Exercices about the Ising Model.

1. **Explore the critical behaviour of the magnetization m of the Ising model i.e. T→T_c, defining t≡(T-T_c)/T_c , remember that k_B T_c=qJ , in the MFT result given in class, using the Taylor expansion: tanh· (x)=x-x^3/3+O(x^5).**

We already know that when there is no external magnetic field, we have $m = 0$ when $T \geq T_c$. Let's explore further what happens in the critical regime just below T_c (i.e., $T \to T_c^-$) at zero field ($h = 0$). Using the expansion

$$\tanh(x) = x - \frac{x^3}{3} + \mathcal{O}(x^5)$$

around $x = 0$, we can rewrite the self-consistency equation for $h = 0$ around $m = 0$ (near T_c) as

$$\begin{aligned} m &= \beta qJm - \frac{1}{3}(\beta qJm)^3 \\ &= \left(\frac{T_c}{T}\right) m - \frac{1}{3}\left(\frac{T_c}{T}\right)^3 m^3 \,, \qquad T \to T_c^- \,, \end{aligned}$$

or moving everything to the same side,

$$m\left[\left(\frac{T_c}{T} - 1\right) - \frac{1}{3}\left(\frac{T_c}{T}\right)^3 m^2\right] = 0 \,, \qquad T \to T_c^- \,.$$

This gives the solutions $m = 0$ and

$$m = \pm\sqrt{3\left(\frac{T}{T_c}\right)^2\left(\frac{T_c - T}{T_c}\right)} \,, \qquad T \to T_c^- \,.$$

Note that this expression is only sensible for $T \leq T_c$, otherwise m would be imaginary (which is unphysical). However, we have to keep in mind that this expression only applies whenever m is very close to 0, meaning that we are looking only at the region below T_c but very close to T_c. In terms of the reduced temperature t,

$$m = \pm\sqrt{-3(1+t)^2 t} \,, \qquad T \to T_c^- \,.$$

Using the binomial approximation

$$(1+x)^\alpha \approx 1 + \alpha x \,, \qquad |x| \ll 1 \,,$$

we can simplify this for $t \to 0^-$ (i.e., $T \to T_c^-$) as

$$m \approx \pm\sqrt{-3(1+2t)t} \approx \pm\sqrt{-3t} \,, \qquad T \to T_c^- \,.$$

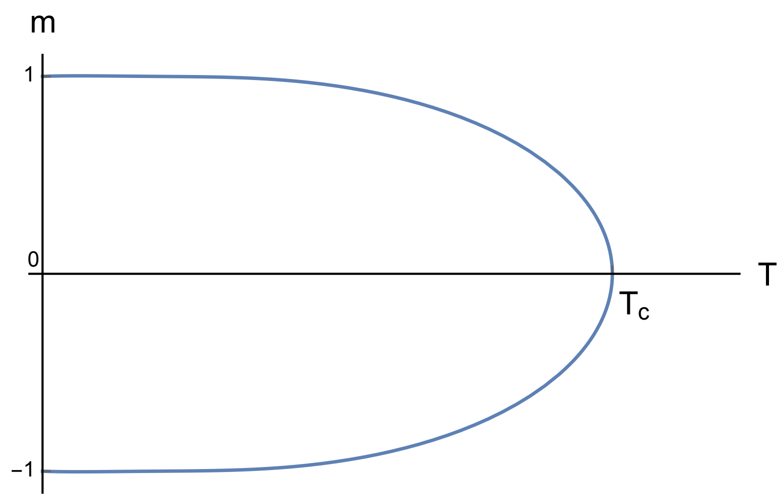

Figure 1: Behavior of the magnetization $m(T,0)$ obtained by solving the Ising model using MFT.

We have thus found that at zero field, the magnetization $m(T,h)$ behaves as

$$\boxed{m(T,0) = \begin{cases} \pm(3|t|)^{1/2}\,, & T \to T_c^- \\ 0\,, & T \to T_c^+ \end{cases}}\,.$$

In the zero-temperature limit ($T \to 0\,,\ \beta \to \infty$), the self-consistency equation gives $m_0 = 1$, so

$$\boxed{m(0,0) = \pm 1}\,.$$

We can use all of this information to sketch the magnetization as a function of temperature in Figure 1. The physical interpretation of this is that above T_c, thermal fluctuations are strong enough to prevent the system from becoming magnetized; this is the paramagnetic phase. However, at T_c a phase transition occurs and the system becomes spontaneously magnetized as you decrease the temperature past T_c; this is the ferromagnetic phase.

2. Compute the isothermal (magnetic) susceptibility χ_T (T,h)≡(∂m/∂h)_T in the MFT approach and explore its behaviour close to T_c. You can use the Taylor expansion of cosh (x).

$$\chi_T(T,h) \equiv \left(\frac{\partial m}{\partial h}\right)_T\,.$$

Taking the derivative of both sides of the self-consistency equation with respect to h while keeping T constant gives

$$\chi_T = \frac{1}{\cosh^2[\beta(h+qJm)]}\beta(1+qJ\chi_T)\,.$$

Solving for χ_T, we find

$$\chi_T(T,h) = \frac{\beta}{\cosh^2[\beta(h+qJm)] - \beta qJ}\,.$$

Let's now look at the behavior of the at zero field ($h=0$):

$$\chi_T(T,0) = \frac{\beta}{\cosh^2(\beta qJm) - \beta qJ}\,.$$

For $T \to T_c^+$, we have $m=0$, so

$$\chi_T(T,0) = \frac{\beta}{1-\beta qJ} = \frac{1}{k_\mathrm{B}(T-T_c)} = \frac{1}{k_\mathrm{B}T_c}\frac{1}{|t|}\,, \qquad T \to T_c^+\,.$$

For $T \leq T_c$ but very close to T_c, we have $m = \pm(3|t|)^{1/2}$ (as found in the previous section), which is very small. We can thus use the expansion

$$\cosh(x) = 1 + \frac{x^2}{2} + \mathcal{O}(x^4)$$

around $x=0$ to write

$$\begin{aligned}
\chi_T(T,0) &= \frac{\beta}{[1+\frac{1}{2}(\beta qJ(3|t|)^{1/2})^2]^2 - \beta qJ} \\
&\approx \frac{\beta}{1+3(\beta qJ)^2|t| - \beta qJ} \\
&\approx \frac{1}{2}\frac{1}{k_\mathrm{B}T_c}\frac{1}{|t|}\,, \qquad T \to T_c^-\,.
\end{aligned}$$

We have thus found that at zero field, the isothermal susceptibility goes as

$$\boxed{\chi_T(T,0) = \begin{cases} A|t|^{-1}\,, & T \to T_c^- \\ 2A|t|^{-1}\,, & T \to T_c^+ \end{cases}\,, \quad \text{where} \quad A = \frac{1}{2}\frac{1}{k_\mathrm{B}T_c}}\,,$$

and diverges at $T = T_c$. We can use this information to sketch the susceptibility as a function of temperature near T_c in Figure 2.

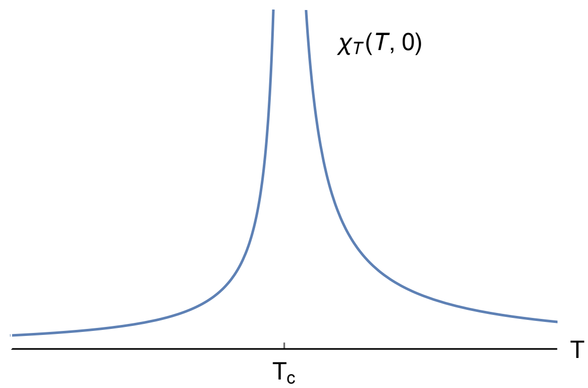

Figure 2: Behavior of the isothermal susceptibility $\chi_T(T, 0)$ near T_c obtained by solving the Ising model using MFT.

3. Compute the MFT solution of the Ising model with single-ion anisotropy given by this Hamiltonian:

$$\mathcal{H} = -J\sum_{\langle ij\rangle} s_i s_j - D\sum_{i=1}^{N}(s_i)^2 - h\sum_{i=1}^{N} s_i\,,$$

where $J > 0$ is a ferromagnetic coupling constant and D is the single-ion anisotropy constant that favors easy-axis magnetization for $D > 0$ and easy-plane magnetization for $D < 0$.

Decoupling the hamiltonian

For the interaction term, we will write $s_i s_j$ in the form

$$s_i = \langle s_i\rangle + \delta s_i\,,$$

where

$$\delta s_i \equiv s_i - \langle s_i\rangle$$

denotes fluctuations about the mean value of s_i. The spin interaction terms $s_i s_j$ thus be-come

$$\begin{aligned} s_i s_j &= (\langle s_i\rangle + \delta s_i)(\langle s_j\rangle + \delta s_j) \\ &= \langle s_i\rangle\langle s_j\rangle + \langle s_j\rangle\delta s_i + \langle s_i\rangle\delta s_j + \delta s_i\delta s_j\,. \end{aligned}$$

We now make the assumption that the fluctuations are very small, so we can ignore the term quadratic in fluctuations:

$$\delta s_i\delta s_j = 0\,.$$

The quantity $s_i s_j$ is then approximately

$$\begin{aligned} s_i s_j &\approx \langle s_i\rangle\langle s_j\rangle + \langle s_j\rangle\delta s_i + \langle s_i\rangle\delta s_j \\ &= \langle s_i\rangle\langle s_j\rangle + \langle s_j\rangle(s_i - \langle s_i\rangle) + \langle s_i\rangle(s_j - \langle s_j\rangle) \\ &= \langle s_j\rangle s_i + \langle s_i\rangle s_j - \langle s_i\rangle\langle s_j\rangle\,. \end{aligned}$$

Since this system is translationally invariant, the expectation value $\langle s_i\rangle$ of any given site i is independent of the site, so we have

$$\langle s_i\rangle = m\,.$$

We can then further simplify $s_i s_j$ to

$$s_i s_j = m(s_i + s_j) - m^2 = m[(s_i + s_j) - m]\,.$$

Similarly, for the single-ion anisotropy term, we will write $(s_i)^2$ as

$$(s_i)^2 = 2ms_i - m^2 = m(2s_i - m)\,.$$

The mean field Hamiltonian is then

$$\begin{aligned}
\mathcal{H}_{\text{MF}} &= -Jm\sum_{\langle ij\rangle}(s_i + s_j - m) - Dm\sum_{i=1}^{N}(2s_i - m) - h\sum_{i=1}^{N} s_i \\
&= -Jm\sum_{\langle ij\rangle}(2s_i - m) - Dm\sum_{i=1}^{N}(2s_i - m) - h\sum_{i=1}^{N} s_i \\
&= -\frac{qJm}{2}\sum_{i=1}^{N}(2s_i - m) - Dm\sum_{i=1}^{N}(2s_i - m) - h\sum_{i=1}^{N} s_i \\
&= \left(\frac{qJ}{2} + D\right) Nm^2 - [h + (qJ + 2D)m]\sum_{i=1}^{N} s_i\,,
\end{aligned}$$

where q is the coordination number. We thus find

$$\mathcal{H}_{\text{MF}} = \left(\frac{qJ}{2} + D\right) Nm^2 - h_{\text{eff}}\sum_{i=1}^{N} s_i\,,$$

where

$$h_{\text{eff}} \equiv h + (qJ + 2D)m$$

is the effective magnetic field felt by the spins.

Let's calculate the partition function using the mean field Hamiltonian:

$$\begin{aligned}
Z_{\text{MF}} &= \operatorname{Tr}(e^{-\beta\mathcal{H}_{\text{MF}}}) \\
&= \prod_{i=1}^{N}\left(\sum_{s_i=\pm 1}\right) e^{-\beta\mathcal{H}_{\text{MF}}} \\
&= \prod_{i=1}^{N}\left(\sum_{s_i=\pm 1}\right) e^{-\beta(\frac{qJ}{2}+D)Nm^2} e^{\beta h_{\text{eff}}\sum_{j=1}^{N} s_j} \\
&= e^{-\beta(\frac{qJ}{2}+D)Nm^2}\prod_{i=1}^{N}\left(\sum_{s_i=\pm 1} e^{\beta h_{\text{eff}} s_i}\right) \\
&= e^{-\beta(\frac{qJ}{2}+D)Nm^2}\prod_{i=1}^{N}\underbrace{(e^{\beta h_{\text{eff}}} + e^{-\beta h_{\text{eff}}})}_{=2\cosh(\beta h_{\text{eff}})} \\
&= e^{-\beta(\frac{qJ}{2}+D)Nm^2}[2\cosh(\beta h_{\text{eff}})]^N\,,
\end{aligned}$$

so we find

$$\boxed{Z_{\rm MF} = e^{-\beta(\frac{qJ}{2}+D)Nm^2}[2\cosh(\beta h_{\rm eff})]^N} .$$

Now, recall from that the magnetization is given by

$$m \equiv \frac{1}{N}\sum_{i=1}^{N} \langle s_i \rangle \ .$$

We can rewrite this as

$$\begin{aligned}
m &= \frac{1}{N}\sum_{i=1}^{N} \frac{\mathrm{Tr}(s_i e^{-\beta \mathcal{H}_{\rm MF}})}{Z_{\rm MF}} \\
&= \frac{1}{N}\frac{1}{Z_{\rm MF}}\sum_{i=1}^{N} s_i e^{-\beta \mathcal{H}_{\rm MF}} \\
&= \frac{1}{N\beta}\frac{1}{Z_{\rm MF}}\frac{\partial Z_{\rm MF}}{\partial h_{\rm eff}} \\
&= \frac{1}{N\beta}\frac{\partial(\ln Z_{\rm MF})}{\partial h_{\rm eff}} ,
\end{aligned}$$

where on the third line we have used the fact that

$$\begin{aligned}
\frac{\partial Z_{\rm MF}}{\partial h_{\rm eff}} &= \frac{\partial}{\partial h_{\rm eff}}\,\mathrm{Tr}(e^{-\beta \mathcal{H}_{\rm MF}}) \\
&= \mathrm{Tr}\left(\frac{\partial}{\partial h_{\rm eff}} e^{-\beta \mathcal{H}_{\rm MF}}\right) \\
&= -\beta\,\mathrm{Tr}\left(\frac{\partial \mathcal{H}_{\rm MF}}{\partial h_{\rm eff}} e^{-\beta \mathcal{H}_{\rm MF}}\right) \\
&= -\beta\,\mathrm{Tr}\left[\left(-\sum_{i=1}^{N} s_i\right) e^{-\beta \mathcal{H}_{\rm MF}}\right] \\
&= \beta\,\mathrm{Tr}\left[\sum_{i=1}^{N} s_i e^{-\beta \mathcal{H}_{\rm MF}}\right] .
\end{aligned}$$

Now, we can calculate $\ln Z_{\rm MF}$:

$$\ln Z_{\rm MF} = -\beta\left(\frac{qJ}{2}+D\right)Nm^2 + N\ln 2 + N\ln[\cosh(\beta h_{\rm eff})] ,$$

so

$$\frac{\partial(\ln Z_{\rm MF})}{\partial h_{\rm eff}} = N\beta\tanh(\beta h_{\rm eff}) .$$

Inserting this back into gives

$$m = \tanh(\beta h_{\rm eff}) .$$

Inserting the definition of h_{eff} back into this equation gives us the self-consistency equation

$$\boxed{m = \tanh\left[\beta\big(h + (qJ + 2D)m\big)\right]}.$$

This corresponds to a system with a phase transition at $k_{\mathrm{B}}T_c = qJ + 2D$. Above this temperature, it is paramagnetic, and below this temperature, it is ferromagnetic. Note that the system will be paramagnetic for all (nonzero) temperatures if $D < -qJ/2$ (remember that $D < 0$ favors easy-plane magnetization).