Recap: Atomic Magnetism

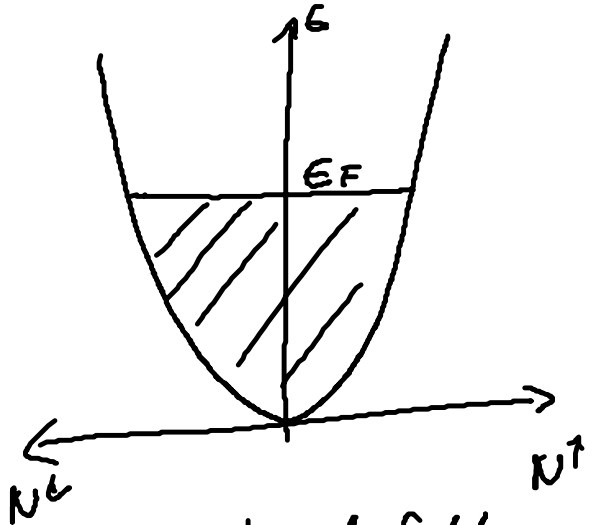
- $J \neq 0$: paramagnetism, $\chi \sim 10^{-2}$
  most free atoms

- Larmor diamagnetism:
  if closed shell → only this survives
  $\chi \sim -10^{-6} - -10^{-4}$

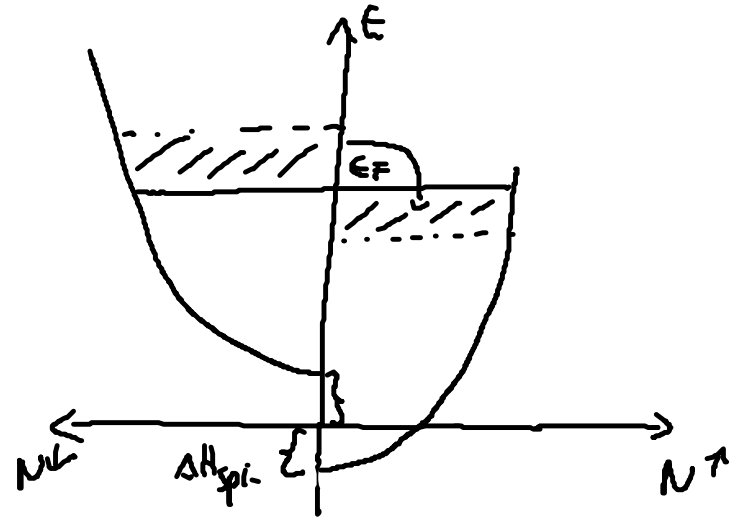
- 2nd order: van Vleck → quantitative agreement
  also for $J=0$ atom

Opposite case: Electron gas

Pauli part: response of electron spins



no external field



$\Delta H_{spin} = \pm \mu_B \cdot B$

We know: Unpolarized e gas:

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

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

$$\rightarrow \epsilon_F = \frac{50.1\,eV}{\left(\frac{r_s}{a_0}\right)} \quad \text{at } T \approx 0$$

$$\rightarrow N(\epsilon_F) = \frac{1}{(20.7\cdot eV\cdot \text{Å}^3)}\left(\frac{r_s}{a_0}\right)^{-1}$$

Spin polarization: Response to external field B

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

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

NB: $\mu_B B \sim 10^{-4}\,eV$

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

$$\Rightarrow \chi^{\text{magn, Pauli}} = \mu_0\mu_B^2\cdot N(\epsilon_F) \sim 10^{-6}\cdot\left(\frac{2.5}{\frac{r_s}{a_B}}\right)$$

small

$$\chi^{\text{magn, Pauli}} \ll \chi^{\text{magn, atom}}$$

For completeness:

Diamagnetic response (Landau; "screening currents" due to cyclar momentum)

$$\chi^{mag,\,Landau} = -\frac{1}{3}\chi^{mag,\,Pauli}$$

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 moment in solid

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

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

Simple metals (Na, Li, Al): paramagnetism

BUT - that's not all.

Magnetic Order

TM, RE elements:

not just superposition of atom, electron gas cases!

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

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

Phenomenology

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

- Ferromagnetism ↑↑↑↑↑ "spontaneous magnetization"
- Antiferromagnetism ↑↓↑↓↑
- Ferrimagnetism ↑↓↑↓↑

- ... but that's not all !

e.g. Spin density wave in Cr:

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

$\delta \approx 0.05$

and two magnetic transitions

$T_N \sim 310\,K$

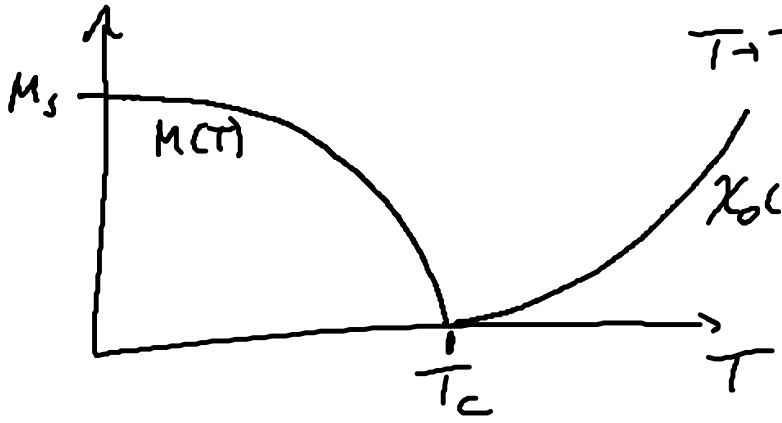
$T_{SF} \sim 130\,K$

Ferromagnetic ordering

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

Without external stimulus $\Leftrightarrow$ certainly not linear response

above T_c: $\underline{M}$ vanishes



$T \to T_c$: $M(T) \sim (T_c - T)^{\beta}$ $\quad \beta \sim \frac{1}{3}$

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

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

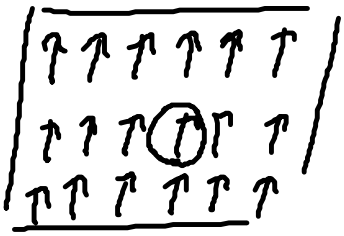
$T \to \infty$: $\chi_0(T) \sim (T - \Theta_c)^{-1}$ "Curie-Weiss law"

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 "DOM"s that each feel an effective field



$$\underline{H}_{eff} = \underline{H} + \lambda \underline{M}$$

$\underline{H}$ ↓ external

$\lambda \underline{M}$ ↘ "molecular field" $\sim \underline{M}$

Paramagnetic spin in this field:

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

$$\eta \sim \frac{H}{T}$$ Last Lecture!

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

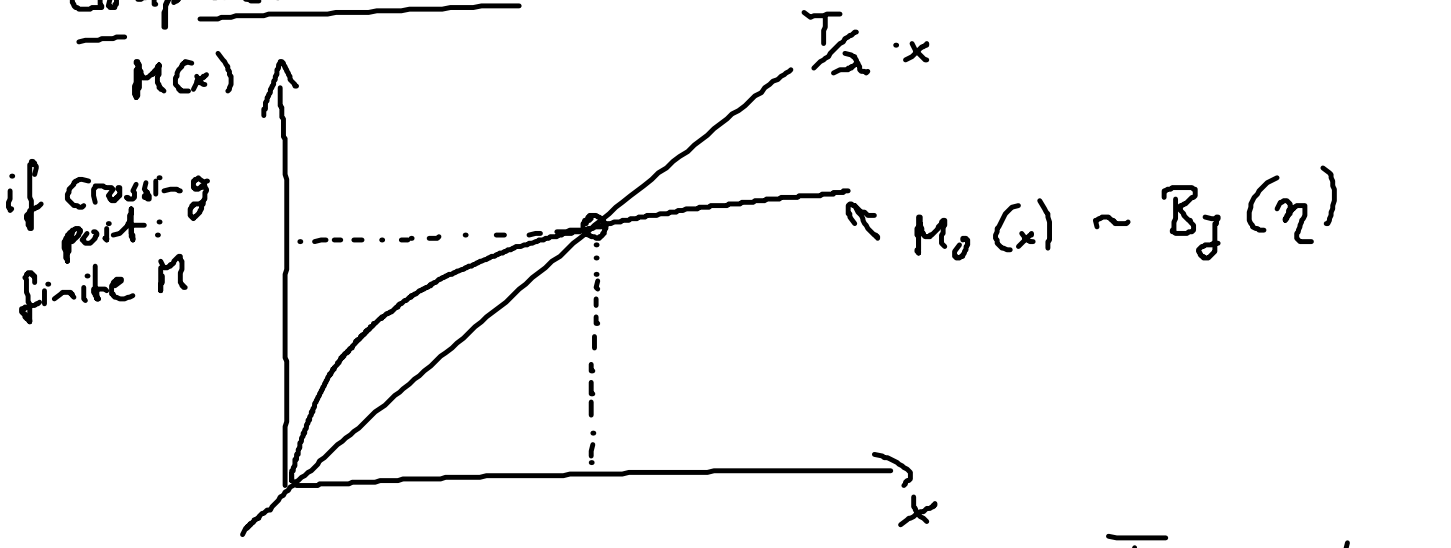
How can this be?

set $x = \frac{\lambda}{T}\cdot M$ →

① $M(T) = M_0(x)$

② $M(T) = \frac{T}{\lambda}\cdot x$

Graphical solution:



if crossing point: finite M

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

qualitatively → T_c exists!

Mean-field susceptibility above T_c:

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

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

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

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

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

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

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

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

Curie – Weiss

However: Mean field says $\Theta_c = T_c$ incorrect

$\gamma = 1$ incorrect.

M in solid: Estimate.

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

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

$$m_{atom} = \mu_B \cdot g(J(S)) \cdot J$$

- "Molecular field" $\lambda M(T=0)$

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

$\bar{m}_s$: effective moment in solid

$$= \frac{3 k_B \Theta_c \bar{m}_s}{(\text{mol})^2}$$

$$\sim \frac{(5 \cdot T_c \text{ in K})}{\left(\frac{\text{mol}}{\mu_B}\right)} \text{ in Tesla!}$$

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

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

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 ≡ required no microscopic understanding of interaction 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!

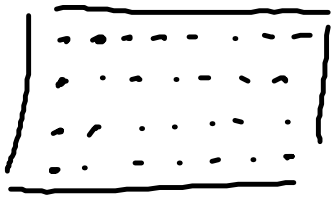
In practice: • J_{ij} are often fitted to experiment

- 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 supercell



- Random or (somehow) ordered starting configuration
- Choose spin j randomly

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

$E(\text{flip}, j) > 0$ accept with probability $e^{-\frac{E_{\text{spin}}}{kT}}$

repeat N times to get averages $\overline{E}(kT)$, fluctuations, C_V, ...

Metropolis algorithm

② Analytical limits:

- mean-field theory (ehrh!)
- "random-phase approximation" (in reciprocal space)

- renormalization 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 : ↑↑↑↓↑↑↑ flip 1 spin ?

However ↑↗→↘↓ ... long-wavelength spin wave "magnon".