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Problem Set 3
The Ising model

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Reminder

1 Paramagnetic-ferromagnetic phase transition

Consider a system of $N(\gg 1)$ atoms whose positions are fixed to the nodes of a crystalline lattice with volume V , which is in equilibrium with a thermostat at the temperature T and subject to an external magnetic field $\boldsymbol{B}_0$. To each atom i is associated a magnetic moment $\boldsymbol{\mu}_i = g\mu_B \boldsymbol{S}_i$, where g is the Landé factor, μ_B the Bohr magneton, and $\boldsymbol{S}_i$ the spin of the i^{th} atom. In what follows, we assume that S_i can only take the values $\pm 1/2$ in the direction of the applied magnetic field.

1.1 Paramagnetism

Let us first neglect the interactions between the magnetic moments. The system can then be described by a Hamiltonian coupling the magnetic moments with the applied field $\boldsymbol{B}_0$ and which simply reads

$$\mathcal{H} = -\sum_{i=1}^{N} \boldsymbol{\mu}_i \cdot \boldsymbol{B}_0 = -g\mu_B \sum_{i=1}^{N} \boldsymbol{S}_i \cdot \boldsymbol{B}_0$$

(a) What is the state of the system at zero temperature (give a concise answer, without performing any calculation) ? What is the effect of a temperature increase on such a state ?

(b) Calculate the canonical partition function Z and the free energy F of the system.

(c) Show that the average magnetization M of the system reads

$$M = \frac{N}{V}\frac{g\mu_B}{2}\tanh\left(\frac{g\mu_B B_0}{2k_B T}\right)$$

Plot M as a function of the applied magnetic field. Does the system showcase a phase transition ?

(d) One defines the magnetic susceptibility as

$$\chi = \lim_{B_0 \to 0} \frac{\partial M}{\partial B_0} \tag{1}$$

Show that χ follows the Curie law

$$\chi = \frac{\mathcal{C}}{T} \tag{2}$$

Give an expression of $\mathcal{C}$ as a function of the parameters of the problem. Notice that for weak magnetic fields, one has $M = \chi B_0$.

1.2 Ferromagnetism

Let us now consider a ferromagnetic interaction between nearest-neighbor magnetic moments. The Hamiltonian of the system then reads

$$\mathcal{H} = -g\mu_B \sum_{i=1}^{N} \boldsymbol{S}_i \cdot \boldsymbol{B}_0 - J \sum_{\langle i,j \rangle} \boldsymbol{S}_i \cdot \boldsymbol{S}_j \tag{3}$$

where $\langle i, j\rangle$ corresponds to a summation over pairs of nearest neighbors i and j on the lattice, and where J is the ferromagnetic coupling constant (what is the sign of J ?).

(a) Within the mean field approximation, one neglects the correlations between the fluctuations of the spins with respect to their mean value $\langle \boldsymbol{S}_i\rangle$. In what follows, we assume that each atom has p nearest neighbors. Show that the effective magnetic field B_{eff} exerted on a lattice site i reads $B_{\text{eff}} = B_0 + \lambda M$, where M is the magnetization of the interacting system. Give an expression of λ as a function of the parameters of the problem. Show that the Hamiltonian 3 reads within the mean field approximation as

$$\mathcal{H} = -g\mu_B B_{\text{eff}} \sum_{i=1}^{N} S_i + J\frac{Np}{2}\left(\frac{VM}{Ng\mu_B}\right)^2$$

$$S_i = \langle S_i\rangle + \delta S_i = S + \delta S_i$$

We call C_{ij} the spin-spin correlation,

$$C_{ij} = \langle S_i S_j\rangle - \langle S_i\rangle\langle S_j\rangle = \langle \delta S_i \delta S_j\rangle \approx 0$$

We make this approximation to 0 in the mean-field approximation.

$$\begin{aligned}
H &= -g\mu_B B_0 \sum_{i=1}^{N} S_i - J\sum_{\langle i,j\rangle}(S+\delta S_i)(S+\delta S_j) \\
&\approx -g\mu_B B_0 \sum_{i=1}^{N} S_i - J\sum_{\langle i,j\rangle}[S^2 + S(\delta S_i + \delta S_j)] \\
&= -g\mu_B B_0 \sum_{i=1}^{N} S_i - J\sum_{\langle i,j\rangle}[S^2 + 2S(\delta S_i)] \\
&= -g\mu_B B_0 \sum_{i=1}^{N} S_i - J\sum_{\langle i,j\rangle}[S^2 + 2S(S_i - S)] \\
&= \frac{JS^2Np}{2} - g\mu_B\left[B_0 + \frac{JSp}{g\mu_B}\right]\sum_{i=1}^{N} S_i
\end{aligned}$$

We can define the magnetization,

$$M = \frac{\langle \text{total magnetic moment}\rangle}{V} = \frac{Ng\mu_B S}{V}$$

Meaning,

$$S = \frac{VM}{Ng\mu_B}$$

So, in the end,

$$\mathcal{H} \approx -g\mu_B B_{\text{eff}} \sum_{i=1}^{N} S_i + J\frac{Np}{2}\left(\frac{VM}{Ng\mu_B}\right)^2$$

With,

$$B_{\text{eff}} = B_0 + \lambda M \qquad\qquad \lambda = \frac{VJp}{N(g\mu_B)^2}$$

(b) Calculate Z and F within the mean field approximation.

$$\begin{aligned} Z &= \sum_{s_1=\pm 1/2} \cdots \sum_{s_N=\pm 1/2} e^{\beta g\mu_B B_{\text{eff}} \sum_i S_i} e^{-\beta J \frac{Np}{2}(VM/Ng\mu_B)^2} \\ &= \sum_{s_1=\pm 1/2} \cdots \sum_{s_N=\pm 1/2} \prod_{i=1}^{N} e^{\beta g\mu_B B_{\text{eff}}} S_i e^{-\beta J \frac{Np}{2}(VM/Ng\mu_B)^2} \\ &= \left[\sum_{s_{27}=\pm 1/2} e^{\beta g\mu_B B_{\text{eff}} s_{27}}\right]^N e^{-\beta J \frac{Np}{2}(VM/Ng\mu_B)^2} \end{aligned}$$

We can write $Z = z^N$ because of the distinguishable lattice sites, with

$$z = 2\cosh\left(\frac{\beta\mu_B B_{\text{eff}}}{2}\right) e^{-\beta pJ/2(VM/Ng\mu_B)^2}$$

$$\begin{aligned} F &= -k_B T \ln Z \\ &= -Nk_B T \ln z \\ &= -Nk_B T \ln\left[2\cosh\left(\frac{\beta\mu_B B_{\text{eff}}}{2}\right)\right] + \frac{NpJ}{2}\left(\frac{VM}{Ng\mu_B}\right)^2 \end{aligned}$$

(c) Use the results of Part 1.1 to determine the following self-consistent equation, which determines the value(s) of the magnetization M :

$$M = \frac{N}{V}\frac{g\mu_B}{2}\tanh\left(\frac{\beta g\mu_B}{2}(B_0 + \lambda M)\right) \tag{4}$$

Rederive the above result by minimizing the free energy found at question 1.2(b) with respect to M.

$$M = -\frac{1}{V}\frac{\partial F}{\partial B_0}$$

At equilibrium,

$$\left.\frac{\partial F}{\partial M}\right|_{\text{eq}} = 0$$

Because it should minimize the free energy.

$$\frac{\partial}{\partial B_0} F(B_0, M(B_0)) = \frac{\partial F}{\partial B_0} + \frac{\partial F}{\partial M}\frac{\partial M}{\partial B_0}$$

Meaning,

$$M = \frac{1}{V} N \frac{g\mu_B}{2} \tanh\left(\frac{\beta g \mu_B}{2} B_{\text{eff}}\right)$$

We can define the magnetization at saturation, M_S,

$$M_S = \frac{N g \mu_B}{2V}$$

Meaning,

$$M = M_S \tanh\left(\frac{\beta g \mu_B}{2} B_{\text{eff}}\right)$$

And so we get the self-consistent equation.

- If we have no interaction (meaning $J = 0$) we recover paramagnetism
- We can make the calculation out-of-minimizing free energy,

$$\frac{\partial F}{\partial M} = -\cancel{N}\cancel{k_B T}\frac{\cancel{\beta} g \mu_B}{2}\lambda \tanh\left(\frac{\beta g \mu_B}{2} B_{\text{eff}}\right) + \cancel{N} pJ \left(\frac{V}{N g \mu_B}\right)^2 M = 0$$

  One can finish this calculation and recover

$$M = M_S \tanh\left(\frac{\beta g \mu_B}{2} B_{\text{eff}}\right)$$

1.2.1 Properties of the system at zero magnetic field

In this part of the problem, we consider a vanishing external magnetic field, i.e., $B_0 = 0$.

(a) How many solutions to the transcendental equation 4 can you find ? (Use a graphical method.) Does the system present a phase transition ? If yes, give an expression for the critical temperature T_c.

$B_0 = 0$, so

$$M = M_S \tanh\left(\beta \frac{g\mu_B}{2}\frac{2}{2}\frac{VJp}{N(g\mu_B)^2}M\right)$$
$$= M_S \tanh\left(\beta \frac{1}{2}\frac{2}{2}\frac{VJp}{N(g\mu_B)}M\right) \qquad = M_S \tanh\left(\frac{pJ}{4k_BT}\frac{M}{M_S}\right)$$

Meaning we get,

$$m = \tanh\left(\frac{pJ}{4k_BT}m\right) \qquad m = \frac{M}{M_S}$$

We can introduce this for now (but will have some sense after),

$$k_BT_C = \frac{pJ}{4}$$

where T_C is the critical temperature, and we can define

$$t = \frac{T}{T_C}$$

Meaning,

$$m = \tanh\left(\frac{T_C}{T}m\right) = \tanh\left(\frac{m}{t}\right)$$

we already solved this equation graphicaly on the lecture
In order to check the stability of the solution, one has to check the sign of the curvature of the free energy, meaning the sign of $\mathrm{d}^2F/\mathrm{d}M^2$

$$F = \frac{JNp}{2}\frac{1}{4}\left(\frac{2VM}{Ng\mu_B}\right)^2 - Nk_BT\ln\left[2\cosh\left(\frac{\beta g\mu_B}{2}\lambda M\right)\right]$$
$$= \frac{JNp}{2}\frac{1}{4}m^2 - Nk_BT\ln\left[2\cosh\left(\frac{T_C}{T}m\right)\right]$$

Meaning,

$$f = \frac{F}{Nk_BT_C} = \frac{1}{2}m^2 - t\ln\left[2\cosh\left(\frac{m}{t}\right)\right]$$
$$= f(m=0) + \frac{m^2}{2} - t\ln\left[\cosh\left(\frac{m}{t}\right)\right]$$

$$\frac{\partial f}{\partial m} = m - \tanh\left(\frac{m}{t}\right)\bigg|_{\mathrm{eq}} = 0$$

Meaning,

$$m = \tanh\left(\frac{m}{t}\right)$$

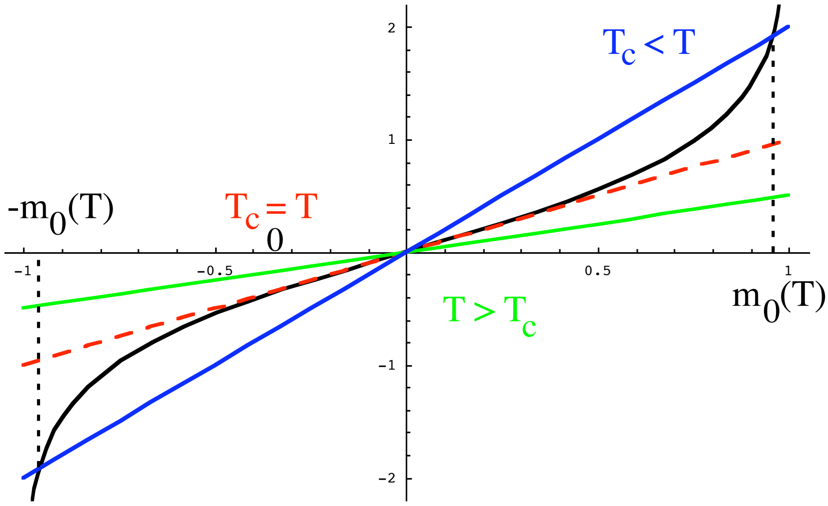

FIGURE (1) – Solution of the self-consistent equation for zero field $h = 0$ and for different temperatures : $T > T_C$ green solid line ($m = 0$), $T < T_C$ blue solid line ($m = -m_0, 0, m_0$) and $T = T_C$ red dashed line.

$$(\tanh x)' = \left(\frac{\sinh x}{\cosh x}\right)' = \frac{\cosh^2 x - \sinh^2 x}{\cosh^2 x} = 1 - \tanh^2 x$$

$$\begin{aligned} \frac{\partial^2 f}{\partial m^2} &= 1 - \frac{1}{t}\left[1 - \tanh^2\left(\frac{m}{t}\right)\right]\Big|_{\text{eq}} \\ &= 1 - \frac{1}{t}[1 - m^2] \end{aligned}$$

if $t > 1$, $m = 0$ is the only solution, and

$$\frac{\partial^2 f}{\partial m^2} = 1 - \frac{1}{t} > 0$$

Meaning it is a stable solution.
if $t < 1$, there is three solutions, $m = 0$, $m = \pm m_0(T)$

$$\frac{\partial^2 f}{\partial m^2} = 1 - \frac{1}{t} < 0$$

the solution for $m = 0$ is unstable,

$$\frac{\partial^2 f}{\partial m^2} = 1 - \frac{1}{t}(1 - m_0^2)$$

We can decide yet if those solutions are stable.

(b) Determine the magnetization in the low-temperature limit $T \ll T_c$, as well as in the vicinity of T_c (*i.e.*,for $0 < 1 - T/T_c \ll 1$).

$$t \ll 1 \longrightarrow m = \pm 1$$

$$t \to 1^- \longrightarrow m \ll 1$$

$$m \approx \frac{m}{t} - \frac{1}{3}\frac{m^3}{t^3}$$

We can divide by m since we can exclude the trivial solution $m = 0$,

$$\begin{aligned} 1 &\approx \frac{1}{t} - \frac{1}{3}\frac{m^2}{t^3} \\ &= \frac{1 - \frac{m^2}{3t^2}}{t} \end{aligned}$$

$$t = 1 - \frac{m^2}{3t^2}$$

$$m^2 = 3t^2(1-t)$$

$$t \to 1^- \qquad\qquad \varepsilon = 1 - t \ll 1$$

$$m^2 = 3(1-\varepsilon)^2\varepsilon \approx 3\varepsilon + \mathcal{O}(\varepsilon^2)$$

$$m^2 = 3(1-t)$$

Meaning,

$$m = \sqrt{3(1-t)}$$

Meaning,

$$M(T \approx T_C) = \pm M_S\sqrt{3\left(1 - \frac{T}{T_C}\right)}$$

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$$\begin{aligned}
\tanh x &= \frac{\sinh x}{\cosh x} = \frac{e^x - e^{-x}}{e^x + e^{-x}} \\
&\approx \frac{1 + x + \frac{x^2}{2} + \frac{x^3}{6} - \left(1 - x + \frac{x^2}{2} - \frac{x^3}{6}\right)}{1 + x + \frac{x^2}{2} + \frac{x^3}{6} + \left(1 - x + \frac{x^2}{2} - \frac{x^3}{6}\right)} \\
&= \frac{2x + \frac{x^3}{3}}{2 + x^2} \\
&= \frac{2x + \frac{x^3}{3}}{2(1 + x^2/2)} \\
&= \frac{2x + x^3/3}{2}\left(1 - \frac{x^2}{2}\right) \\
&\approx x + \frac{x^3}{6} - \frac{x^3}{2} \\
&\approx x - \frac{x^3}{3}
\end{aligned}$$

(c) Calculate the ensemble-averaged energy of the system. Deduce from your result the corresponding specific heat $\mathcal{C}$. How does the latter quantity behave as a function of temperature ? In particular, what happens for $T = T_c$?

$$\begin{aligned}
\langle E \rangle &= -\frac{\partial \ln Z}{\partial \beta} \\
&= \frac{\partial}{\partial \beta}\beta F \\
&= N k_B T_C \frac{m^2}{2} - N k_B T_C m \underbrace{\frac{\sinh(2\cosh(\beta k_B T_C m))}{\cosh(\beta k_B T_C m)}}_{=m} \\
&= -N k_B T_C \frac{m^2}{2}
\end{aligned}$$

Reminder :

$$F = 2N k_B T_C \left(\frac{m}{2}\right)^2 - N k_B T \ln(2\cosh(\beta k_B T_C m)) \qquad m = \frac{M}{M_S}$$

$$\begin{aligned} C_V &= -T\frac{\partial^2 F}{\partial T^2} \\ &= \frac{\partial\langle E\rangle}{\partial t}\frac{\partial t}{\partial T} \\ &= \frac{1}{T_C}\frac{\partial\langle E\rangle}{\partial t} \end{aligned}$$

for $t \to 1^-$, $m^2 \approx 3(1-t)$, and so we found,

$$C_V = \frac{3}{2}Nk_B$$

> **Remark** :
>
> $$\langle E\rangle = \frac{\partial}{\partial\beta}\beta F \qquad\qquad F = F(\beta, m(\beta))$$
>
> So, we should write
>
> $$\frac{\partial F}{\partial\beta} + \frac{\partial F}{\partial m}\frac{\partial m}{\partial\beta}$$
>
> but,
>
> $$\frac{\partial F}{\partial m} = 0$$
>
> since we're at equilibrium.

1.2.2 Properties of the system at finite magnetic field

We now consider the system to be subject to a finite magnetic field ($B_0 \neq 0$).

(a) Solve for the self-consistent equation 4 graphically. Consider first the case $T > T_c$, and then $T < T_c$. You shall consider that the magnetic field is finite, but weak (with respect to what ?)

$$\begin{aligned} m &= \tanh\left(\frac{m}{t} + \frac{\beta g\mu_B}{2}B_0\right) \\ &= \tanh\left(\frac{m}{t} + \frac{b_0}{t}\right) \end{aligned} \qquad\qquad b_0 = \frac{g\mu_B B_0}{2k_B T_C}$$

We can re-write it :

$$\tanh^{-1}(m) = \frac{1}{t}(m + b_0)$$

- $t > 1$
- $t < 1$

> **Remark** : This model predict a phase transition for dimension $d = 1$, but this is wrong.
> The more you increase the dimension d, the more the mean-field approximation is a good approximation.

(b) Use the previous result to calculate the magnetic susceptibility defined in Eq. 1. Compare to the paramagnetic case and to the Curie law 2.

- $t > 1$

$$\begin{aligned}
\chi &= \frac{\partial M}{\partial B_0}\bigg|_{B_0 \to 0} \\
&= \frac{\partial}{\partial B_0}(mM_S) \\
&= M_S \frac{\partial m}{\partial b_0}\frac{\partial b_0}{\partial B_0} \\
&= M_S \frac{g\mu_B}{2k_B T_C}\frac{\partial m}{\partial b_0}\bigg|_{b_0 \to 0} \\
&= M_S \frac{g\mu_B}{2k_B T_C}\xi
\end{aligned}$$

As $b_0 \to 0$, $m \ll 1$,

$$(m + b_0)\frac{1}{t} = \text{arctan}(m)$$

Meaning,

$$\frac{m}{t} + \frac{b_0}{t} = m \longrightarrow m \approx \frac{b_0}{t-1}$$

And so,

$$\xi = \frac{1}{t-1} \qquad\qquad t \geq 1$$

- $t < 1$

$$m = \tanh\left(\frac{m}{t} + \frac{b_0}{t}\right)$$

we take the derivative to have an order of ξ,

$$\begin{aligned}\xi = \frac{\partial m}{\partial b_0}\bigg|_{b_0\to 0} &= \frac{1}{t}(\xi+1)\left[1-\tanh^2\left(\frac{m}{t}+\frac{b_0}{t}\right)\bigg|_{b_0\to 0}\right] \\ &= \frac{1}{t}(\xi+1)\left[1-\frac{m}{t}+m^2\right]\end{aligned}$$

And so $t \to 1^-$, $b_0 = 0$, $m^2 \approx 3(1-t)$,

$$\begin{aligned}\xi &= \frac{1-m^2}{t-1+m^2} \\ &= \frac{3t-2}{2(1-t)} \\ &\approx \frac{1}{2(1-t)} && t < 1^-\end{aligned}$$

1.2.3 Mean-field critical exponants

From your results above, deduce the mean-field critical exponants, which are defined, in the vicinity of the critical temperature, as

$$\begin{aligned}M(T, B_0 = 0) &\sim (T_c - T)^\beta \\ C(T, B_0 = 0) &\sim (T - T_c)^\alpha \\ \chi &\sim (T - T_c)^{-\gamma}\end{aligned}$$

In a couple of weeks, you will compare these results to those of Problem Set 4.

$$\begin{aligned}M(T, B_0 = 0) &\sim (T_c - T)^{1/2} \\ C(T, B_0 = 0) &\sim (T - T_c)^0 \\ \chi &\sim (T - T_c)^{-1}\end{aligned}$$

2 1d Ising model : exact solution with the transfer matrix method

Let us consider a chain of N spins $s_i = \pm 1 (i = 0, 1, ..., N-1)$ at the temperature T and in an external magnetic field H, with a ferromagnetic interaction J between nearest neighbors. The corresponding Hamiltonian reads

$$\mathcal{H} = -J \sum_{i=0}^{N-1} s_i s_i + 1 - H \sum_{i=0}^{N-1} s_i$$

where we use periodic boundary conditions, that is, $s_N = s_0$.

2.1 Thermodynamical properties of the system

(a) Show that the canonical partition function of the system reads

$$Z = \sum_{s_0=\pm1} \sum_{s_1=\pm1} \sum_{s_2=\pm1} \cdots \sum_{s_{N-1}=\pm1} \mathcal{T}_{s_0 s_1} \mathcal{T}_{s_1 s_2} \cdots \mathcal{T}_{s_{N-1} s_0}$$

where the *transfer matrix* $\mathcal{T}$ (with dimensions 2×2) is defined through its matrix elements as

$$\mathcal{T}_{s_i s_{i+1}} = \exp\left(\beta J s_i s_{i+1} + \frac{\beta H}{2} [s_i + s_{i+1}] \right)$$

with $\beta = 1/k_B T$, and where the rows are labelled by $s_i = +1$ and -1, and the columns by $s_{i+1} = +1$ and -1, respectively. In particular, show that

$$\mathcal{T} = \begin{pmatrix} e^{\beta(J+H)} & e^{-\beta J} \\ e^{-\beta J} & e^{\beta(J-H)} \end{pmatrix}$$

We define $K = \beta J$, $h = \beta H$,

$$\begin{aligned} Z &= \sum_{s_0=\pm1} \cdots \sum_{s_{N-1}=\pm1} e^{K \sum_{i=0}^{N-1} s_i s_{i+1} + h \sum_{i=0}^{N-1} s_i} \\ &= \sum_{s_0=\pm1} \cdots \sum_{s_{N-1}=\pm1} e^{K(s_0 s_1 + s_1 s_2 + \cdots + s_{N-1} s_0)} e^{h(s_0 + s_1 + \cdots + s_{N-1}} \\ &= \sum_{s_0=\pm1} \cdots \sum_{s_{N-1}=\pm1} e^{K s_0 s_1 + \frac{h}{2}(s_0+s_1) \cdots} \\ &= \sum_{s_0=\pm1} \cdots \sum_{s_{N-1}=\pm1} \mathcal{T}_{s_0 s_1} \cdots \mathcal{T}_{s_{N-1} s_0} \end{aligned}$$

(b) Using matrix multplication, show that

$$Z = \sum_{s_0=\pm1} \left(\mathcal{T}^N \right)_{s_0 s_0} = \mathrm{Tr}\left\{ \mathcal{T}^N \right\} = \lambda_0^N + \lambda_1^N$$

where λ_0 and λ_1 ($|\lambda_0| > |\lambda_1|$ by convention) are the eigenvalues of $\mathcal{T}$. At the thermodynamical limit ($N \to \infty$), argue that $Z = \lambda_0^N$.

$$\sum_{s_{i+1}=pm1} \mathcal{T}_{s_i s_{i+1}} \mathcal{T}_{s_{i+1} s_{i+2}} = \left(\mathcal{T}^2\right)_{s_{i+1} s_{i+2}}$$

This is the same as the matrix multiplication,

$$\sum_j A_{ij} B_{jk} = \sum_j \langle i| A |j\rangle \langle j| B |k\rangle = \langle i| AB |k\rangle = (AB)_{ik}$$

$$\begin{aligned}
Z &= \sum_{s_0=\pm 1} \cdots \sum_{s_{N-1}=\pm 1} \mathcal{T}_{s_0 s_1} \cdots \mathcal{T}_{s_{N-1} s_0} \\
&= \sum_{s_0=\pm 1} \left(\mathcal{T}^N\right)_{s_0 s_0} \\
&= \mathrm{Tr}\left\{\mathcal{T}^N\right\} \\
&= \lambda_0^N + \lambda_1^N
\end{aligned}$$

Intermezzo :

$$D = \begin{pmatrix} \lambda_1 & 0 \\ 0 & \lambda_n \end{pmatrix} \qquad P = (\vec{\alpha}_1, \cdots, \vec{\alpha}_n) \text{ with } M\vec{\alpha}_i = \lambda_i \vec{\alpha}_i$$

$$M = PDP^{-1}$$

So,

$$\begin{aligned}
\mathrm{Tr}(M) &= \mathrm{Tr}(PDP^{-1}) \\
&= \mathrm{Tr}(DP^{-1}P) \qquad\qquad = \mathrm{Tr}(D) \\
&= \sum_{i=1}^{n} \lambda_i
\end{aligned}$$

$$Z = \lambda_0^N \left[1 + \left(\frac{\lambda_1}{\lambda_0}\right)^N\right]$$

Meaning at the thermodynamic limit,

$$Z_{N \gg 1} \approx \lambda_0^N$$

(c) Deduce from the previous result that

$$Z = \left[e^{\beta J} \cosh(\beta H) + \sqrt{e^{2\beta J} \sinh^2(\beta H) + e^{-2\beta J}}\right]^N$$

(d) Still at the thermodynamical limit, determine the free energy of the system.

$$F = -Nk_BT\ln\left[e^{\beta J}\cosh(\beta H) + \sqrt{e^{2\beta J}\sinh^2(\beta H) + e^{-2\beta J}}\right]$$

> **Remark** :
> If we set $K = 0$, *i.e.*, the non-interacting limit, we find back $Z = (2\cosh(h))^N$, which is the familiar paramagnetic situation.

(e) Deduce from the previous question the average magnetization $M = \langle s_i \rangle$ of the system. Plot your result as a function of the applied magnetic field. What can you tell about the noninteracting case $J = 0$ and the limit $J/k_BT \gg 1$ (strongly-interacting limit). Give a qualitative interpretation to your results. Is there a phase transition for the exactly-solved 1d Ising model ? Compare with the mean-field solution of Problem 1.

$$\begin{aligned} M &= \langle s_i \rangle \\ &= -\frac{1}{N}\frac{\partial F}{\partial N} \\ &= -\frac{1}{N}\frac{\partial F}{\partial h}\frac{\partial h}{\partial H} \\ &= \frac{e^K\sinh(h) + \frac{1}{2}2\sinh(h)\cosh(h)e^{2K}/\sqrt{e^{2K}\sinh^2(h) + e^{-2K}}}{e^K\cosh(h) + \sqrt{e^{2K}\sinh^2(h) + e^{-2K}}} \\ &= \frac{e^K\sinh(h)}{\sqrt{e^{2K}\sinh^2(h) + e^{-2K}}} \end{aligned}$$

Limit cases :

- $K = 0$:

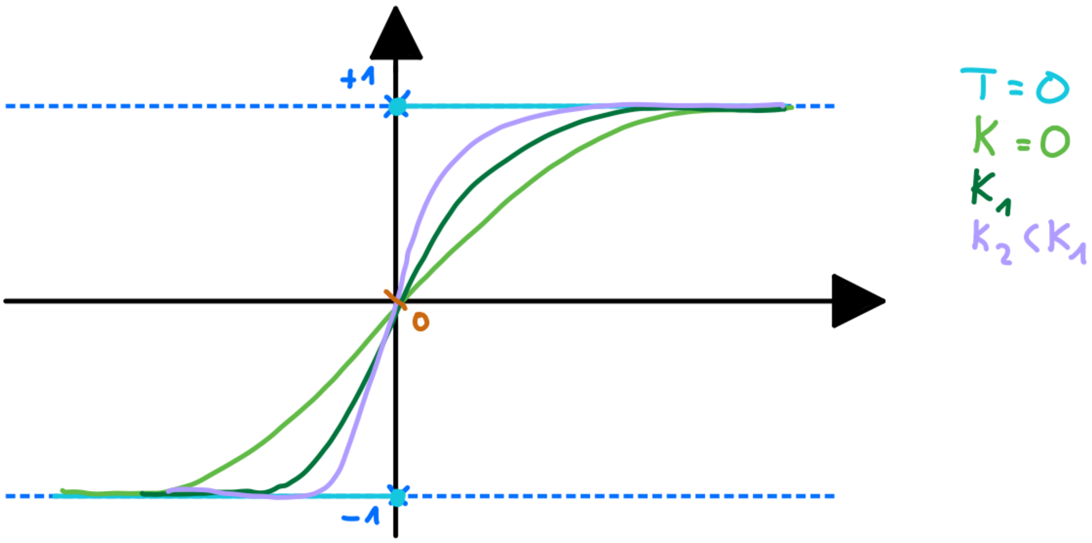
$$M = \tanh(h)$$

- $h \ll 1$:

$$M \approx e^{2K}h$$

- $K \to +\infty$:

$$M \approx \frac{\sinh(h)}{|\sinh(h)|} = \text{sgn}(h)$$



> **Remark** :
> WIthin the mean-field approximation (MFA), for dimension $d = 1$, we found $T_C = 2J/k_B$.
> But, as we seen here, there is **no phase transition in 1D** for the Ising model. This does mean that this approximation is bad in this case.
> In fact, the MFA is always wrong in 1D, because we're doing the mean of too little neighbours.

2.2 Correlation function

The correlation function between two spins separated by $R - 1$ lattice sites is defined as

$$\Gamma_R = \langle s_0 s_R \rangle - \langle s_0 \rangle \langle s_R \rangle$$

and the correlation lenghth ξ by

$$\xi^{-1} = \lim_{R\to\infty} \left\{ -\frac{\ln |\Gamma_R|}{R} \right\} \tag{5}$$

(a) Let us express Γ_R in terms of the transfer matrix $\mathcal{T}$ and the matrix $\mathcal{S}$ representing the spin operator. We write $\mathcal{T}$ and $\mathcal{S}$ in their diagonal form :

$$\mathcal{T} = \sum_{n=0,1} \lambda_n |u_n\rangle \langle u_n|$$

$$\mathcal{S} = \sum_{s_i=\pm 1} s_i |s_i\rangle \langle s_i|$$

The vectors $|s_i = +1\rangle = (1,0)$ and $|s_i = -1\rangle = (0,1)$ correspond to the two possible spin states. Using $\mathcal{T}$ and $\mathcal{S}$, show that

$$\langle s_0 \rangle = \langle s_R \rangle = \langle u_0 | \mathcal{S} | u_0 \rangle$$

in the thermodynamical limit.

$$\begin{aligned}
\langle s_0 \rangle &= \sum_{s_0} \cdots \sum_{s_{N-1}} s_0 \mathcal{T}_{s_0 s_1} \cdots \mathcal{T}_{s_{N-1} s_0} \frac{1}{Z} \\
&= \frac{1}{Z} \sum_{s_0} s_0 \mathcal{T}^N_{s_0 s_0} \\
&= \frac{1}{Z} \sum_{s_0} s_0 \langle s_0 | \sum_{n=0}^{1} \lambda_n^N | u_n \rangle \langle u_n | s_0 \rangle \\
&= \frac{1}{Z} \sum_{s_0} \langle u_n | s_0 \rangle s_0 \langle s_0 | \sum_{n=0}^{1} \lambda_n^N | u_n \rangle \\
&= \frac{1}{Z} \sum_{n=0}^{1} \lambda_n^N \langle u_n | \sum_{s_0} s_0 | s_0 \rangle \langle s_0 | u_n \rangle \\
&= \frac{1}{Z} \sum_{n=0}^{1} \lambda_n^N \langle u_n | \mathcal{S} | u_n \rangle \\
&= \frac{1}{\sum_{n=0}^{1} \lambda_n^N} \sum_{n=0}^{1} \lambda_n^N \langle u_n | \mathcal{S} | u_n \rangle \\
&= \frac{\lambda_0^N \left[\langle u_0 | \mathcal{S} | u_0 \rangle + \left(\frac{\lambda_1}{\lambda_0} \right)^N \langle u_1 | \mathcal{S} | u_1 \rangle \right]}{\lambda_0^N \left[1 + \left(\frac{\lambda_1}{\lambda_0} \right)^N \right]} \\
&\approx \langle u_0 | \mathcal{S} | u_0 \rangle
\end{aligned}$$

We see that this result is independant of i in $\langle s_i \rangle$, meaning,

$$\langle s_0 \rangle = \langle s_R \rangle = \langle u_0 | \mathcal{S} | u_0 \rangle$$

(b) Then, show that

$$\langle s_0 s_R \rangle = \sum_{n=0}^{1} \left(\frac{\lambda_n}{\lambda_0} \right)^R \langle u_0 | \mathcal{S} | u_0 \rangle \langle u_n | \mathcal{S} | u_0 \rangle$$

for $N \gg 1$.

$$
\begin{aligned}
\langle s_0 s_R \rangle &= \sum_{s_0} \cdots \sum_{s_R} \cdots \sum_{S_{N-1}} \frac{1}{Z} s_0 \mathcal{T}_{s_0 s_1} \cdots \mathcal{T}_{s_{R-1} s_R} s_R \mathcal{T}_{s_R s_{R+1}} \cdots \mathcal{T}_{s_{N-1} s_0} \\
&= \frac{1}{Z} \sum_{s_0} \sum_{s_R} s_0 \mathcal{T}^R_{s_0 s_R} s_R \mathcal{T}^{N-R}_{s_R s_0} \\
&= \frac{1}{Z} \sum_{s_0, s_R} s_0 \langle s_0 | \sum_{n=0}^{1} \lambda_n^R |u_n\rangle \langle u_n | s_R \rangle s_R \langle s_R | \sum_{m=0}^{1} \lambda_m^{N-R} |u_m\rangle \langle u_m | s_0 \rangle \\
&= \frac{1}{Z} \sum_{s_0} s_0 \langle s_0 | \sum_{n=0}^{1} \lambda_n^R |u_n\rangle \langle u_n | \mathcal{S} \sum_{m=0}^{1} \lambda_m^{N-R} |u_m\rangle \langle u_m | s_0 \rangle \\
&= \frac{1}{Z} \sum_{n,m=0}^{1} \sum_{s_0} s_0 \langle s_0 | \lambda_n^R |u_n\rangle \langle u_n | \mathcal{S} \lambda_m^{N-R} |u_m\rangle \langle u_m | s_0 \rangle \\
&= \frac{1}{Z} \sum_{n,m=0}^{1} \langle u_m | s_0 \rangle \sum_{s_0} s_0 \langle s_0 | \lambda_n^R |u_n\rangle \langle u_n | \mathcal{S} \lambda_m^{N-R} |u_m\rangle \\
&= \frac{1}{Z} \sum_{n,m=0}^{1} \langle u_m | \sum_{s_0} |s_0\rangle s_0 \langle s_0 | \lambda_n^R |u_n\rangle \langle u_n | \mathcal{S} \lambda_m^{N-R} |u_m\rangle \\
&= \frac{1}{Z} \sum_{n,m=0}^{1} \langle u_m | \mathcal{S} \lambda_n^R |u_n\rangle \langle u_n | \mathcal{S} \lambda_m^{N-R} |u_m\rangle \\
&= \frac{1}{Z} \sum_{n,m=0}^{1} \lambda_n^R \lambda_m^{N-R} \langle u_m | \mathcal{S} |u_n\rangle \langle u_n | \mathcal{S} |u_m\rangle \\
&= \frac{1}{Z} \sum_{n} \lambda_n^R \lambda_0^{N-R} \left[\langle u_0 | \mathcal{S} |u_n\rangle \langle u_n | \mathcal{S} |u_0\rangle + \left(\frac{\lambda_1}{\lambda_0}\right)^{N-R} \langle u_1 | \mathcal{S} |u_n\rangle \langle u_n | \mathcal{S} |u_1\rangle \right] \\
&\approx \sum_{n=0}^{1} \left(\frac{\lambda_n}{\lambda_0}\right)^R \langle u_0 | \mathcal{S} |u_n\rangle \langle u_n | \mathcal{S} |u_0\rangle
\end{aligned}
$$

(c) Deduce from the two previous questions that

$$
\Gamma_R = \left(\frac{\lambda_1}{\lambda_0}\right)^R \langle u_0 | \mathcal{S} |u_1\rangle \langle u_1 | \mathcal{S} |u_0\rangle \tag{6}
$$

$$
\begin{aligned}
\Gamma_R &= \langle s_0 s_R \rangle - \langle s_0 \rangle \langle s_R \rangle \\
&= \left(\frac{\lambda_1}{\lambda_0}\right)^R \langle u_0 | \mathcal{S} |u_1\rangle \langle u_1 | \mathcal{S} |u_0\rangle
\end{aligned}
$$

(d) Calculate explicitly the correlation function 6. It will be accepted without calculating them that the eigenvectors of the transfer matrix read $|u_0\rangle = (\alpha_+, \alpha_-)$ and $|u_1\rangle = (\alpha_-, -\alpha_+)$, with

$$\alpha_{\pm} = \frac{1}{\sqrt{2}}\left(1 \pm \frac{e^{\beta J}\sinh(\beta H)}{\sqrt{e^{2\beta J}\sinh^2(\beta H) + e^{-2\beta J}}}\right)^{1/2}$$

In particular, study the zero-magnetic field limit. In the latter case, plot the correlation function as a function of R.

$$\langle u_0|\,\mathcal{S}\,|u_1\rangle = \begin{pmatrix}\alpha_+ & \alpha_-\end{pmatrix}\begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix}\begin{pmatrix}\alpha_-\\ -\alpha_+\end{pmatrix} = 2\alpha_+\alpha_- = \langle u_1|\,\mathcal{S}\,|u_0\rangle$$

Meaning,

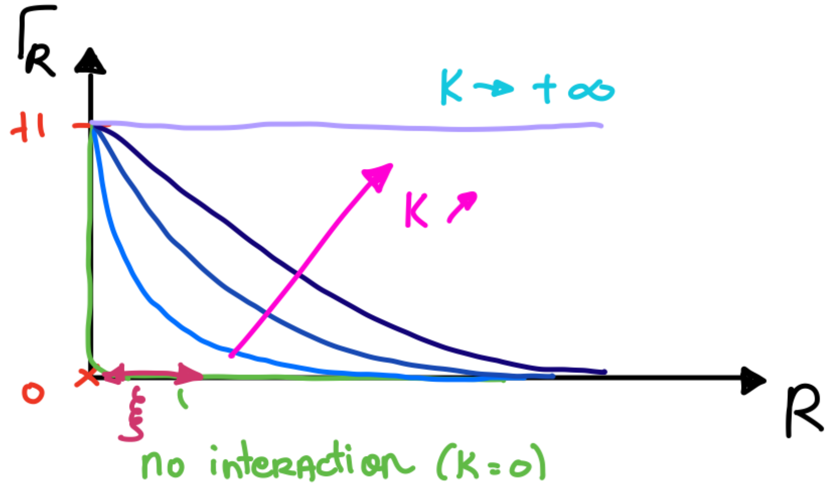
$$\Gamma_R = \left(\frac{\lambda_1}{\lambda_0}\right)^R (2\alpha_+\alpha_-)^2$$

(e) Calculate the correlation length 5 using the expression 6. Comment on the low-and high-temperature limits.

$$\begin{aligned}\Gamma_R &= \left(\frac{\lambda_1}{\lambda_0}\right)^R (2\alpha_+\alpha_-)^2\\ &= \left(\frac{e^K\cosh(h) - \sqrt{e^{2K}\sinh^2(h) + e^{-2K}}}{e^K\cosh(h) + \sqrt{\cdots}}\right)^R \frac{e^{-2K}}{e^{2K}\sinh^2(h) + e^{-2K}}\end{aligned}$$

for $h = 0$,

$$\begin{aligned}\Gamma_R &= (\tanh(K))^R\\ &= e^{\ln(\tanh(K))^R}\\ &= e^{R\ln(\tanh(K))}\\ &= e^{-R|\ln(\tanh(K))|}\\ &= e^{-R/\xi}\end{aligned}$$



Γ_R
+1
0
$K \to +\infty$
$K \nearrow$
ξ
1
R
no interaction (K=0)