Homework 7
Due Wednesday, November 25 in class

1. Consider mean-field theory for a spin-1/2 Heisenberg ferromagnet we discussed in class.

   (a) Starting from the mean-field Hamiltonian

   $$H = -\frac{JzM}{g\mu_B}\sum_i S_i^z + \frac{JzNM^2}{2g^2\mu_B^2},$$

   calculate the free energy per spin $f = F/N$ (N is the number of lattice sites) as a function of the magnetization M (recall that $F = -k_B T \ln Z$, where Z is the partition function).

   (b) Expand f to fourth order in M. Such an expansion is valid near the transition temperature T_c, where the magnetization is small. Analyze how the coefficient of the M^2 term in the expansion behaves as a function of T.

   (c) Plot the (expanded to M^4) free energy as a function of M for $T > T_c$ and for $T < T_c$. What is the difference?

   (d) Minimize f and recover $M(T)$ for T near T_c we obtained in class.

   While you obtained the above results on the behavior of the free energy of a magnet near T_c using mean-field theory for a specific model, they are in fact valid quite generally and form the basis of Landau's famous theory of phase transitions.

2. In class we discussed the behavior of the magnetic susceptibility χ of a spin-1/2 ferromagnet for $T > T_c$. Find the mean-field theory result for χ for $T < T_c$. Analyze in detail the behavior of χ for T near T_c and T near 0.
   Hint: start from the mean-field equation for M we derived in class. Let $M = M^0 + \delta M$, where M^0 satisfies the mean-field equation at zero external magnetic field and $\delta M \propto B$ is a small correction due to the external field. Expand the mean-field equation to first order in δM and B assuming they are small.

Problem 1

ⓐ Partition function for single spin:

$$\tilde{Z} = \sum_{S^z = \pm\frac{1}{2}} e^{\frac{JzM}{g\mu_B k_B T} S^z} = 2\cosh\left(\frac{JzM}{2g\mu_B k_B T}\right)$$

Total partition function $Z = \tilde{Z}^N$

Thus the free energy per spin is given by:

$$f = -k_B T \ln\left[2\cosh\left(\frac{JzM}{2g\mu_B k_B T}\right)\right] + \frac{JzM^2}{2g^2\mu_B^2}$$

ⓑ Expanding to 4th order in M we obtain:

$$f \simeq -k_B T \cdot \frac{1}{2}\left(\frac{JzM}{2g\mu_B k_B T}\right)^2 + k_B T \cdot \frac{1}{12}\left(\frac{JzM}{2g\mu_B k_B T}\right)^4 +$$

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

$$+ \frac{1}{12(k_B T)^3}\left(\frac{Jz}{2g\mu_B}\right)^4 M^4$$

Use $T_c = \frac{Jz}{4k_B}$

$$f = \frac{M^2}{(g\mu_B)^2}\left[2k_B T_c - \frac{2}{k_B T}(k_B T_c)^2\right] +$$

$$+\ \frac{16}{12\left(k_B T_c\right)^3}\left(k_B T_c\right)^4 \frac{M^4}{(g\mu_B)^4}$$

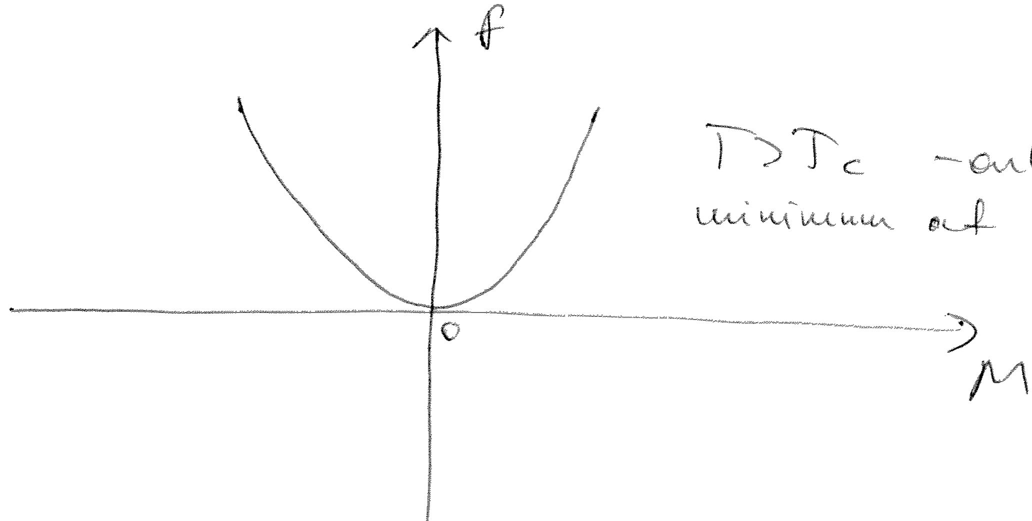
In the ~~xxxxx~~ second term I put $T = T_c$ since the expansion is valid for T near T_c. Thus we obtain:

$$f = 2k_B T_c \left(\frac{M}{g\mu_B}\right)^2 \left(1 - \frac{T_c}{T}\right) +$$

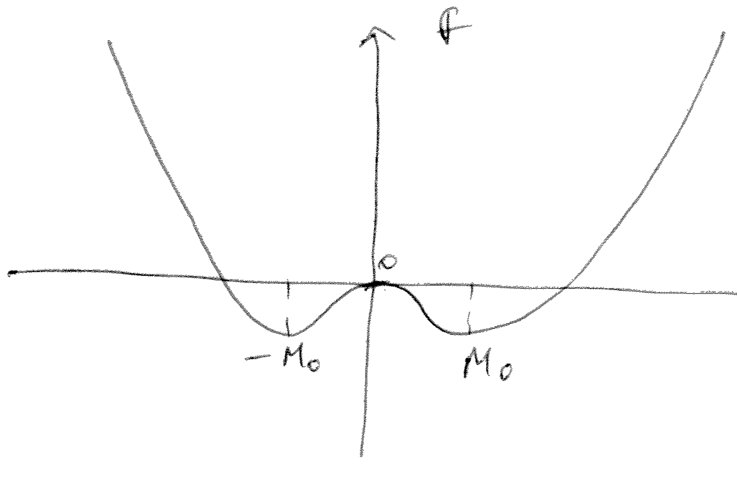
$$+\ \frac{4\, k_B T_c}{3}\left(\frac{M}{g\mu_B}\right)^4$$

The coefficient of the M^2 term in the expansion is positive for $T > T_c$ and negative for $T < T_c$.

(c)



$T > T_c$ – only 1 minimum at $M = 0$



$T < T_c$ – two minima at $\pm M_0 \neq 0$.

(d) $$\frac{df}{dM} = \frac{4k_BT_c}{(g\mu_B)^2}\left(1-\frac{T_c}{T}\right)M + \frac{16k_BT_c}{3(g\mu_B)^4}M^3 = 0.$$

$$M^2 = -\frac{4k_BT_c}{(g\mu_B)^2}\cdot\frac{3(g\mu_B)^4}{16k_BT_c}\left(1-\frac{T_c}{T}\right) =$$

$$= \frac{3(g\mu_B)^2}{4T}(T_c-T) \simeq \frac{3(g\mu_B)^2}{4T_c}(T_c-T)$$

$$M = \frac{\sqrt{3}\,g\mu_B}{2\sqrt{T_c}}\sqrt{T_c-T}$$

Problem 2

Mean-field equation for M in the presence of magnetic field B is:

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

Let $M = M^0 + \delta M$ where $\delta M \sim B$ and

$$M^0 = \frac{g\mu_B}{2}\tanh\left(\frac{JzM^0}{2g\mu_Bk_BT}\right) \quad (**)$$

Expand the right-hand-side of $(*)$ assuming δM and B are small.

$$M^0 + \delta M = \frac{g\mu_B}{2} \tanh\left(\frac{g\mu_B B + \frac{Jz}{g\mu_B} M^0 + \frac{Jz}{g\mu_B}\delta M}{2k_B T} \right)$$

$$\simeq \frac{g\mu_B}{2} \tanh\left(\frac{Jz M^0}{2 g\mu_B k_B T} \right) +$$

$$+ \frac{g\mu_B}{2} \left[1 - \tanh^2 \left(\frac{Jz M^0}{2 g\mu_B k_B T} \right) \right] \left(\frac{g\mu_B B + \frac{Jz}{g\mu_B}\delta M}{2k_B T} \right)$$

Here I've used the Taylor expansion of $\tanh x$:

$$\tanh(x_0 + \delta x) \approx \tanh x_0 + (1 - \tanh^2 x_0)\,\delta x$$

Using (**), we obtain:

$$\delta M = \frac{g\mu_B}{2} \left(1 - \frac{4(M^0)^2}{(g\mu_B)^2} \right) \left(\frac{g\mu_B B + \frac{Jz}{g\mu_B}\delta M}{2k_B T} \right)$$

$$\delta M \left[1 - \frac{Jz}{4k_B T} \left(1 - \frac{4M^{0\,2}}{(g\mu_B)^2} \right) \right] =$$

$$= \frac{(g\mu_B)^2 B}{4k_B T} \left(1 - \frac{4M^{0\,2}}{(g\mu_B)^2} \right)$$

$$\chi = \frac{\delta M}{B} = \frac{\frac{(g\mu_B)^2}{4k_B T} \left(1 - \frac{4M^{0\,2}}{(g\mu_B)^2} \right)}{1 - \frac{T_c}{T} \left(1 - \frac{4M^{0\,2}}{(g\mu_B)^2} \right)}$$

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

For T close to T_c: $\mu^0 = \frac{\sqrt{3}\, g\mu_B}{2\sqrt{T_c}} \sqrt{T_c - T}$

$$1 - \frac{4\mu^{0\,2}}{(g\mu_B)^2} = 1 - \frac{3}{T_c}\left(T_c - T\right) =$$

$$= -2 + \frac{3T}{T_c}$$

$$\chi \simeq \frac{\frac{(g\mu_B)^2}{4k_B T_c}}{1 - \frac{T_c}{T}\left(\frac{3T}{T_c} - 2\right)}$$

$$= \frac{(g\mu_B)^2}{4k_B T_c} \frac{1}{-2 + \frac{2T_c}{T}} \simeq \frac{(g\mu_B)^2}{8k_B} \frac{1}{T_c - T}$$

Thus $\chi(T)$ diverges at T_c, just as for $T > T_c$. The coefficient of $\frac{1}{T_c - T}$ term is $\frac{1}{2}$ of the coefficient of $\frac{1}{T - T_c}$ term for $T > T_c$.

For $T \to 0$ we have:

$$\mu^0(T) \simeq \frac{g\mu_B}{2}\left(1 - 2e^{-\frac{2T_c}{T}}\right)$$

Substituting this into the general expression for χ, we obtain :

$$\chi = \frac{(g\mu_B)^2}{4k_B} \frac{1 - \frac{4\mu_0^2}{(g\mu_B)^2}}{T - T_c\left(1 - \frac{4\mu_0^2}{(g\mu_B)^2}\right)} \simeq$$

$$\simeq \frac{(g\mu_B)^2}{4k_B T}\left[1 - \left(1 - 2e^{-\frac{2T_c}{T}}\right)^2\right] \simeq$$

$$\simeq \frac{(g\mu_B)^2}{k_B T} e^{-\frac{2T_c}{T}}$$

Thus $\chi(T) \to 0$ as $T \to 0$.