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Mean Field Approximation for the Heisenberg model

We will study the ferromagnetic ($J>0$) Heisenberg model in this section

- rewrite Hamiltonian as

$$H = \sum_i \left(- \sum_j J_{ij} S_j + g\mu_B \vec{B} \right) \cdot \vec{S}_i \qquad (*)$$

Writing the Hamiltonian this way reminds us of the Hamiltonian for independent spins in a magnetic field, except that here the magnetic field is an operator that depends on all spins in the system: $\vec{B} - \sum_j \frac{J_{ij}}{g\mu_B} \vec{S}_j$

If we replace the operator by its expectation value, we obtain

$$H_{eff} = \sum_i \left(- \sum_j J_{ij} \langle S_j \rangle + g\mu_B \vec{B} \right) \cdot \vec{S}_j = \sum_j g\mu_B \vec{B}_{eff} \cdot \vec{S}_j$$

where $\vec{B}_{eff} = \vec{B} - \sum_j \frac{J_{ij}}{g\mu_B} \langle \vec{S}_j \rangle$

Note: H_{eff} is only an approximation to H in $(*)$

The approximation is motivated by the idea that each spin feels an effective magnetic field generated by all other spins

"Mean Field Approximation"

We alredy solved the problem of independent spins in a magnetic field. For the magnetization, we have

$$\vec{M} = N\langle\vec{\mu}\rangle = -Ng\mu_B\langle\vec{S}_i\rangle$$

To calculate this expectation value, we need to know the field $\vec{B}_{eff}$ which in turn depends on the expectation value $\langle\vec{S}_i\rangle$: "selfconsistency problem"

- choose $\vec{B}_{eff}$ along $\hat{z}$-direction (external $\vec{B}$ along $\hat{z}$ and quantization axis for $\vec{S}$ is $\hat{z}$ axis)

- consider spin-$\frac{1}{2}$:

Brillouin function $B_{\frac{1}{2}}(x) = \tanh(x)$

$$\Rightarrow M = N\mu_B \tanh\left(\frac{\mu_B B}{k_B T}\right)$$

$$M = N\mu_B \tanh(\beta\mu_B B_{eff}) = N\mu_B \tanh\left(\beta\mu_B\left(B - \sum_j \frac{J_{ij}}{g\mu_B}\langle S_j^z\rangle\right)\right)$$

$$= N\mu_B \tanh\left[\beta\mu_B\left(B + \frac{zJ}{N(g\mu_B)^2}M\right)\right]$$

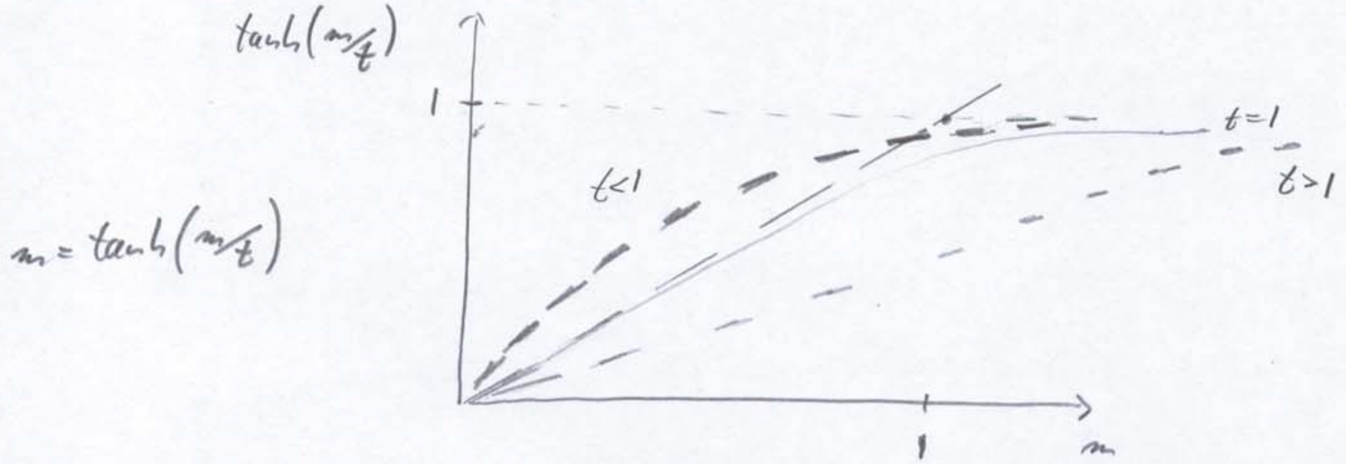
where we assumed that J_{ij} is a nearest neighbor coupling J and that z is the number of nearest neighbors (coordination number)

The magnetization per lattice site becomes

$$\boxed{m = \frac{M}{N} = \mu_B \tanh\left[\frac{\mu_B}{k_B T}\left(B + W m\right)\right]}$$

where $W = \frac{Z J}{g^2 \mu_B^2}$ and in particular, for $B = 0$:

$$m = \mu_B \tanh\left(\frac{\mu_B W}{k_B T} m\right)$$



$\rightsquigarrow$ $m = 0$ is always a solution but if the slope of $f(x) = \tanh\left(\frac{\mu_B^2 W}{k_B T} x\right)$ at $x = 0$ is larger than 1, i.e. if

$$1 < f'(0) = \frac{\mu_B^2 W}{k_B T} \frac{1}{\cosh^2\left(\frac{\mu_B^2 W}{k_B T} x\right)}\Bigg|_{x=0} = \frac{\mu_B^2 W}{k_B T}$$

2 additional solutions m^* and $-m^*$ exist.

→ It exists a critical temperature T_c so that for $T < T_c$ a finite magnetization $m^* \neq 0$ exists even if $B = 0$.

The critical temperature is often called <u>Curie temperature</u>

$$\boxed{k_B T_C = \mu_B^2 W = \frac{z J}{g^2}}$$

At T_c (and $B = 0$), <u>spontaneous symmetry breaking</u> occurs. The Heisenberg model is spin-rotational symmetric but below T_c a particular direction (which we choose to be the z-direction) is favored. This is the direction of the spontaneous magnetization.

The magnetization is the <u>order parameter</u> for the ferromagnetic phase transition.

$$m \begin{cases} = 0 & \text{above } T_c, \text{ "disordered phase"} \\ \neq 0 & \text{below } T_c, \text{ "symmetry-broken phase"} \end{cases}$$

For arbitrary spin S, the mean-field approximation yields

$$\boxed{k_B T_c = \frac{1}{3} z J S(S+1)}$$

We can estimate the behavior of m near T_c (where m is small) using $\tanh(x) \simeq x - \frac{1}{3}x^3 + \dots$

$$\Rightarrow \quad m = \frac{\mu_B^2 W}{k_B T} m - \frac{1}{3} \frac{\mu_B^4 W^3}{(k_B T)^3} m^3 + \dots$$

and as $m \neq 0$ for $T < T_c$:

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

$$\text{or} \quad m^2 = 3\mu_B^2 \left(\frac{T}{T_c}\right)^3 \left(\frac{T_c}{T} - 1\right)$$

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

For T near T_c, we therefore find ($t = \frac{T_c - T}{T_c}$ small)

$$m \simeq 3\mu_B^2 \sqrt{t}$$

The magnetization vanishes near T_c in a square-root singularity

$$m \sim (T_c - T)^\beta \quad \text{with } \beta = \tfrac{1}{2}$$

β is a <u>critical exponent</u>

and $\beta = \frac{1}{2}$ is characteristic for mean-field behavior

The correct value of β is $\beta \simeq \frac{1}{3}$

For $T \ll T_c$, the mean-field approximation predicts

$$\frac{m}{\mu_B} = \tanh\left(\frac{T_c}{T}\frac{m}{\mu_B}\right) = \frac{1-e^{-2\frac{T_c}{T}\frac{m}{\mu_B}}}{1+e^{-2\frac{T_c}{T}\frac{m}{\mu_B}}}$$

$$\approx 1 - e^{-2\frac{T_c}{T}\frac{m}{\mu_B}}$$

$$\approx 1 - e^{-2\frac{T_c}{T}}$$

which, again, does not reflect the true behavior.

The susceptibility within the mean-field approximation is

$$\chi = \frac{\partial \mathcal{M}}{\partial B} = \frac{\partial \mathcal{M}}{\partial B_{eff}}\frac{\partial B_{eff}}{\partial B} = N\mu_B^2\beta\frac{1}{\cosh^2(\beta\mu_B B_{eff})}\left(1+\frac{zJ}{N(g\mu_B)^2}\frac{\partial \mathcal{M}}{\partial B}\right)$$

above T_c: $\mathcal{M}\to 0$ for $B\to 0$ and therefore $B_{eff}\to 0$ for $B\to 0$

$$\Rightarrow \quad \chi = \frac{N\mu_B^2}{k_B T}\left(1+\frac{k_B T_c}{N\mu_B^2}\chi\right)$$

$$\left(1-\frac{T_c}{T}\right)\chi = \frac{N\mu_B^2}{k_B T}$$

or $\boxed{\chi(B=0) = \frac{C}{T-T_c}}$ Curie-Weiss law

with Curie constant $C = \frac{N\mu_B^2}{k_B}$

$$\chi \sim (T-T_c)^{-\gamma}, \quad \gamma = 1$$

- divergence of χ at T_c signals the (2^{nd} order) phase transition

Advantages and Disadvantages of the Mean-Field Theory

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- predicts existence of a phase transition and critical temperature
- qualitative predictions of possible types of order (here: ferromagnetic order)
- critical temperatures have the right order of magnitude
- qualitative behavior of many observables (here m and χ) is correctly captured.

(−)

- critical temperatures are generally overestimated as fluctuations are ignored
- critical exponents are incorrect
- mean field theory predicts phase transitions independent of dimension of the system while the Heisenberg model in one and two dimensions cannot have a phase transition at finite ($T \neq 0$) temperatures (Mermin - Wagner theorem)
- the analytic behavior of magnetization and specific heat at low T is not described correctly (as spin wave excitations are absent in MF).