

Using the constraints

$$\begin{cases} \text{Tr}^{(i)}(\rho_i) = 1 & \rightarrow a + b = 1 \\ \text{Tr}^{(i)}(\rho_i S_i) = m_i & \rightarrow a - b = m_i \end{cases}$$

where a, b are the functions of the order parameter. In that case we have not to write the functions for all the i . For $S_i = 1$ we have one value, for all the other values another one. The results of the previous equation are:

$$\begin{cases} a = \frac{1-m_i}{2} \\ b = \frac{1+m_i}{2} \end{cases}$$

Hence,

$$\rho_i = \frac{1-m_i}{2}(1 - \delta_{S_i,1}) + \frac{1+m_i}{2}\delta_{S_i,1} \quad (1)$$

that in matrix form can be expressed as

$$\rho_i = \begin{pmatrix} \frac{(m_i+1)}{2} & 0 \\ 0 & \frac{(1-m_i)}{2} \end{pmatrix} \quad (2)$$

Mean field energy term

Let us consider the average of the Hamiltonian

$$\langle \mathcal{H} \rangle_{\rho_{MF}} = \left\langle -J \sum_{\langle ij \rangle} S_i S_j - \sum_i H_i S_i \right\rangle_{\rho_{MF}} = -J \sum_{\langle ij \rangle} \langle S_i S_j \rangle_{\rho_{MF}} - \sum_i H_i \langle S_i \rangle_{\rho_{MF}} \quad (3)$$

Since we have

$$\rho_{MF} = \prod_{i=1}^N \rho_i$$

the term $\langle S_i S_j \rangle_{\rho_{MF}}$ will transform into

$$\langle S_i S_j \rangle_{\rho_{MF}} = \langle S_i \rangle_{\rho_{MF}} \langle S_j \rangle_{\rho_{MF}}$$

Moreover, for all function g of S_i we can write

$$\begin{aligned} \langle g(S_i) \rangle_{\rho_{MF}} &= \text{Tr}^{(i)}(g(S_i) \rho_i) = \sum_{S_i=\pm 1} g(S_i) \rho_i \\ &= \sum_{S_i=\pm 1} g(S_i) \left[\frac{1+m_i}{2} \delta_{S_i,1} + \frac{1-m_i}{2} (1 - \delta_{S_i,1}) \right] \\ &= \frac{1+m_i}{2} g(1) + \frac{1-m_i}{2} g(-1) \end{aligned}$$

Note that, if $g(S_i) = S_i$, we have $g(1) = +1$ and $g(-1) = -1$, hence

$$\langle S_i \rangle_{\rho_{MF}} = m_i$$

as expected. Taken this into account, the Hamiltonian can be rewritten as

$$\langle \mathcal{H} \rangle_{\rho_{MF}} = -J \sum_{\langle ij \rangle} m_i m_j - \sum_i H_i m_i \quad (4)$$

Remark. This has the form of the original Hamiltonian where S_i had been replaced by their statistical averages.

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The entropy term is:

$$\begin{aligned}\langle \ln \rho \rangle_{\rho_{MF}} &= \text{Tr}(\rho \ln \rho) \stackrel{MF}{=} \sum_i \text{Tr}^{(i)}(\rho_i \ln \rho_i) \\ &= \sum_i \left[\frac{1+m_i}{2} \ln \frac{1+m_i}{2} + \frac{1-m_i}{2} \ln \frac{1-m_i}{2} \right]\end{aligned}\quad (5)$$

The total free energy in Eq.(??) becomes:

$$\begin{aligned}F_{\rho_{MF}} &= \langle \mathcal{H} \rangle_{\rho_{MF}} + k_B T \langle \ln \rho \rangle_{\rho_{MF}} \\ &= -J \sum_{\langle ij \rangle} m_i m_j - \sum_i H_i m_i + k_B T \sum_i \left[\frac{1+m_i}{2} \ln \frac{1+m_i}{2} + \frac{1-m_i}{2} \ln \frac{1-m_i}{2} \right]\end{aligned}\quad (6)$$

We now look for the values $m_i = \bar{m}_i$, that minimizes $F_{\rho_{MF}}$ (equilibrium phases):

$$\left. \frac{\partial F_{\rho_{MF}}}{\partial m_i} \right|_{m_i = \bar{m}_i} = 0$$

This gives:

$$0 = -J \sum_{j \in n.n. \text{ of } i} \bar{m}_j - H_i + \frac{k_B T}{2} \ln \left[\frac{1+\bar{m}_i}{1-\bar{m}_i} \right]$$

To solve it, remember that

$$\tanh^{-1}(x) = \frac{1}{2} \ln \frac{1+x}{1-x} \quad |x| < 1$$

Hence,

$$k_B T \tanh^{-1}(\bar{m}_i) = J \sum_{j \in n.n. \text{ of } i} \bar{m}_j + H_i$$

which implies

$$\bar{m}_i = \tanh \left[(k_B T)^{-1} \left(J \sum_{j \in n.n. \text{ of } i} \bar{m}_j + H_i \right) \right]$$

We have again found the self-consistency equation for the magnetization that we have already encountered in the Weiss mean field theory for the Ising model! This is again a confirmation that all mean field theories are equivalent. Defining

$$z\bar{m}_i \equiv \sum_{j \in n.n. \text{ of } i} \bar{m}_j$$

we get

$$\bar{m}_i = \tanh [\beta (J z \bar{m}_i + H_i)] \quad (7)$$

this is the Bragg-William approximation.

Example 1: Ising anti-ferromagnet in an external field

Let us consider the model

$$\mathcal{H} = +J \sum_{\langle ij \rangle} S_i S_j - H \sum_i S_i, \quad (8)$$

Note the + sign before J , this means that the interactions are anti-ferromagnetic. Let us consider two cases:

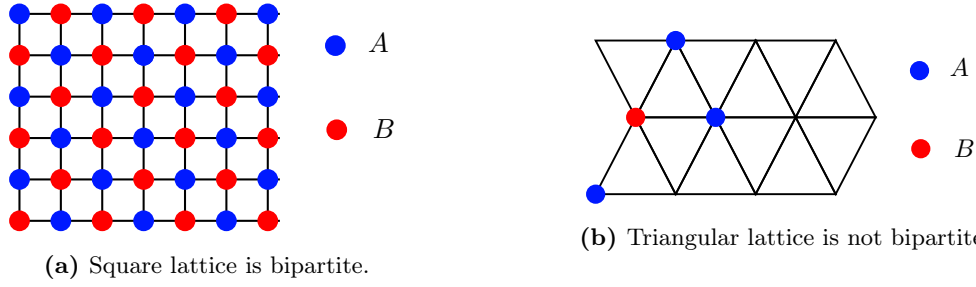


Figure 1: Ising anti-ferromagnet in an external field.

- If $H = 0$ ferromagnetic and anti-ferromagnetic behave similarly when the interactions are between nearest neighbours on a *bipartite lattice*, i.e. a lattice that can be divided into two sublattices, say A and B , such that a A site has only B neighbours and a B site only A ones.

Remark. FCC is not bipartite, while BCC it is. See Figure 1.

If the lattice is bipartite and J_{ij} is non zero only when i and j belong to different sublattices (they do not have to be only n.n!), one can redefine the spins such that

$$S'_j = \begin{cases} +S_j & j \in A \\ -S_j & j \in B \end{cases}$$

Clearly, $S'_i S'_j = -S_i S_j$. It is like if the J_{ij} have changed sign and we are formally back to ferromagnetic model for the two sublattices:

$$\mathcal{H}^* = -J \sum_{\langle ij \rangle} S'_i S'_j \quad (9)$$

i.e. a ferromagnetic Ising.

- In presence of a magnetic field H , we need to reverse its sign when applied to sites B .

The thermodynamic of a ferromagnetic Ising model on a bipartite lattice in a uniform magnetic field H is identical to the one of the Ising antiferromagnetic model in presence of the so called *staggered field*, i.e. $H_A = H$ and $H_B = -H$. The Hamiltonian is

$$\mathcal{H}^*[S] = -J \sum_{\langle r_A r_B \rangle} S(r_A) S(r_B) - H \sum_{r_A} S(r_A) + H \sum_{r_B} S(r_B), \quad J > 0, H > 0 \quad (10)$$

The average magnetization per spin is

$$m \equiv \frac{1}{2}(m_A + m_B)$$

while

$$m_S = \frac{1}{2}(m_A - m_B)$$

is the *staggered magnetization*.

In order to use the variational density matrix method for this problem we consider two independent variational parameters m_A and m_B for sublattice

A and B respectively. On each sublattice, the model is like the standard Ising

$$\begin{cases} \rho_A^{(1)}(S) = \frac{1+m_A}{2}\delta_{S,1} + \frac{1-m_A}{2}\delta_{S,-1} \\ \rho_B^{(1)}(S) = \frac{1+m_B}{2}\delta_{S,1} + \frac{1-m_B}{2}\delta_{S,-1} \end{cases}$$

Remark. Note that, being H uniform, $\langle S_i \rangle = m$, i.e. does not depend on i . Same for the 1-particle distribution functions $\rho_A^{(1)}(S)$ and $\rho_B^{(1)}(S)$.

By performing the calculation for the terms

$$\langle \mathcal{H} \rangle_{\rho_{MF}} = -J \sum_{\langle ij \rangle} \langle S_i S_j \rangle_{\rho_{MF}} - H \sum_i \langle S_i \rangle_{\rho_{MF}}$$

$$\langle \ln \rho \rangle_{\rho_{MF}} = \sum_i \text{Tr}^{(i)}(\rho_i \ln \rho_i)$$

as before, but remembering to partition the procedure into the two sublattices A and B , one can show that the variational free energy is given by

$$\frac{F(m_A, m_B)}{N} = \frac{z\hat{J}}{2} m_A m_B - \frac{1}{2} H(m_A + m_B) - \frac{1}{2} k_B T s(m_A) - \frac{1}{2} k_B T s(m_B) \quad (11)$$

where the entropy term is

$$s(m) = \left[\frac{1+m}{2} \ln \left(\frac{1+m}{2} \right) + \frac{1-m}{2} \ln \left(\frac{1-m}{2} \right) \right]$$

By differentiating $\frac{F}{N}$ with respect to m_A and m_B , one gets

$$\begin{aligned} \frac{\partial(F/N)}{\partial m_A} = 0 & \Rightarrow m_B = \frac{H}{z\hat{J}} - \frac{k_B T}{z\hat{J}} \ln \left(\frac{1+m_A}{1-m_A} \right) \\ \frac{\partial(F/N)}{\partial m_B} = 0 & \Rightarrow m_A = \frac{H}{z\hat{J}} - \frac{k_B T}{z\hat{J}} \ln \left(\frac{1+m_B}{1-m_B} \right) \end{aligned}$$

As before, since

$$\tanh^{-1}(x) = \frac{1}{2} \ln \frac{1+x}{1-x}$$

these self-consistent equations can be written as

$$\begin{cases} m_A = \tanh \left(\beta \left(H - z\hat{J}m_B \right) \right) \\ m_B = \tanh \left(\beta \left(H - z\hat{J}m_A \right) \right) \end{cases} \quad (13)$$

The sites $\in A$ experience an internal field $H_{A,MF} = -z\hat{J}m_B$ from the B neighbours and vice versa for the sites $\in B$.

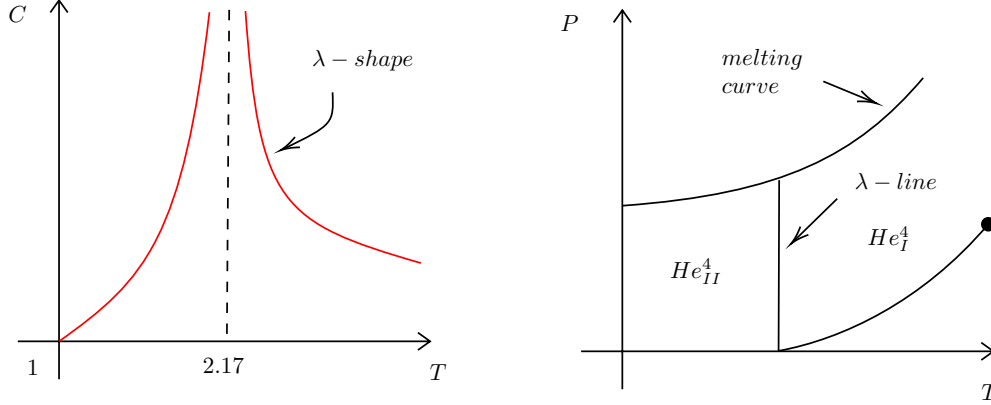
0.0.1 Second approach: Blume-Emery-Griffith model

We apply this approach to the so called *Blume-Emery-Griffith model*. This is a spin model with vacancies that describes the phase diagram and the critical properties of an interacting system displaying a *tricritical point*. Perhaps the most famous of these systems is the $\text{He}^3 - \text{He}^4$ mixture undergoing a fluid-superfluid transition.

Remark. He^4 is a non radiative isotope with two protons and two neutrons. Roughly

1/4 of the universe matter is He^4 ! From a quantum statistical point of view He^4 is a *boson*.

A gas of He^4 undergoes a fluid-superfluid transition at $T_\lambda = 2.17\text{K}$ and $P = P_0$. It is known as λ -transition since at $T \sim T_\lambda$ the specific heat $c(T)$ behaves as in Figure 2a: the plot of the specific heat as a function of the temperature has a shape that resembles a λ . The λ -transition is a genuine critical point (second order). For $T < T_\lambda$, He^4 is in the superfluid phase and it can be described by a two-fluids model in which one component has zero viscosity and zero entropy.



(a) Plot of the specific heat $c(T)$. It has the shape of a λ .

(b) (P, T) phase diagram.

Figure 2

The BEG model is used to describe what happens when we add some He^3 to the system constituted by He^4 ; it does not consider quantum effects, but only the "messing up" due to the He^3 impurities.

Remark. He^3 is a non-radioactive isotope with 2 protons and 1 neutron. From a quantum statistical point of view is a *fermion*.

Experimentally when He^3 is added to He^4 the temperature of the fluid-superfluid transition decreases. More specifically, if inserted in a system of He^4 it will "dilute" its bosonic property. Then, one expects that T_λ decreases, as observed. Denoting by x the concentration of He^3 , one observes

$$T_\lambda = T_\lambda(x)$$

with $T_\lambda(x)$ that decreases as x increases.

For small concentration of He^3 the mixture remains homogeneous, and the only effect is the change of T_λ . However, when the concentration x of He^3 reaches the critical value x_t

$$x > x_t = \frac{n_3}{n_3 + n_4} \sim 0.67$$

He^3 and He^4 separate into two phases (just like oil separates from water, the mixture undergoes a separation between a phase rich and a phase poor of He^3) and the λ transition becomes first-order (namely, discontinuous). The transition point (x_t, T_t) where the system shifts from a continuous λ -transition to a discontinuous one is that where the phase separation starts and is called tricritical point (i.e. it is a critical point that separates a line of second order transition from a line of first order transition). The BEG model was introduced to describe such a situation.

BEG Model

As we have anticipated, the BEG Model is a lattice gas model and so it is based on an Ising-like Hamiltonian. In particular, it is the model of a diluted ferromagnetic

system. On the sites of this lattice we define a variable S_i which can assume the values $-1, 0$ and $+1$: we decide that when an He^4 atom is present in a lattice site then $S_i = \pm 1$, while when $S_i = 0$ it means that the site is occupied by an He^3 atom. We then define our order parameter to be

$$\langle S_i \rangle = m_i$$

In the Ising model $\langle S_i^2 \rangle$ can only be equal to 1, while in this case it can be either 0 or 1: we can thus interpret $\langle S_i^2 \rangle$ as the concentration of He^4 atoms, and

$$x \equiv 1 - \langle S_i^2 \rangle$$

as the fraction of He^3 . We also define

$$\Delta \propto \mu_{\text{He}^3} - \mu_{\text{He}^4}$$

to be the difference of the chemical potentials of He^3 and He^4 ; since this parameter is related to the number of He^3 and He^4 atoms, we expect that when

- $x \rightarrow 0$ (namely, there is only He^4), we have $\Delta \rightarrow -\infty$.
- $x \rightarrow 1$ (namely, there is only He^3), we have $\Delta \rightarrow +\infty$.

and the order parameter for the λ -transition becomes

$$\langle S_i \rangle = \begin{cases} 0 & T > T_\lambda \\ m & T < T_\lambda \end{cases}$$

We consider the following Hamiltonian for the system:

$$\mathcal{H} = -J \sum_{\langle ij \rangle}^N S_i S_j + \Delta \sum_{i=1}^N S_i^2 - \Delta N \quad (14)$$

Remark. N is the total number of lattice sites. The ΔN term is a typical term for a gas in grand canonical ensemble.

Variational mean field approach to BEG

Since we want to apply the second variational method that we have seen, we write the mean field probability density as:

$$\rho_{MF} = \prod_i \rho_i = \prod_i \rho(S_i)$$

and the free energy:

$$G(T, J, \Delta) = \langle \mathcal{H} \rangle_{\rho_{MF}} + k_B T \sum_i \text{Tr}(\rho_i \ln \rho_i) \quad (15)$$

The mean value of the Hamiltonian is:

$$\langle \mathcal{H} \rangle_{\rho_{MF}} = -J \sum_{\langle ij \rangle} \langle S_i S_j \rangle + \Delta \sum_i \langle S_i^2 \rangle - N\Delta$$

and since $\langle S_i S_j \rangle = \langle S_i \rangle \langle S_j \rangle$ (it's the fundamental hypothesis of mean field theories) we get

$$\langle \mathcal{H} \rangle_{\rho_{MF}} \stackrel{MF}{\simeq} -J \sum_{\langle ij \rangle} \langle S_i \rangle \langle S_j \rangle + \Delta \sum_i \langle S_i^2 \rangle - N\Delta$$

We have also

$$\langle S_i \rangle = \langle S_j \rangle \equiv m$$

Therefore, the free energy of the system is:

$$G(T, J, \Delta)_{MF} = -\frac{1}{2}NJz(\text{Tr}_{S_i}(\rho_i S_i))^2 + N\Delta \text{Tr}_{S_i}(\rho_i S_i^2) - N\Delta + Nk_B T \text{Tr}_{S_i}(\rho_i \ln \rho_i) \quad (16)$$

where z is the coordination number of the lattice.

We now must minimize this expression with respect to ρ_i , with the constraint $\text{Tr}_{S_i}(\rho_i) = 1$:

$$\frac{dG}{d\rho_i} = 0$$

Let us consider each term

$$\begin{aligned} \frac{d}{d\rho_i}(\text{Tr}(\rho_i S_i))^2 &= 2(\text{Tr}(\rho_i S_i))S_i = 2\langle S_i \rangle S_i = 2mS_i \\ \frac{d}{d\rho_i}(\text{Tr}(\rho_i S_i^2)) &= S_i^2 \\ \frac{d}{d\rho_i}(\text{Tr}(\rho_i \ln \rho_i)) &= \ln \rho_i + 1 \end{aligned}$$

then,

$$\frac{dG}{d\rho_i} = -JNzmS_i + N\Delta S_i^2 + Nk_B T \ln \rho_i + Nk_B T = 0$$

Dividing by $Nk_B T$,

$$\ln \rho_i \equiv \ln \rho^{(1)}(S_i) = \beta JzmS_i - \beta \Delta S_i^2 - 1$$

which leads to

$$\rho^{(1)}(S_i) = \frac{1}{A} e^{\beta(zJmS_i - \Delta S_i^2)} \quad (18)$$

where we have reabsorbed e^{-1} into the normalization constant A . The constant A can be found by imposing the constraint $\text{Tr}_{S_i} \rho^{(1)}(S_i) = 1$, we find

$$A = 1 + 2e^{-\beta\Delta} \cosh(\beta z Jm) \quad (19)$$

Example 2: How to compute A

By imposing the constraint $\text{Tr}_{S_i} \rho^{(1)}(S_i) = 1$ (recall that $S_i = \pm 1, 0$), we get

$$1 = \frac{1}{A} \left(e^{\beta(zJm(+1) - \Delta(+1)^2)} + e^{\beta(zJm(-1) - \Delta(-1)^2)} + e^{\beta(zJm(0) - \Delta(0)^2)} \right)$$

Hence, by rearranging

$$1 = \frac{1}{A} \left(2e^{-\beta\Delta} \cosh(\beta z Jm) + 1 \right) \Rightarrow A = 1 + 2e^{-\beta\Delta} \cosh(\beta z Jm)$$

Given $\rho^{(1)}(S_i)$ it is possible to show

$$\langle S_i^2 \rangle = \text{Tr}_{S_i}(\rho_i S_i^2) = \frac{1}{A} 2e^{-\beta\Delta} \cosh(\beta z Jm)$$

and

$$x = 1 - \langle S_i^2 \rangle = \frac{A - 2e^{-\beta\Delta} \cosh(\beta z Jm)}{A} \Rightarrow x = \frac{1}{A}$$

Hence, substituting this expression of ρ_i into G , after some mathematical rearrangement we get:

$$\frac{G(T, \Delta, m, J)}{N} = \frac{z}{2} J m^2 - \Delta - k_B T \ln A \quad (20)$$

In order to find the equilibrium state for any T and Δ , we must minimize this expression of $G(T, \Delta, m, J)$ with respect to m . If we expand G for small values of m , keeping in mind the Taylor expansions

$$\cosh(t) = 1 + \frac{t^2}{2} + \frac{t^4}{24}, \quad \ln(1+t) = t - \frac{t^2}{2}$$

we get

$$G(T, \Delta, J, m) = a_0(T, \Delta) + a(T, \Delta)m^2 + b(T, \Delta)m^4 + \frac{c(T, \Delta)}{6}m^6 \quad (21)$$

where

$$\begin{cases} a_0(T, \Delta) = -k_B T \ln(1 + 2e^{-\beta\Delta}) - \Delta \\ a(T, \Delta) = \frac{zJ}{2} \left(1 - \frac{zJ}{\delta k_B T}\right) \\ b(T, \Delta) = \frac{zJ}{8\delta^2} (\beta z J)^3 \left(1 - \frac{\delta}{3}\right) \\ c(T, \Delta) > 0 \end{cases} \quad (22)$$

and the parameter δ is

$$\delta \equiv 1 + \frac{e^{\beta\Delta}}{2} = \delta(T, \Delta) \quad (23)$$

Note that unlike the Ising model in the Weiss approximation in this case both the quadratic and the quartic terms, a and b , can change sign when the parameters assume particular values. Let us also note that the order parameter of the system, namely the concentration of He^3 , is:

$$x(T, \Delta, J) = 1 - \langle S_i^2 \rangle = \frac{1}{A} = \frac{1}{1 + 2e^{-\beta\Delta} \cosh(\beta z J m)}$$

Therefore, in the disordered phase (both He^3 and He^4 are present) we have $m = 0$ and the concentration of He^3 becomes:

$$x(T, \Delta, J) = \frac{1}{1 + 2e^{-\beta\Delta}} = 1 - \frac{1}{\delta} \quad (24)$$

This way we can determine how the temperature of the λ -transition depends on x ; in fact, the critical temperature will be the one that makes a change sign, so we can determine it from the condition $a = 0$:

$$a(T_c(\Delta)) = \frac{zJ}{2} \left(1 - \frac{zJ}{\delta k_B T_c}\right) = 0 \quad \Rightarrow T_c = \frac{zJ}{k_B \delta}$$

Since as we have just seen $1/\delta = 1 - x$, we have

$$T_c(x) = T_c(0)(1 - x) \quad (25)$$

where $T_c(0) = zJ/k_B$. The other transition (from the continuous λ to the discontinuous one) will occur when the quartic term b changes sign, and so we can determine the critical value of x_c at which it occurs from the condition $b = 0$. Hence, the tricritical point is the one that satisfies the conditions

$$\begin{cases} a(T_t, \Delta_t) = 0 \\ b(T_t, \Delta_t) = 0 \end{cases} \Rightarrow \begin{cases} \delta_t = \frac{zJ}{k_B T_t} \\ \delta_t = 3 \end{cases}$$

and the value of the concentration of He^3 results

$$x(T_t, \Delta_t) = 1 - \frac{1}{\delta_t} = \frac{2}{3} \quad (26)$$

which is in astonishingly good agreement with the experimental result of $x_t \sim 0.67$.

Exercise 1: Expansion of G for small values of m

Expand the free-energy per site

$$\frac{G}{N} = \frac{z}{2} J m^2 - \Delta - k_B T \ln A$$

where $A = 1 + 2e^{-\beta\Delta} \cosh(\beta z J m)$ for small values of m .

Solution. Let us define

$$x \equiv \beta z J m, \quad B \equiv 2e^{-\beta\Delta}$$

Since $\cosh x \simeq 1 + \frac{x^2}{2} + \frac{x^4}{24}$, we can expand A as

$$A = 1 + B \cosh x \simeq 1 + B \left(1 + \frac{x^2}{2} + \frac{x^4}{24} \right)$$

Hence,

$$\begin{aligned} \ln A &= \ln \left(1 + B + \frac{Bx^2}{2} + \frac{Bx^4}{24} \right) \\ &\simeq \ln \left[(1+B) \left(1 + \frac{B}{2(1+B)} x^2 + \frac{B}{24(1+B)} x^4 \right) \right] \\ &= \ln(1+B) + \ln(1+t) \end{aligned}$$

where

$$t \equiv \frac{B}{2(1+B)} x^2 + \frac{B}{24(1+B)} x^4$$

Let us first consider the term

$$\frac{B}{1+B} = \frac{2e^{-\beta\Delta}}{1+2e^{-\beta\Delta}} = \frac{2}{2+e^{\beta\Delta}} = \frac{1}{\delta}$$

Since $\ln(1+t) = t - \frac{t^2}{2}$, we have

$$\Rightarrow \ln A = \ln(1+B) + \frac{x^2}{2\delta} + \left(\frac{1}{24\delta} - \frac{1}{4\delta^2} \right) x^4 - \frac{1}{24\delta^2} x^6$$

If we remember that $x \equiv \beta z J m$, we obtain

$$\begin{aligned} -\frac{\ln A}{\beta} + \frac{z}{2} J m^2 - \Delta &\simeq a_0(T, \Delta) + \left(\frac{z}{2} J - \frac{\beta z^2 J^2}{2\delta} \right) m^2 \\ &\quad + \left(\frac{1}{8\delta} - \frac{1}{24\delta} \right) \beta^3 z^4 J^4 m^4 + \frac{1}{24\delta^2} \beta^5 z^6 J^6 m^6 \end{aligned}$$

Hence, the free energy G for small values of m is

$$G(T, \Delta, J, m) = a_0(T, \Delta) + a(T, \Delta) m^2 + b(T, \Delta) m^4 + c(T, \Delta) m^6$$

where

$$\begin{aligned} a(T, \Delta) &= \frac{zJ}{2} \left(1 - \frac{\beta z J}{\delta} \right) \\ b(T, \Delta) &= \frac{\beta^3 z^4 J^4}{8\delta} \left(\frac{1}{\delta} - \frac{1}{3} \right) = \frac{\beta^3 z^4 J^4}{8\delta^2} \left(1 - \frac{\delta}{3} \right) \\ c(T, \Delta) &= \frac{\beta^5 z^6 J^6}{24\delta^2} > 0 \end{aligned}$$

0.0.2 Mean field again

Another way to introduce the variational approach and the mean field approximation often discussed starts from the general expression of the variational free energy

$$F_{var} = \langle \mathcal{H} \rangle_{\rho_{TR}} + k_B T \langle \ln \rho_{TR} \rangle_{\rho_{TR}} \quad (28)$$

We have to choose a family of distribution. If one assumes that the family of trial distribution is of the Gibbs-Boltzmann form

$$\rho_{TR} = \frac{e^{-\beta \mathcal{H}_{TR}}}{Z_{TR}} \quad (29)$$

with

$$Z_{TR} = e^{-\beta F_{TR}} = \sum_{\{\Phi_i\}} e^{-\beta \mathcal{H}_{TR}(\{\Phi_i\})} \quad (30)$$

then, since

$$\ln \rho_{TR} = -\beta \mathcal{H}_{TR} - \ln Z_{TR}$$

we have

$$k_B T \langle \ln \rho_{TR} \rangle_{\rho_{TR}} = k_B T \left\langle \frac{-\mathcal{H}_{TR}}{k_B T} \right\rangle + k_B T \underbrace{\langle -\ln Z_{TR} \rangle}_{\beta F_{TR}}$$

By rearranging,

$$k_B T \langle \ln \rho_{TR} \rangle_{\rho_{TR}} = \langle -\mathcal{H}_{TR} \rangle + F_{TR}$$

Hence, the variational free energy becomes

$$F_{var} = \langle \mathcal{H} \rangle_{\rho_{TR}} - \langle \mathcal{H}_{TR} \rangle_{\rho_{TR}} + F_{TR} = \langle \mathcal{H} - \mathcal{H}_{TR} \rangle_{\rho_{TR}} + F_{TR} \quad (31)$$

Clearly, $F \leq F_{var}$ and one has to look for the minima of F_{var} by varying ρ_{TR} . Within this approach, the mean field approximation is still given by

$$\rho_{TR}^{MF}(\Phi_1, \dots, \Phi_N) = \prod_{i=1}^N \rho_{TR}^{(1)}(\Phi_i)$$

that in this case becomes

$$\prod_{i=1}^N \rho_{TR}^{(1)}(\Phi_i) = \frac{1}{Z_{TR}^{MF}} e^{-\beta \sum_i b_i \Phi_i} \quad (32)$$

and

$$Z_{TR} = \sum_{\{\Phi\}} e^{-\beta \sum_i b_i \Phi_i} \quad (33)$$

where b_i are the variational parameters. The Hamiltonian is

$$\mathcal{H}_{TR} = - \sum_i b_i \Phi_i \quad (34)$$

If we consider again the Ising model (remind that it means $\Phi_i \rightarrow S_i = \pm 1$), the Hamiltonian is

$$\mathcal{H} = -J \sum_{\langle ij \rangle} S_i S_j - H \sum_i S_i$$

Hence, Eq.(31) becomes

$$\begin{aligned}
F_{var} &= \langle \mathcal{H} - \mathcal{H}_{TR} \rangle_{\rho_{TR}} + F_{TR} \\
&= F_{TR} + \left\langle \left(-J \sum_{\langle ij \rangle} S_i S_j - H \sum_i S_i \right) - \left(- \sum_i b_i S_i \right) \right\rangle_{\rho_{TR}} \\
&= F_{TR} + \left\langle -J \sum_{\langle ij \rangle} S_i S_j + \sum_i (b_i - H) S_i \right\rangle_{\rho_{TR}} \\
&= F_{TR} - J \sum_{\langle ij \rangle} \langle S_i S_j \rangle_{\rho_{TR}} + \sum_i (b_i - H) \langle S_i \rangle_{\rho_{TR}}
\end{aligned}$$

Since $\rho_{TR} = \prod_{i=1}^N \rho_i$, we have

$$\langle S_i S_j \rangle_{\rho_{TR}} = \langle S_i \rangle_{\rho_{TR}} \langle S_j \rangle_{\rho_{TR}}$$

Therefore,

$$F_{var} = F_{TR} - J \sum_{\langle ij \rangle} \langle S_i \rangle_{\rho_{TR}} \langle S_j \rangle_{\rho_{TR}} + \sum_i (b_i - H) \langle S_i \rangle_{\rho_{TR}}$$

Let us minimize the last equation, we consider the condition:

$$\frac{\partial F_{var}}{\partial b_i} = 0, \quad \forall i$$

which gives

$$0 = \frac{\partial F_{var}}{\partial b_i} = \left[-J \sum_{j \in n.n.i} \langle S_i \rangle_{\rho_{TR}} + b_i - H \right] \frac{\partial \langle S_i \rangle}{\partial b_i}$$

The variational parameters are equal to

$$b_i = J \sum_{j \in n.n.i} \langle S_j \rangle_{\rho_{TR}} + H$$

Let us calculate the average of the spin $\langle S_i \rangle_{\rho_{TR}}$:

$$\begin{aligned}
\langle S_i \rangle_{\rho_{TR}} &= \frac{1}{Z_{TR}} \sum_{\{S\}} S_i e^{\beta \sum_k S_k b_k} = \frac{\prod_k \sum_{S_k} S_i e^{\beta S_k b_k}}{\prod_k \sum_{S_k} e^{\beta S_k b_k}} \\
&= \frac{\sum_{S_i=\pm 1} S_i e^{\beta S_i b_i}}{\sum_{S_i=\pm 1} e^{\beta S_i b_i}} = \frac{\sinh(\beta b_i)}{\cosh(\beta b_i)} = \tanh(\beta b_i)
\end{aligned}$$

Finally, the variational parameters are

$$b_i = J \sum_{j \in n.n.i} \tanh(\beta b_j) + H \quad (35)$$

Remark. The main step to understand is how to derive F_{var} from a ρ_{TR} . This is nice to see a variation with respect to the real hamiltonian. Consider a bunch of data, for instance a million of configuration, which is the distribution of the configuration? Usually, we build up a model with a distribution that depends on parameters and what we want to do is statistical inference. Starting from the model and the data we have to obtain the real distribution.

Exercise 2

Consider again the antiferromagnetic Ising model

$$\mathcal{H}[\{S\}] = -J \sum_{\langle \vec{r}_A \vec{r}_B \rangle} S(\vec{r}_A) S(\vec{r}_B) - H \sum_{\vec{r}_A} S(\vec{r}_A) + H \sum_{\vec{r}_B} S(\vec{r}_B)$$

with $J > 0$ and $H > 0$. Remember that

- \vec{r}_A denotes the site on the A sublattice.
- \vec{r}_B denotes the site on the B sublattice.

Let us find again the mean-field solution, but now using the variational ansatz

$$F \leq F_{var} = \langle \mathcal{H} \rangle_{\rho_{TR}} - \langle \mathcal{H}_{TR} \rangle_{\rho_{TR}} + F_{TR} = \langle \mathcal{H} - \mathcal{H}_{TR} \rangle_{\rho_{TR}} + F_{TR}$$

Remark. Since the problem can be splitted in two sublattices, it is convenient to use

$$\mathcal{H}_{TR} = -H_A \sum_{r_A} S(r_A) - H_B \sum_{r_B} S(r_B)$$

In particular:

- show that F_{var} has the following expression:

$$F_{var} = F_{TR}(\beta H_A, \beta H_B) - 4NJ \langle S_A \rangle_{\rho_{TR}} \langle S_B \rangle_{\rho_{TR}} - \frac{1}{2}NH \left(\langle S_A \rangle_{\rho_{TR}} - \langle S_B \rangle_{\rho_{TR}} \right) + \frac{1}{2}N \left(H_A \langle S_A \rangle_{\rho_{TR}} + H_B \langle S_B \rangle_{\rho_{TR}} \right)$$

where

$$\begin{aligned} \langle S_A \rangle_{\rho_{TR}} &\equiv m_A + n \\ \langle S_B \rangle_{\rho_{TR}} &\equiv m_B - n \end{aligned}$$

with $m = m_A + m_B$, and

$$\begin{aligned} m_A &= \tanh(\beta H - 4\beta J m_B) \\ m_B &= \tanh(\beta H - 4\beta J m_A) \end{aligned}$$

- Expand the free energy F_{var} in powers of m of the form

$$F_{var} = A + Bm^2 + cm^4 + O(m^6)$$

and find the explicit expression of A, B and C as a function of T, H and n .