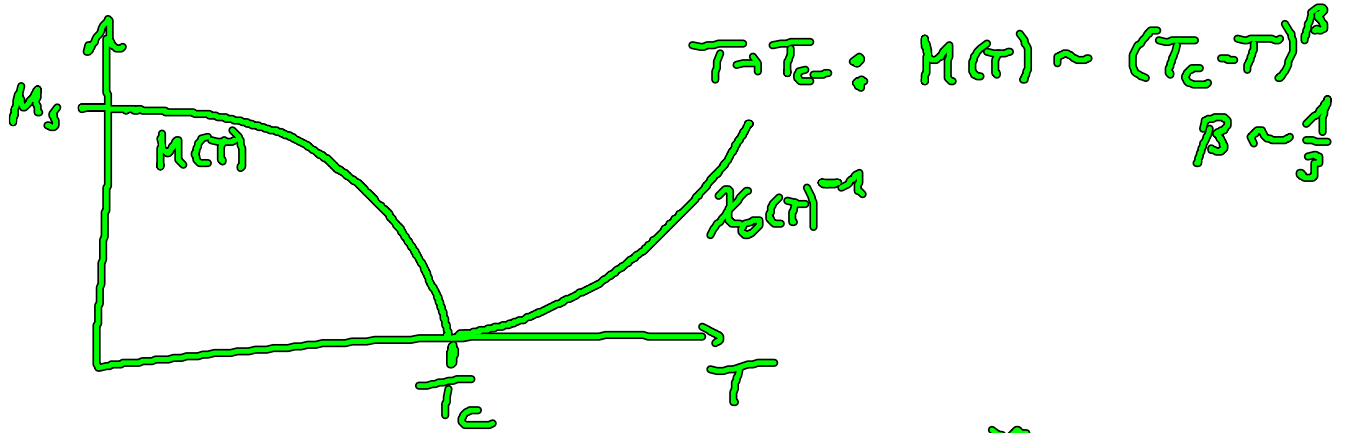
$$T_{SF} \sim 130 \text{ K}$$

Ferromagnetic ordering

Observation: FM materials show spontaneous, non-vanishing magnetization \underline{M} at $T \rightarrow 0 \text{ K}$

Without external stimulus \Leftrightarrow certainly not linear response

above T_c : \underline{M} vanishes



above $T_c: \chi_0(T) |_{B=0} \sim (T - T_c)^{-\gamma} \quad \gamma \sim \frac{4}{3}$

$C_v(T) |_{B=0} \sim (T - T_c)^{-\alpha} \quad \alpha \sim 0.1$

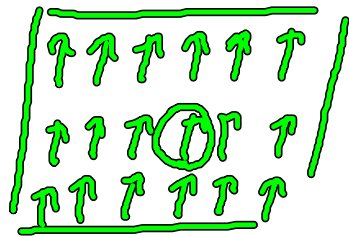
$T \rightarrow \infty: \chi_0(T) \sim (T - \Theta_c)^{-1}$ "Curie-Weiss law"

NB: $\Theta_c \neq T_c$

Phenomenological theories

Mean-Field theory: Curie-Weiss

Without knowing anything about the microscopic magnetic interaction, assume that there are "DLH"s that each feel an effective field



$$\underline{H}_{\text{eff}} = \underbrace{\underline{H}}_{\text{external}} + \lambda \underbrace{\underline{M}}_{\text{"molecular field"} \sim \underline{M}}$$

Paramagnetic spin in this field:

$$M_0(T) = \frac{g(JLS) \mu_B \cdot J}{V} B_J(\eta)$$

$$\eta \sim \frac{H}{T}$$

Last Lecture!

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

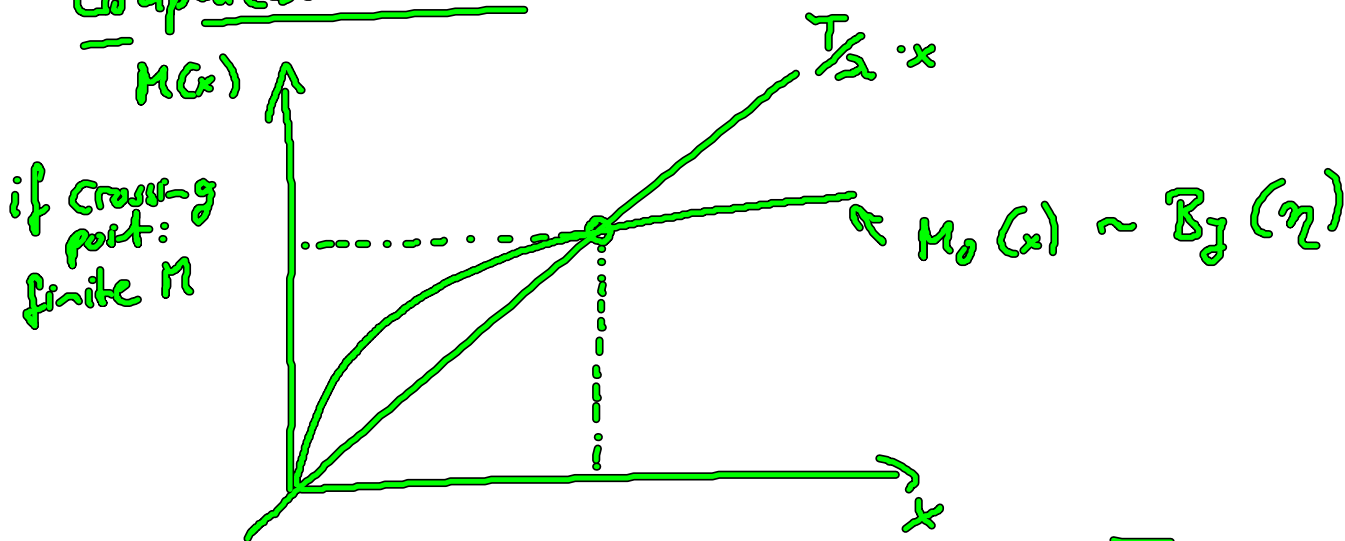
How can this be?

$$\text{set } x = \frac{\lambda}{T} \cdot M \rightarrow$$

$$\textcircled{1} M(T) = M_0(x)$$

$$\textcircled{2} M(T) = \frac{T}{\lambda} \cdot x$$

Graphical solution:



FM solution $M \neq 0$ if slope $\frac{T}{\lambda} < M_0'(0)$

qualitatively $\rightarrow T_c$ exists!

Mean-field susceptibility above T_c :

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

$$\Rightarrow \chi = \frac{\partial M}{\partial H} = \frac{\partial M_0}{\partial H_{\text{eff}}} \cdot \frac{\partial H_{\text{eff}}}{\partial H}$$

$$\rightarrow \frac{\partial M_0}{\partial H_{\text{eff}}} \equiv \chi_0 \text{ for paramagnet at } H = H_{\text{eff}}$$

Curie's law! $\chi_0 = \frac{C}{T}$

$$\frac{\partial H_{\text{eff}}}{\partial H} = \frac{\partial}{\partial H} (H + \lambda M) = \frac{\partial}{\partial H} (H + \lambda \chi H) = (1 + \lambda \chi)$$

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

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

$$\Theta_c = \lambda \cdot C$$

Curie - Weiss

However: Mean field says $\Theta_c = T_c$ incorrect
 $\gamma = 1$ incorrect.

M in solid: Estimate.

$$\text{Recall: } C = \frac{N}{V} \frac{\mu_0 \mu_B^2 g^2 (J \text{ (eV)})^2 J \cdot (g \mu)}{3 k_B}$$

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

$$\mu_{\text{atom}} = \mu_B \cdot g (J \text{ (eV)}) \cdot J$$

• "Molecular field" $\propto M(T=0)$

$$\rightarrow B_{\text{mol}} = \mu_0 \lambda M(0\text{K}) = \mu_0 \frac{Q}{c} \left(\frac{N}{V} \bar{m}_s \right)$$

$$= \frac{3k_B Q_c \bar{m}_s}{4\pi a^3}$$

effective
moment in
solid

$$\sim \frac{(5 T_c \text{ in K})}{\left(\frac{\text{nm}^3}{\mu_B} \right)} \text{ in Tesla!}$$

$$B_{\text{mol}} \sim 10^3 \text{ T} \quad \text{HUGE}$$

• Decay of $M(T)$ as $T \rightarrow 0 \rightarrow T = T_c$

can show that $M(T \rightarrow T_c^-) \sim (T_c - T)^{1/2}$

(e.g. Ashcroft

at variance with $\gamma \sim \frac{1}{3}$!

Heisenberg model

So far: mean field \equiv required no microscopic understanding of interactions between spins.

Better picture: assume fixed, discrete local moments \underline{m}_i on lattice sites i

Interaction: $H_{ij} = -\frac{J_{ij}}{\mu_B^2} \underline{m}_i \cdot \underline{m}_j$

$$\Rightarrow H^{\text{Heisenberg}} = - \sum_{i,j}^{M,M} \frac{J_{ij}}{\mu_B^2} \underline{m}_i \cdot \underline{m}_j$$

Heisenberg Hamiltonian

NB1: This is an approximation:
 We have postulated that something can be treated as discrete local moments - no band structure?

NB2: No physical motivation yet for J_{ij}
 but in principle: FM, AFM, spin waves ...
 all possible!

NB3: pair-only approximation.
 Not necessary!

Can show that a generalized Heisenberg Hamiltonian can always be found that describes every spin configuration of a real system - as long as we can find meaningful local moments!

\Rightarrow in principle, an exact spin Hamiltonian could be found!

In practice:

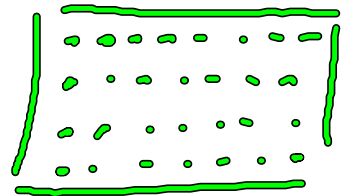
- J_{ij} are often fitted to experiment
- J_{ij} can be fitted to / extracted from electronic structure theory.

Solution strategies

① Numerical (today): e.g. Monte Carlo method

- obtain suitable J_{ij}

- map out lattice sites in e.g. periodic square



- Random or (sometimes) ordered starting configuration

- Choose spin j randomly

if $E(\text{flip}, j) < 0$

accept flip

$E(\text{flip}, j) > 0$

accept with probability $e^{-\frac{E_{\text{flip}}}{kT}}$

repeat N times to get

averages $\bar{E}(kT)$, fluctuations, C_V, \dots

Metropolis algorithm

② Analytical limits:

- mean-field theory (ohh!)

- "random-phase approximation" (in reciprocal space)

- Kohnshilber's group theory

- ...

③ Further simplification: Ising Model

• replace $\underline{m}_i \cdot \underline{m}_j \rightarrow \underbrace{\hat{m}_{i,z} \cdot \hat{m}_{j,z}}_{\pm 1}$

→ useful in many contexts

1D: NN: solve exactly but no phase transition

2D: NN: can solve exactly but difficult

3D: no analytical solution

Heisenberg: Some limits

① Low temperature excitations.

naively: $\uparrow \uparrow \uparrow \downarrow \uparrow \uparrow \uparrow$
flip 1 spin?

However $\uparrow \uparrow \rightarrow \rightarrow \rightarrow \downarrow \downarrow \downarrow \downarrow \dots$ long-wavelength
spin wave
"magnon".