Lecture 26 | Magnetism in metals, Stoner instability

Magnetism for localized spins

Interaction of the localized moments is described by the Heisenberg Hamiltonian

$$\mathcal{H} = \underbrace{-\sum_{ij} J_{ij}\vec{S}_i\vec{S}_j}_{\text{Exchange interaction}} \underbrace{-2\mu_B\sum_i S_i\vec{B}}_{\text{Zeeman term}}$$

Positive J_{ij} favors parallel spin configuration (ferromagnet), negative J_{ij} favors anti parallel orientation (antiferromagnet)

If spins do not interact ($J_{ij}=0$) we can easily calculate the average spin in the presence of the magnetic field B

$$\langle S\rangle = \frac{\sum_s s\, e^{-\frac{H}{T}}}{\sum e^{-\frac{H}{T}}} = \frac{1}{2}\,\frac{\left(e^{\frac{\mu_B B}{T}} - e^{-\frac{\mu_B B}{T}}\right)}{e^{\frac{\mu_B B}{T}} + e^{\frac{\mu_B B}{T}}} \Rightarrow$$

$$\langle S\rangle = \frac{1}{2}\tanh\left(\frac{\mu_B B}{T}\right)$$

Magnetization is $2\mu_B S$

$$M = 2\mu_B \langle S \rangle = \mu_B \tanh\left(\frac{\mu_B B}{T}\right)$$

For small fields $B \to 0$ we have

$$M = \chi B \quad \text{with } \chi = \frac{\mu_B^2}{T} \quad \text{(Curie law)}$$

Let us return back to the interacting spin. We will use the mean field approximation where we assume that spins values are close to their average value (P. Weiss)

$$\vec{S}_i = \langle \vec{S} \rangle + \underbrace{\vec{S}_i - \langle \vec{S} \rangle}_{\delta \vec{S}_i \ll \langle S \rangle}$$

Then $\vec{S}_i \cdot \vec{S}_j = \langle \vec{S} \rangle^2 + \langle \vec{S} \rangle \delta \vec{S}_i + \langle \vec{S} \rangle \delta \vec{S}_j + \cancel{\delta \vec{S}_i \delta \vec{S}_j}$

Keeping only linear in δs terms we obtain

$$\vec{S}_i \cdot \vec{S}_j = \langle S \rangle^2 + \langle \vec{S} \rangle (\vec{S}_i - \langle \vec{S} \rangle) + \langle \vec{S} \rangle (\vec{S}_j - \langle \vec{S} \rangle) =$$

$$= \langle S \rangle (\vec{S}_i + \vec{S}_j) - \langle \vec{S} \rangle^2$$

Then the interaction term can be written as

$$-\sum_{ij} J_{ij} S_i S_j = -\langle S\rangle \sum_{ij} J_{ij}(S_i + S_j) + \langle S\rangle^2 \sum_{ij} J_{ij}$$

Introducing $J = \sum_i J_{ij} = \sum_j J_{ij}$

we obtain

z is the coordination number

$$H = -\sum_i 2J\langle S\rangle S_i + NJ\frac{z}{2}\langle S\rangle^2 - 2\mu_B \sum_i S_i B$$

The first term has the same form as the last (magnetic field) term, adding the <u>exchange field</u> $\frac{J\langle S\rangle}{\mu_B}$ to B

Then for the average spin is

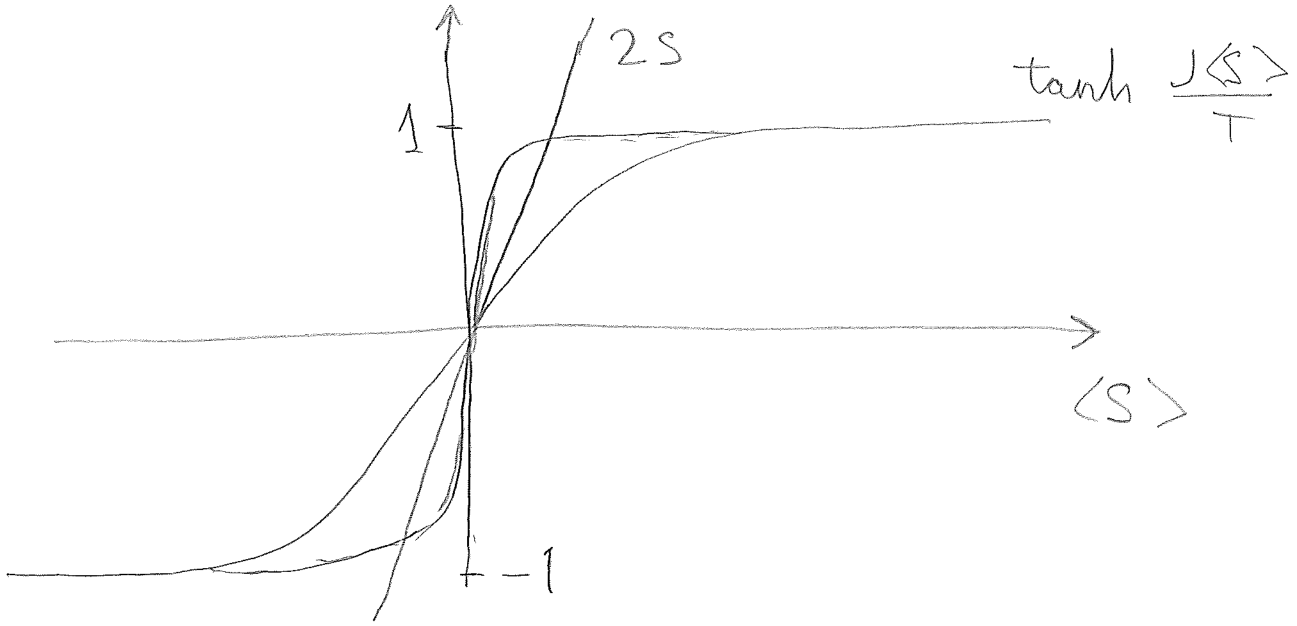
$$\langle S\rangle = \frac{1}{2}\tanh\left(\frac{J\langle S\rangle + \mu_B B}{T}\right)$$

This is the self consistent <u>mean field</u> equation for $\langle S\rangle$

In zero field we should solve

$$\langle S \rangle = \frac{1}{2} \tanh\left(\frac{J\langle S \rangle}{T}\right)$$

We can solve this equation graphically



Nonzero $\langle S \rangle$ appears for $T > T_c = \frac{J}{2}$

This temperature is the Curie temperature.

Below it material is ferramagnetic.

Close to T_c expanding $\tanh x = x - \frac{x^3}{3}$ e.t.c.

we obtain $\langle S \rangle = \frac{T_c}{T}\langle S \rangle - 4\left(\frac{T_c \langle S \rangle}{T}\right)^3 \Rightarrow$

$\langle S \rangle \propto (T_c - T)^{1/2}$

slightly above T_c in the field

$$\langle S \rangle = \frac{T_c}{T} + \frac{\mu_B B}{2T} \Rightarrow \langle S \rangle = \frac{\mu_B B}{2(T - T_c)}$$ Curie Weis law

Band ferromagnetism

Elemental magnetic metals are Fe, Co, Ni. They belong to the 3d transition metals. The 3d orbitals are rather bound to the nuclei. Mobility is reduced which favors interaction. As we found in the Lecture 17 about the Fermi liquid, interaction enhances the susceptibility

$$\chi = \frac{\mu_B^2 \, N(\varepsilon_F)}{1 + \langle Z(\theta) \rangle}$$

when $\langle Z(\theta) \rangle$ approaches -1 the susceptibility diverges. Consider the model for conduction electrons with a repulsive contact interaction

$$H = \sum_{k,s} \varepsilon_k \, c^+_{ks} c_{ks} + U \int d^3r \, d^3r' \, \hat{\rho}_\uparrow(r) \, \delta(r-r') \, \hat{\rho}_\downarrow(r')$$

Here $\rho_\uparrow(r) = c^+_{r\uparrow} c_{r\uparrow}$

The contact interaction is an approximation of the screened Coulomb interaction. Because of the Pauli principle this interaction is active between electrons with the opposite spins. That's why we have $\hat{\rho}_\uparrow(r)\,\hat{\rho}_\downarrow(r)$. Using the mean field approximation we rewrite

$$\hat{\rho}_s = n_s + (\hat{\rho}_s(r) - n_s)$$

with $n_s = \langle \hat{\rho}_s(r) \rangle$

Substituting it and dropping $\delta\rho^2$ terms we obtain similarly to the case of localised spins

$$H = \sum_{k,s} \varepsilon_k c^+_{ks} c_{ks} + U \int d^3r \left[\hat{\rho}_\uparrow(r) n_\downarrow + \hat{\rho}_\downarrow(r) n_\uparrow - n_\uparrow n_\downarrow \right]$$

$$= \sum (\varepsilon_k + U n_{-s}) c^+_{ks} c_{ks} - U V n_\uparrow n_\downarrow$$

This mean field Hamiltonian describes electrons that move in the uniform background of electrons of opposite spins

Then

$$n_{\uparrow} = \frac{1}{V} \sum_{k} c^{+}_{k\uparrow} c_{k\uparrow} = \frac{1}{V} \sum_{k} f(\varepsilon_k + U n_{\downarrow}) =$$

$$= \int d\varepsilon \, \frac{1}{V} \sum_{k} \delta(\varepsilon - \varepsilon_k - U n_{\downarrow}) \, f(\varepsilon) =$$

$$= \int d\varepsilon \, \frac{1}{2} N(\varepsilon - U n_{\downarrow}) \, f(\varepsilon)$$

And the similar result for $n_{\downarrow}$

The total number of electrons

$$n_0 = \frac{n_{\uparrow} + n_{\downarrow}}{2} = \frac{1}{2} \int d\varepsilon \left[N(\varepsilon - U n_{\downarrow}) + N(\varepsilon - U n_{\uparrow}) \right] f(\varepsilon)$$

and the difference $m = n_{\uparrow} - n_{\downarrow}$

$$n_{\uparrow} - n_{\downarrow} = \frac{1}{2} \int d\varepsilon \left[N(\varepsilon - U n_{\downarrow}) - N(\varepsilon - U n_{\uparrow}) \right] f(\varepsilon)$$

These equations can be rewritten as

$$n_0 = \frac{1}{2} \sum_{s} \int d\varepsilon \, N\left(\varepsilon - \frac{U n_0}{2} - s \frac{U m}{2}\right) f(\varepsilon)$$

$$m = \frac{1}{2} \sum_{s} s \int d\varepsilon \, N\left(\varepsilon - \frac{U n_0}{2} - s \frac{U m}{2}\right) f(\varepsilon)$$

In general case this system of equations should be solved numerically

Experimentaly T_c for iron is $1043K \ll \mathcal{E}_F \simeq 1eV$

This means that $m \ll n_0$ which allows for a simplification. Let us write magnetization in a field

$$m = \frac{1}{V}\int \Big[f\,(\mathcal{E}_k + U n_\downarrow - \mu_B B) - f\,(\mathcal{E}_k + U n_\uparrow + \mu_B B)\Big]\, d\mathcal{E}$$

Without the Un terms these are integrals that we calculated for the Pauli susceptibility. Expanding we obtain for $T, B \to 0$

$$m = N(\mathcal{E}_F)\left[\mu_B B + U\frac{(n_\uparrow - n_\downarrow)}{2}\right]$$

$$m = N(\mathcal{E}_F)\,\mu_B B + m\,\frac{N(\mathcal{E}_F)\,U}{2} \Rightarrow$$

$$m = \frac{N(\mathcal{E}_F)\,\mu_B B}{1 - \frac{N(\mathcal{E}_F)\,U}{2}}$$

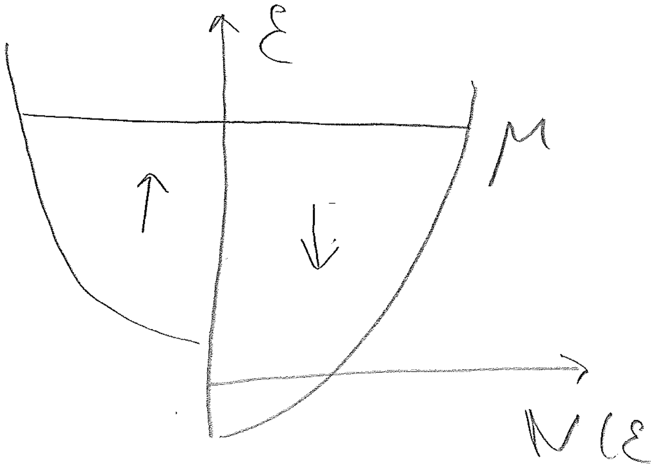
and susceptibility

$$\chi = \frac{\mu_B^2\, N(\mathcal{E}_F)}{1 - \frac{1}{2} U N(\mathcal{E}_F)}$$

Zero temperature susceptibility diverges at $\frac{U N(\varepsilon_F)}{2} = 1$. (Stoner criterion)

For $\frac{U N(\varepsilon_F)}{2} > 1$ we have transition to the ferromagnetic state.

We can find transition temperature calculating the magnetization in zero field



Result is (see e.g. M. Sigrist lectures)

$$T_c \propto \sqrt{U - U_c}\,, \quad U_c = \frac{2}{N(\varepsilon_F)}$$

Not surprisingly below T_c

$$m(T) \propto \sqrt{T_c - T}.$$

The Landau theory of ferromagnetic transition

L. D. Landau suggested that one can describe magnetic transition (as well as many others) from a very simple point of view.

Close to the transition point we can expand the free energy in the powers of magnetisation

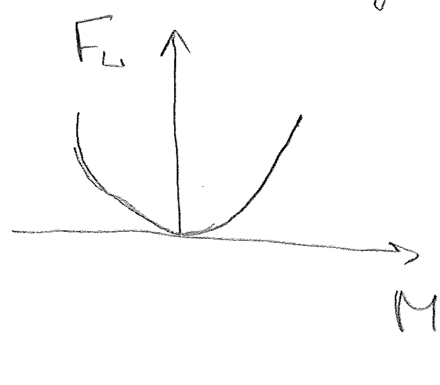
$$F_L(M) = \sum_n a_n \vec{M}^n \quad \text{(homogeneous case)}$$

Since $\vec{M}$ and $-\vec{M}$ have the same energy the free energy should contain only even powers of $\vec{M}$

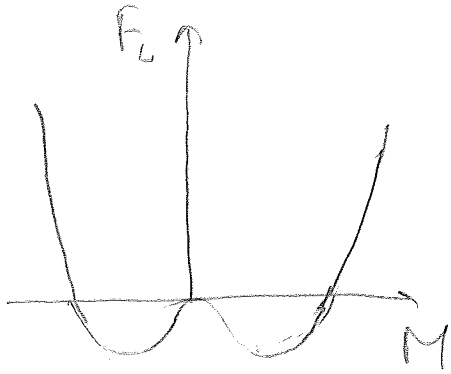
$$F_L = a_0 + a_2(T)\vec{M}^2 + a_4 \vec{M}^4 + \dots$$

If $a_2(T) > 0$ then the minimum of F_L corresponds to $\vec{M} = 0$ and we have paramagnet

This is the situation above T_c



If $a_2 < 0$, $a_4 > 0$ then



$\vec{M} \neq 0$ – ferromagnet

It is naturally to assume the regular behavior of $a_2(T)$ around T_c

$$a_2(T) = a_2' \frac{T - T_c}{T_c} = at \;, \quad a = a_2' \;, \; t = \frac{T - T_c}{T_c}$$

Then we get the free energy

$$F_L = at\, \vec{M}^2 + \frac{b\, \vec{M}^4}{2} - \vec{B} \cdot \vec{M}$$

external field

Minimizing it we obtain

$$2(at\, M + b\, M^3) = B$$

For $B = 0$ we have $M = \left(-\frac{at}{b}\right)^{1/2} \propto \sqrt{T_c - T}$

as we obtained by doind the mean field calculation:

Magnetic susceptibility

$$\chi_T(B) = \frac{\partial M(B)}{\partial B} = \frac{1}{2at + 3b\, M^2(B)} = \begin{cases} \frac{1}{2at}, & t>0 \\ -\frac{1}{4at}, & t<0 \end{cases}$$

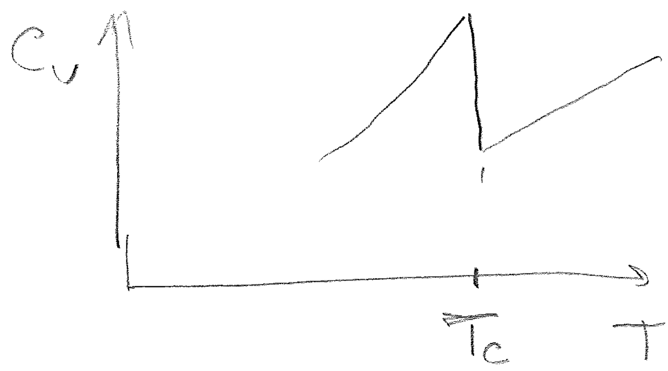
$\longrightarrow$ Curie-Weiss law.

Below T_c the free energy $F = -\frac{a^2 t^2}{2b}$

and the specific heat

$$C_V = -T \frac{\partial^2 F}{\partial T^2} = \frac{a^2}{b T_c} \Rightarrow$$

there is a jump in the heat capacity



Landau theory provides the general framework to describe second order phase transitions.