E5642: Long-range Ising model

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The problem:

Consider a cluster of N spins $s_i = \pm 1$. The interaction between *any* two spins is $-\epsilon s_i s_j$, with $\epsilon > 0$. The interaction of each spin with the external magnetic field H is $-Hs_i$. The total magnetization is defined as $\mathsf{m} = \sum s_i$. The inverse temperature is β.

(a) Show that the partition function can be written as $Z(\beta, H) = \sum_{\mathsf{m}} g(\mathsf{m}) \exp\left(\frac{1}{2}Bm^2 + h\mathsf{m}\right)$. Express $g(\mathsf{m})$ and B and h using (N, ϵ, H, β).

(b) Assume that $B = \frac{b}{N}$, define the magnetization as $M = \frac{\mathsf{m}}{N}$, and write the partition function as $Z(b, h) = \sum_M \exp(-N * A(M))$.

Write the expressions for $A(M)$ and for its derivatives $A'(M)$ and $A''(M)$.

(c) Determine the critical temperature T_c, and write an equation for the mean field value of M. Make a qualitative plot of $A(M)$ below and above the critical temperature.

(d) Write an approximation for $A(M)$ up to order M^4. On the basis of this expression determine the temperature range where mean filed theory cannot be trusted. Hint: you have to estimate the variance $\langle M^2 \rangle$ in the Gaussian approximation. What happens with this condition in the thermodynamic limit $(N \to \infty)$?

(e) What is the susceptibility for $T > T_c$.

(f) What is the heat capacity.

The solution:

(a) Hamiltonian of a system:

$$H = -\epsilon \sum_{<i,j>} s_i s_j - H \sum_{i=1}^{N} s_i \tag{1}$$

where $< i, j >$ means summation over all i and j from 1 to N except duplcations (for example i=1,j=2 and i=2,j=1 it's duplication) and cases when i=j.
First term in Hamiltonian describes interactions of spin s_i with all other spins s_j In view of mean field approximation we assume that each spin s_j has average value $< s >$, thus Hamiltonian takes following form:

$$H = -\epsilon \frac{N}{2} \sum_{i=1}^{N} s_i \langle s \rangle - H \sum_{i=1}^{N} s_i \tag{2}$$

Where factor $\frac{1}{2}$ appears to exclude duplications and N comming from summation over j. Average spin value given by:

$$\langle s \rangle = \frac{1}{N} \sum_{i=1}^{N} s_i = \frac{m}{N} \tag{3}$$

Thus we can rewrite Hamiltonian in following form:

$$H = -\frac{1}{2}\epsilon m^2 - Hm \tag{4}$$

Let us find function g(m) which gives number of possible spin's configuration for given m. We use follwoing notations:
$N_\uparrow$ - total number of "up" spins
$N_\downarrow$ - total number of "down" spins
$m = N_\uparrow - N_\downarrow$
$N_\uparrow = \frac{N+m}{2}$
$N_\downarrow = \frac{N-m}{2}$

$$g(m) = \frac{N!}{N_\uparrow! N_\downarrow!} = \frac{N!}{\left[\frac{1}{2}(N+m)\right]!\left[\frac{1}{2}(N-m)\right]!} \tag{5}$$

Now we can write partition function:

$$Z = \sum_{m=-N}^{N} g(m)\exp\left(-\beta H(m)\right) = \sum_{m=-N}^{N} g(m)\exp\left(\frac{1}{2}Bm^2 + hm\right) \tag{6}$$

Where $B \equiv \beta\epsilon$ and $h \equiv \beta H$

(b) We assume $B = \frac{b}{N}$ and define the magnetization as $M = \frac{\mathsf{m}}{N}$ we can rewrite partition function (6):

$$Z = \sum_{M=-1}^{1} \exp\left[-N\left(-\frac{1}{2}bM^2 - hM - \frac{ln(g(M))}{N}\right)\right] = \sum_{M=-1}^{1} \exp\left(-N * A(M)\right) \tag{7}$$

Where $A(M) \equiv -\frac{1}{2}bM^2 - hM - \frac{ln(g(M))}{N}$.

First we would like to simplify expression (5) for ln(g(m)) and after Stirling's approximation $ln(x!) \approx xln(x) - x$ and little bit algebra we have:

$$ln(g(m)) \approx N\left(ln(2) - \frac{M}{2}ln\left(\frac{1+M}{1-M}\right) - \frac{1}{2}ln(1-M^2)\right) \tag{8}$$

Thus A(M) gets following form:

$$A(M) = -\frac{1}{2}bM^2 - hM - ln(2) + \frac{M}{2}ln\left(\frac{1+M}{1-M}\right) + \frac{1}{2}ln(1-M^2) \tag{9}$$

First and second derivatives of $A(M)$ with respect to M:

$$A'(M) = -bM - h + \frac{1}{2}ln\left(\frac{1+M}{1-M}\right) = -bM - h + arctanh(M) \tag{10}$$

$$A''(M) = -b + \frac{1}{1-M^2} \tag{11}$$

Here relation $arctanh(x) = \frac{1}{2}ln\left(\frac{1+x}{1-x}\right)$ has been used.

(c) In order to find minima of $A(M)$ we equal first derivative (10) to zero:

$$A'(M) = -bM - h + arctanh(M) = 0 \tag{12}$$

From here we deduce:

$$M = tanh(bM + h) \tag{13}$$

We solve graphically this equation with zero external magnetic field ($h \to 0$):

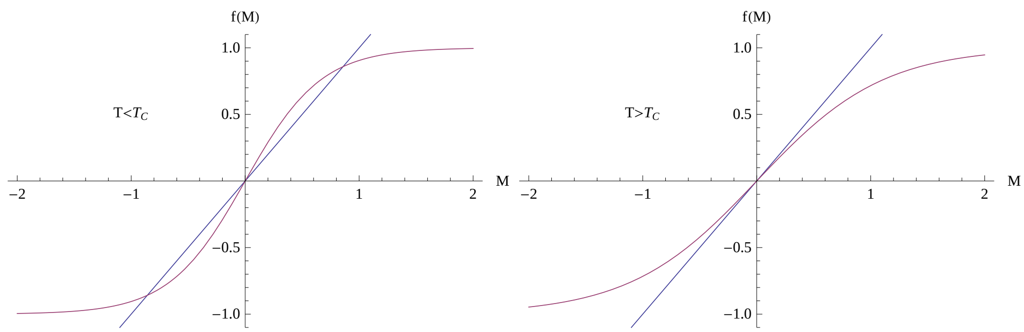

Figure 1: Graphs of $f_1(M) = M$ and $f_2(M) = tanh(bM)$ for different values of b.

Parameter b influences on curvature of $tanh(bM)$ (red line on graph) and starting from some critical value of b the equation has two additional solutions (intersection points on a graph). It happens when slope of blue line is equal to slope of red line near point $M = 0$. Expanding $tanh(bM)$ by Taylor expansion about point $M = 0$ we get:

$$tanh(bM) \approx bM + ... \tag{14}$$

By comparing between slope b of $tanh$ and slope 1 of line we get critical temperature:

$$T_c = \frac{\epsilon N}{k_B} \tag{15}$$

Using (6) and (7) we can rewrite $A(M)$ in following terms:

$$A(M) = \beta(-\frac{1}{2}\epsilon\frac{m^2}{N} - H\frac{m}{N} - \frac{1}{\beta}\frac{ln(g(m))}{N}) = \frac{\beta}{N}(E(m) - TS(m)) = \frac{\beta}{N}F(m) \tag{16}$$

Where $E(m)$ is energy of given magnitization defined by (4), $S(m) \equiv ln(g(m))$ is entropy for given magnitization and F(m) is nothing else Helmholtz free energy for given magnitization.

To understand $A(M)$ function behavior under and above T_c with and without magnetic field we plot following qualitative graphs:

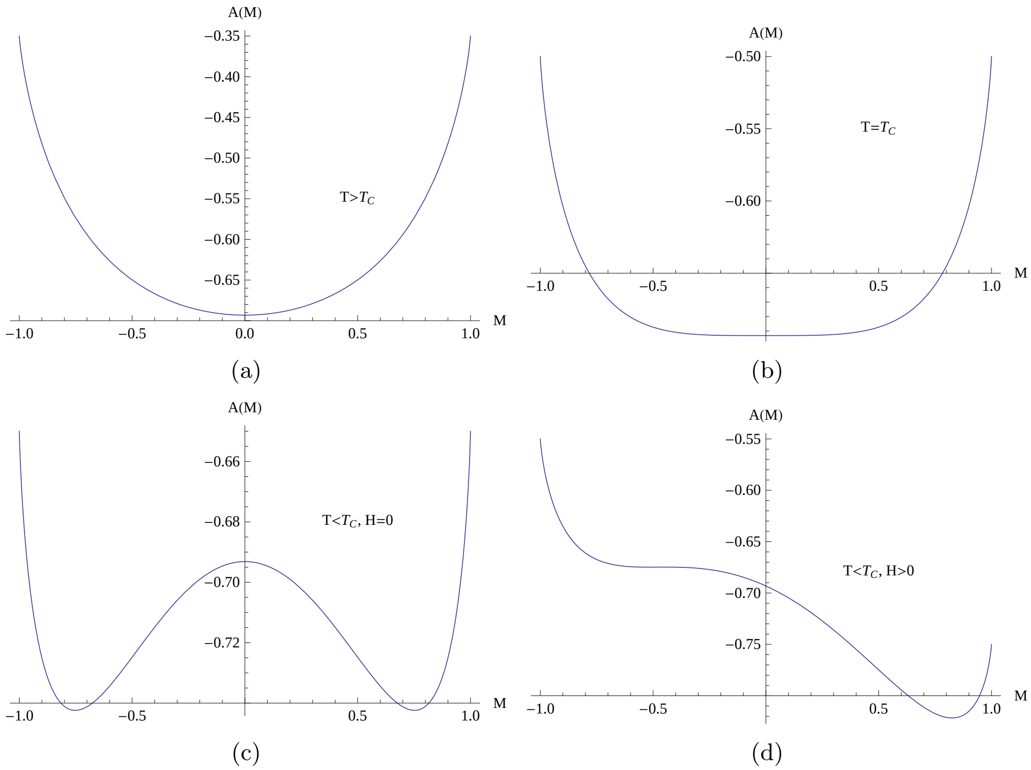

Figure 2: $A(M)$ for different values of temerature and external magnetic field.

We note that above T_c in average magnitization of a system is zero. Under T_c and without external magnetic field system can be in one of two possible magnitizations are different from zero. Magnitudes both of them are equal, because without external magnetic field system is symmetric and there is no preference to be in one of possible magnitizations. If we add external magnetic field spins get preference direction (direction of magnetic field) symmetry is broken and we see in graph that one minima is above the other.

(d) We can expand $A(M)$ defined by (9) about $M = 0$ up to order M^4:

$$A(M) = -ln(2) - hM + \frac{1}{2}(1-b)M^2 + \frac{1}{12}M^4 \tag{17}$$

We can rewrite $1-b$ by using previous definitions $b = BN = \beta\epsilon N$, $T_c = \frac{\epsilon N}{k_B}$ and $\beta = 1/(k_B T)$ and we get:

$$1 - b = \frac{T - T_c}{T} \equiv t \tag{18}$$

and thus A(M) becomes:

$$A(M) = const - hM + \frac{1}{2}tM^2 + \frac{1}{12}M^4 \tag{19}$$

Case of $T > T_c$ ($t > 0$)

We can neglect term of M^4 in (19) in case it's much smaller than contribution from M^2 term:

$$tM^2 \gg M^4 \quad \Rightarrow \quad t \gg M^2 \tag{20}$$

In the absence of external magnetic field from (7) and (19) we get that partition function is:

$$Z \sim \sum \exp\left(-\frac{1}{2}NtM^2\right) = \sum \exp\left(-\frac{M^2}{2\sigma^2}\right) \tag{21}$$

"Width" or variance of Gaussian is σ^2, where $\sigma \equiv \frac{1}{\sqrt{Nt}}$.
In mean field approximation we neglect fluctuations, therefore $\langle M^2 \rangle = \langle M \rangle^2 = M^2$.
Gaussian approximation (21) is valid if disperssion of M^2 is of order σ^2 or smaller.

$$M^2 \sim \sigma^2 = \frac{1}{Nt} \tag{22}$$

By substitution (22) into (20) we get following condition:

$$t \gg \frac{1}{Nt} \quad \Rightarrow \quad t \gg \frac{1}{\sqrt{N}} \tag{23}$$

Case of $T < T_c$ ($t < 0$)

We define $t' \equiv -t$.
When $T < T_c$ function $A(M)$ has two minima (see figure 2(c)), which in the absence of external magnetic field are:

$$M_{1,2} = \pm\sqrt{3\left(\frac{T_c - T}{T}\right)} = \pm\sqrt{3t'} \tag{24}$$

The disctance between two minima is:

$$d = M_2 - M_1 = 2\sqrt{3t'} \sim \sqrt{t'} \tag{25}$$

In this case Gaussian approximation is valid if dispersion of magnitization is much smaller than distance between minima. Comparing (22) with last result we have:

$$d \sim \sqrt{t'} \gg M \sim \frac{1}{\sqrt{Nt'}} \quad \Rightarrow \quad t' \gg \frac{1}{\sqrt{N}} \tag{26}$$

We can combine two conditions (23) and (26) and we have:

$$|t| \gg \frac{1}{\sqrt{N}} \tag{27}$$

In thermodynamic limit $N \to \infty$ this condition is always satisfied excluding cases when temperature is in the vicinity of critical temperature.

(e) Expression (13) we can be written as $arctanh(M) = bM + h$. We derivate both side with respect to external magnetic field H and write magnetic susceptibility of the system:

$$\chi = \left(\frac{\partial M}{\partial H}\right)_T = N\beta \left(\frac{\partial M}{\partial h}\right)_T = \frac{N}{k_B} \frac{1 - M^2}{T - T_c(1 - M^2)} \tag{28}$$

At high temperature ($T > T_c$) $M \ll 1$ and we obtain Curie-Weiss law:

$$\chi \approx \frac{N}{k_B} \frac{1}{T - T_c} \tag{29}$$

(f) To calculate heat capacity we use definition $C_V = \left(\frac{\partial E}{\partial T}\right)_{N,V}$. From (4) we can write in the absence of magnetic field:

$$E(M) = -\frac{1}{2}\epsilon M^2 N^2 \tag{30}$$

Thus heat capacity is:

$$C_V = -\epsilon N^2 M \left(\frac{\partial M}{\partial T}\right) \tag{31}$$

Expression (13) we can be written as $arctanh(M) = bM$. We derivate both side with respect to T (taking into account dependence of b on T) and after a little bit algebra we have:

$$\left(\frac{\partial M}{\partial T}\right) = \frac{M/T_c}{T/T_c - (T/T_c)^2 \frac{1}{1-M^2}} \tag{32}$$

Substituting this result into (31) we get expression for heat capacity:

$$C = \frac{k_B N M^2}{(T/T_c)^2 \frac{1}{1-M^2} - T/T_c} \tag{33}$$

Heat capacity for $T > T_c$ is always zero (mean value of magnitization is zero).
In $T = T_c$ straight line is tangent to $tanh(bM)$ see figure 1 and only one possible solution of $M = tanh(bM)$ is $M(T = T_c) = 0$, therefore near $T = T_c$ we can expand $tanh$ by Teylor series and using fact that $T \simeq T_c$ we get:

$$M(T) = tanh(bM) \approx bM - \frac{1}{3}(bM)^3 \quad \Rightarrow \quad M(T) \approx \sqrt{3(1 - T/T_c)} \tag{34}$$

We substitute our result into (33) and take a limit:

$$\lim_{T \to T_c^-} \frac{3k_B N(1 - T/T_c)}{(T/T_c)^2 \frac{1}{1-3(1-T/T_c)} - T/T_c} = \frac{3}{2} k_B N \tag{35}$$

When $T \to 0$ we can expand (13) about $T = 0$:

$$M(T) \approx 1 - 2\exp\left(-2T/T_c\right) \tag{36}$$

We again substitute our result into (33) and get heat capacity for low temperature:

$$C(T) \approx 4Nk_B \left(\frac{T_c}{T}\right)^2 \exp\left(-2T_c/T\right) \tag{37}$$