Lecture 28

Continue mean-field theory of the Heisenberg model.

The mean-field Hamiltonian of a Heisenberg ferromagnet has the following form:

$$\mathcal{H} = -g\mu_B \left(\vec{B} + \vec{B}_M\right) \cdot \sum_i \vec{S}_i$$

$\vec{B}_M$ – "molecular field"; $\vec{B}_M = \frac{Jz}{g\mu_B} \langle \vec{S} \rangle$.

$\vec{B}_M$ needs to be determined self-consistently.

Assume the external field $\vec{B}$ is in the z-direction:

$\vec{B} = B\hat{z}$. Then the spins will also align in the z-direction since $\vec{B}$ is the only thing in the Hamiltonian that chooses a particular direction. The spin-spin interaction part of the Hamiltonian is rotationally invariant.

Then we have:

$$\mathcal{H} = -g\mu_B \left(B + B_M\right) \sum_i S_i^z$$

Given this $\mathcal{H}$, we can calculate $\langle S_i^z \rangle$.

We will assume $S = \frac{1}{2}$ for simplicity.

$$\langle S^z \rangle = \frac{\sum_{S^z = \pm\frac{1}{2}} e^{\frac{g\mu_B (B+B_M) S^z}{k_B T}} S^z}{\sum_{S^z = \pm\frac{1}{2}} e^{\frac{g\mu_B (B+B_M) S^z}{k_B T}}} =$$

$$= \frac{1}{2} \frac{e^{\frac{g\mu_B(B+B_M)}{2k_BT}} - e^{-\frac{g\mu_B(B+B_M)}{2k_BT}}}{e^{\frac{g\mu_B(B+B_M)}{2k_BT}} + e^{-\frac{g\mu_B(B+B_M)}{2k_BT}}} =$$

$$= \frac{1}{2} \tanh\left(\frac{g\mu_B(B+B_M)}{2k_BT}\right)$$

On the other hand:

$$B_M = \frac{Jz}{g\mu_B}\langle S^z\rangle$$

Thus we obtain a nonlinear equation for B_M:

$$B_M = \frac{Jz}{2g\mu_B}\tanh\left(\frac{g\mu_B(B+B_M)}{2k_BT}\right)$$

Usually this equation is written not in terms of B_M, but in terms of the macroscopic magnetization per spin M:

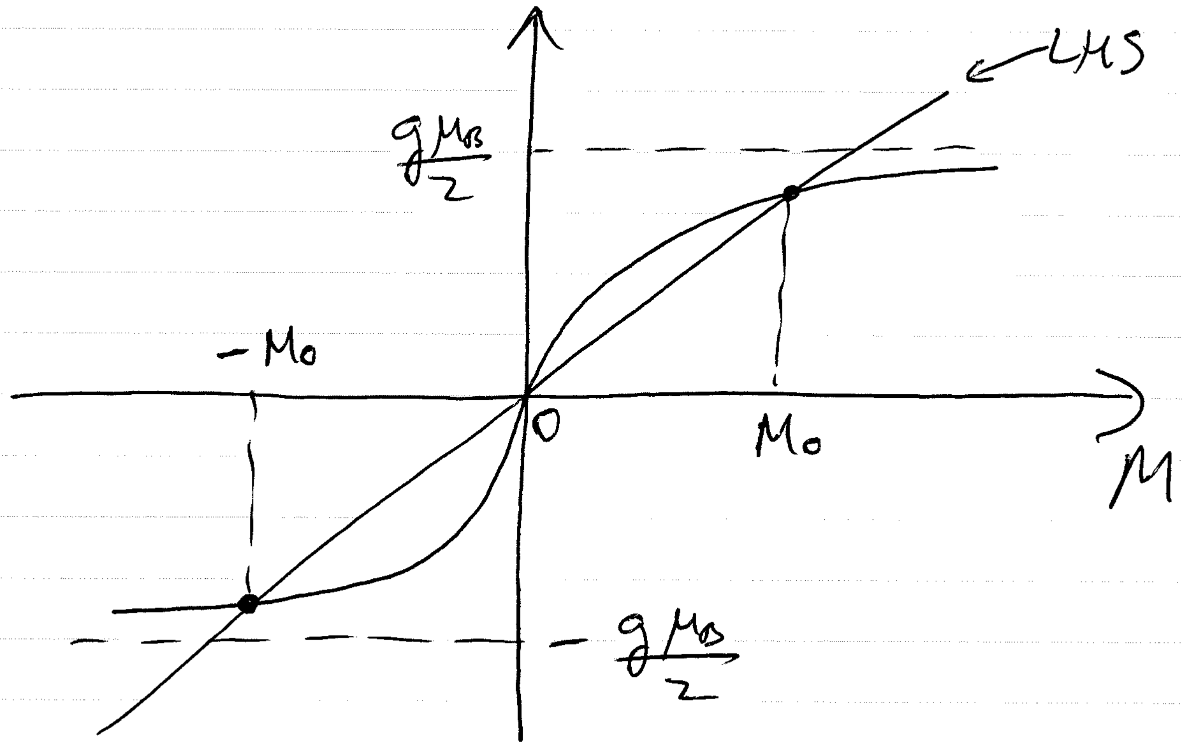
$$M = g\mu_B \frac{1}{N}\sum_i \langle S_i^z\rangle = g\mu_B\langle S^z\rangle.$$

Then we obtain:

$$M = \frac{g\mu_B}{2}\tanh\left(\frac{g\mu_B B + \frac{Jz}{g\mu_B}M}{2k_BT}\right)$$

Analyze this equation at zero external field, $B=0$.

$$M = \frac{g\mu_B}{2} \tanh\left(\frac{JzM}{2g\mu_B k_B T}\right)$$



The slope of the RHS at $M=0$ changes as a function of T: it increases with decreasing T. Thus at low enough T a solution with nonzero M exists.

To determine the critical temperature T_c at which a nontrivial solution appears, expand tanh at small M:

$$\tanh\left(\frac{JzM}{2g\mu_B k_B T}\right) \approx \frac{JzM}{2g\mu_B k_B T}$$

Thus $M = \dfrac{Jz}{4k_B T_c} M \Rightarrow T_c = \dfrac{Jz}{4k_B}$ - Curie temperature.

$$k_B T_c \sim J \sim \frac{e^2}{r} \sim 1\,eV \sim 10^4\,K$$

Real T_c's in magnetic metals are $\sim 10^3$ K.

MFT overestimates T_c because it neglects fluctuations.

We can calculate $M(T)$ analytically in two limits:

$T \to T_c$ and $T \to 0$.

Near T_c we expect M to be small $\Rightarrow$ can expand tanh in Taylor series:

$\tanh x \approx x - \frac{x^3}{3}$.

Then we obtain:

$$M \approx \frac{g\mu_B}{2}\left[\frac{JzM}{2g\mu_B k_B T} - \frac{1}{3}\left(\frac{JzM}{2g\mu_B k_B T}\right)^3\right]$$

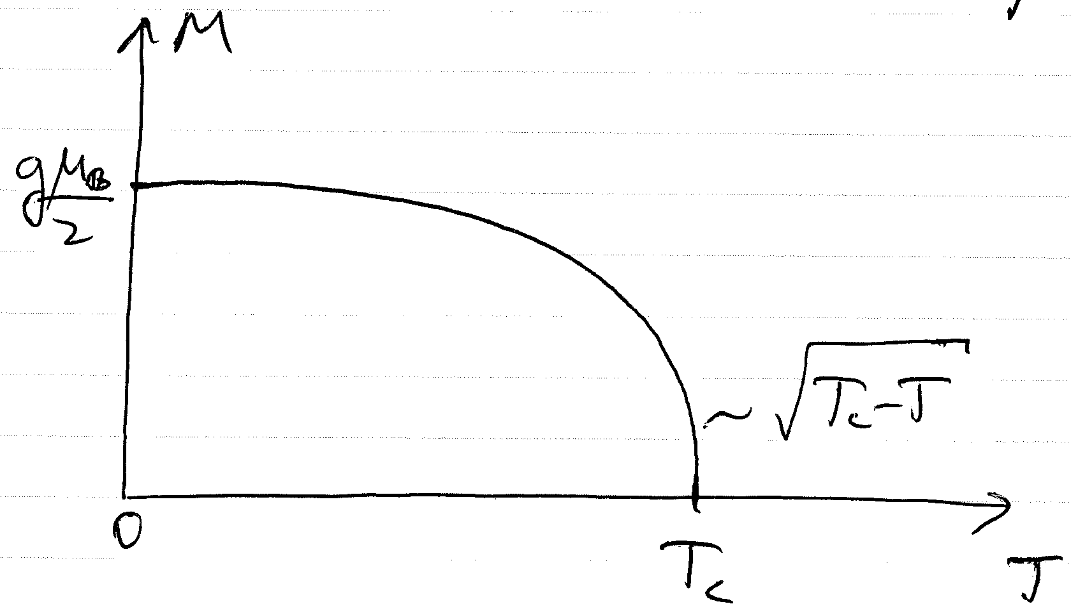
$$1 = \frac{T_c}{T} - \frac{4}{3(g\mu_B)^2}\left(\frac{T_c}{T}\right)^3 M^2$$

$$\left(\frac{M}{g\mu_B}\right)^2 = \frac{3}{4}\left(\frac{T}{T_c}\right)^3 \cdot \left(\frac{T_c}{T} - 1\right) =$$

$$= \frac{3}{4}\left(\frac{T}{T_c}\right)^2\left(1 - \frac{T}{T_c}\right)$$

Thus we obtain:

$$M(T) = \frac{g\mu_B}{2} \frac{T}{T_c} \sqrt{3\left(1-\frac{T}{T_c}\right)}$$



MFT correctly captures the basic fact – that there is a transition at some finite T_c.
It also captures the fact that M vanishes at T_c as a powerlaw:

$$M(T) \sim (T_c - T)^\beta, \quad \beta = \frac{1}{2}$$

The mean-field value of $\beta = \frac{1}{2}$ is, however, incorrect.

The ferromagnet to paramagnet transition is an example of a second order phase transition (in MFT): transition at which the order parameter vanishes continuously. Second order phase transitions are characterised by critical exponents – β is one of them.

Now find $M(T)$ as $T \to 0$.

$$M = \frac{g\mu_B}{2} \tanh\left(\frac{JzM}{2g\mu_B k_B T}\right)$$

Now we need to find the behavior of $\tanh x$ at large x.

$$\tanh x = \frac{e^x - e^{-x}}{e^x + e^{-x}} = \frac{1-e^{-2x}}{1+e^{-2x}} \approx 1 - 2e^{-2x}$$

$$M = \frac{g\mu_B}{2}\left[1 - 2e^{-\frac{JzM}{g\mu_B k_B T}}\right] \approx$$

$$\approx \frac{g\mu_B}{2}\left[1 - 2e^{-\frac{Jz}{2k_B T}}\right] =$$

$$= \frac{g\mu_B}{2}\left[1 - 2e^{-\frac{2T_c}{T}}\right]$$

let $\Delta M = M(0) - M(T)$

$$\frac{\Delta M}{M(0)} = 2e^{-\frac{2T_c}{T}}$$ – MFT prediction.

In reality $\frac{\Delta M}{M(0)} \sim T^{3/2}$ – much faster – due to fluctuations, neglected by MFT.

Calculate magnetic susceptibility.

$$\chi = \frac{\partial M}{\partial B}$$

$$M = \frac{g\mu_B}{2} \tanh\left(\frac{g\mu_B B + \frac{JZ}{g\mu_B} M}{2k_B T} \right)$$

Calculate χ for $T > T_c$.

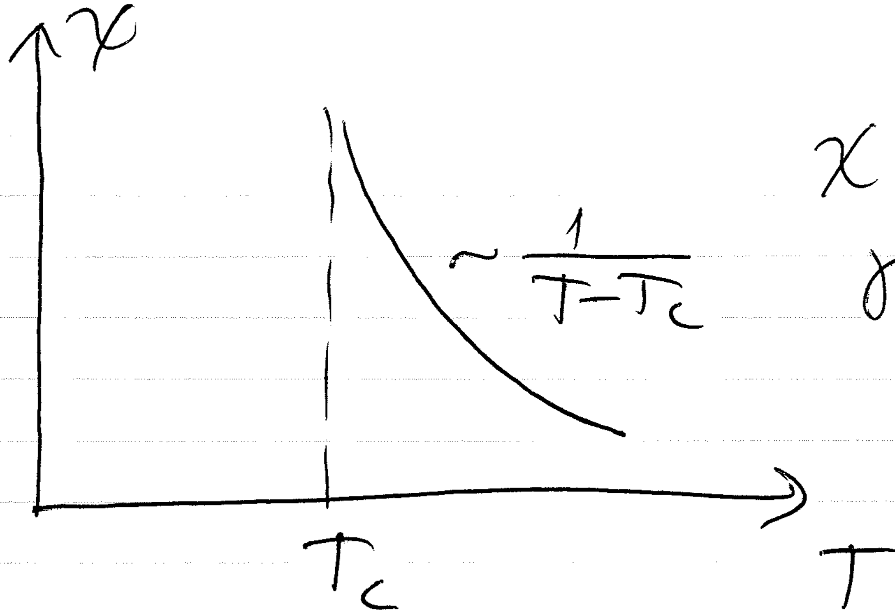
In this case $M = 0$ when $B = 0$.
Assume B is small $\Rightarrow$ M is small and expand the mean-field equation to leading order in M and B:

$$\tanh x \approx x$$

$$M = \frac{g\mu_B}{2} \cdot \frac{g\mu_B B + \frac{JZ}{g\mu_B} M}{2k_B T}$$

$$M \left(1 - \frac{JZ}{4k_B T} \right) = \frac{(g\mu_B)^2}{4k_B T} B$$

$$\chi = \frac{\partial M}{\partial B} = \frac{(g\mu_B)^2}{4k_B} \frac{1}{T - T_c}$$ – Curie-Weiss law.



$$\chi \sim (T-T_c)^{-\gamma}$$

$\gamma = 1$ - also incorrect.

Other kinds of magnetic ordering.

when $J<0$ we get antiferromagnetism:

$$\begin{matrix} \uparrow & \downarrow & \uparrow & \downarrow \\ \downarrow & \uparrow & \downarrow & \uparrow \end{matrix}$$

This does not lead to macroscopic magnetization and thus is much harder to detect. Wasn't discovered until neutron scattering techniques were developed. Antiferromagnetism most commonly occurs in insulators.

Ferrimagnetic ordering is also possible:

$$\uparrow \; \downarrow \; \uparrow \; \downarrow \; \uparrow$$