

Using the constraints

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

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:

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

Hence,

$$\rho_i = \frac{1-m_i}{2}(1 - \delta_{S_i, -1}) + \frac{1+m_i}{2}\delta_{S_i, -1} \quad (3)$$

In matrix form

$$\begin{pmatrix} \frac{(m_i+1)}{2} & 0 \\ 0 & \frac{(1-m_i)}{2} \end{pmatrix} \quad (4)$$

Mean-field energy term

Let us consider the Hamiltonian

$$\langle \mathcal{H} \rangle_{\rho_{MF}} = \left\langle -J \sum_{\langle ij \rangle} S_i S_j - \sum_i H_i S_i \right\rangle_{\rho_{MF}} = -J \sum_{\langle ij \rangle} \langle S_i S_j \rangle_{\rho_{MF}} - \sum_i H_i \langle S_i \rangle_{\rho_{MF}} \quad (5)$$

Since

$$\rho_{MF} = \prod_{i=1}^N \rho_i \quad (6)$$

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

$$\langle S_i S_j \rangle_{\rho_{MF}} = \langle S_i \rangle_{\rho_{MF}} \langle S_j \rangle_{\rho_{MF}} \quad (7)$$

Moreover, for all function g of S_i we can write

$$\begin{aligned} \langle g(S_i) \rangle_{\rho_{MF}} &= \text{Tr}^{(i)}(g(S_i) \rho_i) = \sum_{S_i=\pm 1} g(S_i) \rho_i \\ &= \sum_{S_i=\pm 1} g(S_i) \left[\frac{1+m_i}{2} \delta_{S_i, 1} + \frac{1-m_i}{2} (1 - \delta_{S_i, 1}) \right] \\ &= \frac{1+m_i}{2} g(1) + \frac{1-m_i}{2} g(-1) \end{aligned} \quad (8)$$

Note that, if $g(S_i) = S_i$,

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

as expected.

Hence,

$$\langle \mathcal{H} \rangle_{\rho_{MF}} = -J \sum_{\langle ij \rangle} m_i m_j - \sum_i H_i m_i \quad (9)$$

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 This has the form of the original Hamiltonian where S_i have been replaced by their statistical averages.

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The entropy term is:

$$\begin{aligned}\langle \ln \rho \rangle_{\rho_{MF}} &= \text{Tr}(\rho \ln \rho) \stackrel{MF}{=} \sum_i \text{Tr}^{(i)}(\rho_i \ln \rho_i) \\ &= \sum_i \left[\frac{1+m_i}{2} \ln \frac{1+m_i}{2} + \frac{1-m_i}{2} \ln \frac{1-m_i}{2} \right]\end{aligned}\quad (10)$$

The total free energy becomes:

$$\begin{aligned}F_{\rho_{MF}} &= \langle \mathcal{H} \rangle_{\rho_{MF}} + k_B T \langle \ln \rho \rangle_{\rho_{MF}} \\ &= -J \sum_{\langle ij \rangle} m_i m_j - \sum_i H_i m_i + k_B T \sum_i \left[\frac{1+m_i}{2} \ln \frac{1+m_i}{2} + \frac{1-m_i}{2} \ln \frac{1-m_i}{2} \right]\end{aligned}\quad (11)$$

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

$$\left. \frac{\partial F_{\rho_{MF}}}{\partial m_i} \right|_{m_i = \bar{m}_i} = 0 \quad (12)$$

This gives:

$$0 = -J \sum_{j \in n.n. \text{ of } i} \bar{m}_j - H_i + \frac{k_B T}{2} \ln \left[\frac{1+\bar{m}_i}{1-\bar{m}_i} \right] \quad (13)$$

To solve it, remember that

$$\tanh^{-1}(x) = \frac{1}{2} \ln \frac{1+x}{1-x} \quad (TO DO) \quad (14)$$

Hence,

$$k_B T \tanh^{-1}(\bar{m}_i) = J \sum_{j \in n.n. \text{ of } i} \bar{m}_j + H_i \quad (15)$$

which implies

$$\bar{m}_i = \tanh \left[(k_B T)^{-1} \left(J \sum_{j \in n.n. \text{ of } i} \bar{m}_j + H_i \right) \right] \quad (16)$$

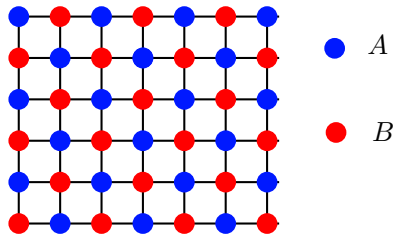
Defining

$$z \bar{m}_i \equiv \sum_{j \in n.n. \text{ of } i} \bar{m}_j \quad (17)$$

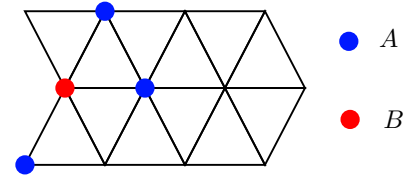
we get

$$\bar{m}_i = \tanh [\beta (J z \bar{m}_i + H_i)] \quad (18)$$

this is the Bragg-William approximation.



(a) Square lattice is bipartite.



(b) Triangular lattice is not bipartite.

Figure 1

Example 1: Ising antiferromagnet in an external field

Consider the model

$$\mathcal{H} = +J \sum_{\langle ij \rangle} S_i S_j - H \sum_i S_i, \quad (19)$$

Remark. Note the $+$ before J . This means that the interactions are antiferromagnetic.

- If $H = 0$ ferromagnetic and antiferromagnetic 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

$$S'_j \begin{cases} +S_j & j \in A \\ -S_j & j \in B \end{cases} \quad (20)$$

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:

$$\mathcal{H}^* = -J \sum_{\langle ij \rangle} S'_i S'_j \quad (21)$$

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 $H_B = -H$.

$$\mathcal{H}^*[S] = -J \sum_{\langle r_A r_B \rangle} S(r_A) S(r_B) - H \sum_{r_A} S(r_A) + H \sum_{r_B} S(r_B), \quad J > 0, H > 0 \quad (22)$$

The average magnetization per spin is

$$m \equiv \frac{1}{2}(m_A + m_B) \quad (23)$$

while

$$m_S = \frac{1}{2}(m_A - m_B) \quad (24)$$

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

$$\begin{cases} \rho_A^{(1)}(S) = \frac{1+m_A}{2} \delta_{S,1} + \frac{1-m_A}{2} \delta_{S,-1} \\ \rho_B^{(1)}(S) = \frac{1+m_B}{2} \delta_{S,1} + \frac{1-m_B}{2} \delta_{S,-1} \end{cases} \quad (25)$$

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

$$\langle \mathcal{H} \rangle_{\rho_{MF}} = -J \sum_{\langle ij \rangle} \langle S_i S_j \rangle_{\rho_{MF}} - H \sum_i \langle S_i \rangle_{\rho_{MF}} \quad (26)$$

$$\langle \ln \rho \rangle_{\rho_{MF}} = \sum_i \text{Tr}^{(1)}(\rho_i \ln \rho_i) \quad (27)$$

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

$$\frac{F(m_A, m_B)}{N} = \frac{z\hat{J}}{2} m_A m_B - \frac{1}{2} H(m_A + m_B) - \frac{1}{2} k_B T s(m_A) - \frac{1}{2} k_B T s(m_B) \quad (28)$$

where the entropy is given by

$$s(m) = \left[\frac{1+m}{2} \ln \left(\frac{1+m}{2} \right) + \frac{1-m}{2} \ln \left(\frac{1-m}{2} \right) \right] \quad (29)$$

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

$$\frac{\partial(F/N)}{\partial m_A} = 0 \quad \Rightarrow m_B = \frac{H}{z\hat{J}} - \frac{k_B T}{z\hat{J}} \ln \left(\frac{1+m_A}{1-m_A} \right) \quad (30a)$$

$$\frac{\partial(F/N)}{\partial m_B} = 0 \quad \Rightarrow m_A = \frac{H}{z\hat{J}} - \frac{k_B T}{z\hat{J}} \ln \left(\frac{1+m_B}{1-m_B} \right) \quad (30b)$$

As before, since

$$\tanh^{-1}(x) = \frac{1}{2} \ln \frac{1+x}{1-x} \quad (31)$$

these self-consistent equations can be written as

$$\begin{cases} m_A = \tanh \left(\beta \left(H - z\hat{J}m_B \right) \right) \\ m_B = \tanh \left(\beta \left(H - z\hat{J}m_A \right) \right) \end{cases} \quad (32)$$

The sites $\in A$ experience an internal field $H_{A,MF} = -z\hat{J}m_B$ from the B neighbours and viceversa 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 $T_\lambda = 2.17K$ and a $P = P_0$. It is known as λ -transition since at $T \sim T_\lambda$ the specific heat $C(T)$ behaves as in

Figure 2a.

Remark. 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.

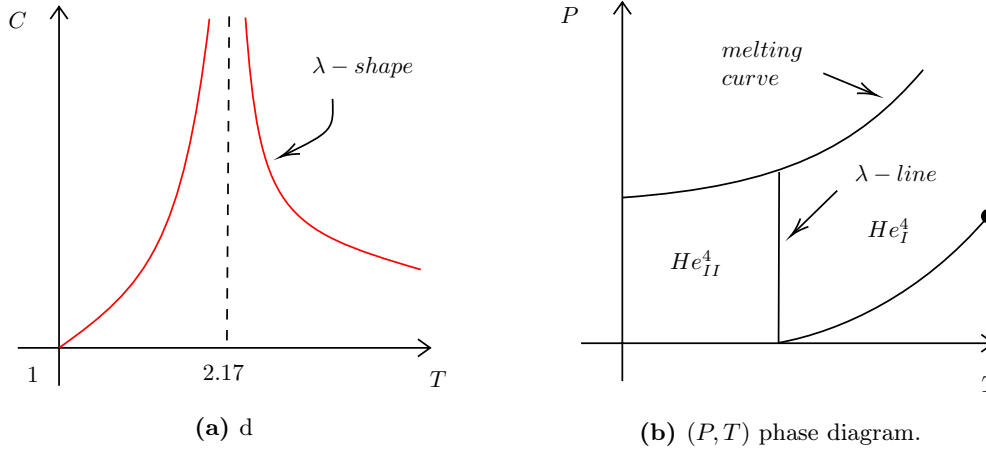


Figure 2

Now, the question is: what happens to the system if a given amount of He^3 is inserted to form a $\text{He}^3 - \text{He}^4$ mixture? He^3 is a non-radiative isotope with 2 protons and 1 neutron. From a quantum statistical point of view it is a *fermion*.

Hence, if inserted in a system of He^4 it will "dilute" its bosonic property. Then, one expects that T_λ decreases. Indeed, denoting by x the concentration of He^3 one observes

$$T_\lambda = T_\lambda(x) \quad (33)$$

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

At the same time, at a given point the mixture undergoes a separation between a phase rich and a phase poor of He^3 . In particular one observes that, for

$$x > x_t = \frac{n_3}{n_3 + n_4} \sim 0.67 \quad (34)$$

the fluid-superfluid transition becomes first order! It is accompanied by a phase separation. The point (x_T, T_t) is a *tricritical point*, i.e. a critical point that separates a line of second order transition from a line of first order transition.

BEG Model

The BEG Model is the model of a diluted ferromagnetic system. The spins are $S_i = \pm 1, 0$ (similar to a lattice gas model), we have $S_i = \pm 1$ for He^4 atom at site i , $S_i = 0$ for He^3 atom at site i .

Let us consider:

- $\langle S_i \rangle = m_i$, order parameter.
- $\langle S_i^2 \rangle$ is the density He^4 atoms.

Let us define the density of He^3 atoms as

$$x \equiv 1 - \langle S_i^2 \rangle \quad (35)$$

The chemical potentials difference is

$$\Delta \propto \mu_3 - \mu_4 \quad (36)$$

and controls the number of He^3 atoms.

If:

- $\Delta \rightarrow -\infty \Rightarrow x \rightarrow 0.$
- $\Delta \rightarrow +\infty \Rightarrow x \rightarrow 1.$

and the order parameter for the λ -transition becomes

$$\langle S_i \rangle = \begin{cases} 0 & T > T_\lambda \\ m & T < T_\lambda \end{cases} \quad (37)$$

The minimal version of the model is:

$$\mathcal{H} = -J \sum_{\langle ij \rangle} S_i S_j + \Delta \sum_{i=1}^N S_i^2 - \Delta N \quad (38)$$

Remark. The ΔN term is a typical term for a gas in gran canonical ensemble.

Variational mean field approach to BEG

Since $\rho_{MF} = \prod_i \rho_i$,

$$G(T, J, \Delta) = \langle \mathcal{H} \rangle_{\rho_{MF}} + k_B T \sum_i \text{Tr}(\rho_i \ln \rho_i) \quad (39)$$

where the first term can be written as

$$\begin{aligned} \langle \mathcal{H} \rangle_{\rho_{MF}} &= -J \sum_{\langle ij \rangle} \langle S_i S_j \rangle + \Delta \sum_i \langle S_i^2 \rangle - N\Delta \\ &\stackrel{MF}{\simeq} -J \sum_{\langle ij \rangle} \langle S_i \rangle \langle S_j \rangle + \Delta \sum_i \langle S_i^2 \rangle - \Delta N \end{aligned} \quad (40)$$

where

$$\langle S_i \rangle = \langle S_j \rangle \equiv m \quad (41)$$

Hence,

$$G(T, J, \Delta)_{MF} = -\frac{1}{2} N J z (\text{Tr}_{S_i}(\rho_i S_i))^2 + N \Delta \text{Tr}_{S_i}(\rho_i S_i^2) - N \Delta + N k_B T \text{Tr}_{S_i}(\rho_i \ln \rho_i) \quad (42)$$

We now minimize $G(T, J, \Delta)_{MF}$ with respect to the function ρ_i with constraint $\text{Tr}_{S_i}(\rho_i) = 1$:

$$\frac{dG}{d\rho_i} = 0 \quad (43)$$

Let us consider each term

$$\frac{d}{dp_i} (\text{Tr}(\rho_i S_i))^2 = 2(\text{Tr}(\rho_i S_i)) S_i = 2 \langle S_i \rangle S_i = 2m S_i \quad (44a)$$

$$\frac{d}{dp_i} (\text{Tr}(\rho_i S_i^2)) = S_i^2 \quad (44b)$$

$$\frac{d}{dp_i} (\text{Tr}(\rho_i \ln \rho_i)) = \ln \rho_i + 1 \quad (44c)$$

Remark. Remind that $\rho_i = \rho^{(1)}(S_i)$.

$$0 = -JNzmS_i + \Delta NS_i^2 + Nk_B T \ln \rho_i + Nk_B T \quad (45)$$

Dividing by $Nk_B T$,

$$\ln \rho_i \equiv \ln \rho^{(1)}(S_i) = \beta JzmS_i - \beta \Delta S_i^2 - 1 \quad (46)$$

which implies

$$\rho^{(1)}(S_i) = A^{-1} e^{\beta(zJmS_i - \Delta S_i^2)} \quad (47)$$

Remark. In A^{-1} it is included the term e^{-1} .

The constant A can be found by imposing $\text{Tr}_{S_i} \rho^{(1)}(S_i) = 1$, (TO DO)

$$A = 1 + 2e^{-\beta\Delta} \cosh(\beta zJm) \quad (48)$$

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

$$\langle S_i^2 \rangle = \text{Tr}_{S_i}(\rho_i S_i^2) = \frac{1}{A} 2e^{-\beta\Delta} \cosh(\beta zJm) \quad (49)$$

and

$$x = 1 - \langle S_i^2 \rangle = \frac{A - 2e^{-\beta\Delta} \cosh(\beta zJm)}{A} \Rightarrow x = \frac{1}{A} \quad (50)$$

Hence,

$$\frac{G(T, \Delta, m, J)}{N} = \frac{z}{2} Jm^2 - \Delta - k_B T \ln A \quad (51)$$

Remark. Now we should minimize $G(T, \Delta, m, J)$ with respect to m to obtain the equilibrium phases.

The expansion for small values of m is

$$\cosh(t) = 1 + \frac{t^2}{2} + \frac{t^4}{24}, \quad \ln(1+t) = t - \frac{t^2}{2} \quad (52)$$

(TO DO)

$$G(T, \Delta, J, m) = a_0(T, \Delta) + a(T, \Delta)m^2 + b(T, \Delta)m^4 + \frac{c(T, \Delta)}{6}m^6 \quad (53)$$

where

$$\begin{cases} a(T, \Delta) = \frac{zJ}{2} \left(1 - \frac{zJ}{8k_B T}\right) \\ b(T, \Delta) = k \left(1 - \frac{\delta}{3}\right) \\ c(T, \Delta) > 0 \end{cases} \quad (54)$$

and the parameter

$$\delta \equiv 1 + \frac{e^{\beta\Delta}}{2} = \delta(T, \Delta) \quad (55)$$

is related to the concentration of $\text{He}^3 - x$. This can be seen as follows.

Since

$$x(T, \Delta, J) \equiv 1 - \langle S_i^2 \rangle = \frac{1}{A} = \left(1 + 2e^{-\beta\Delta} \cosh(\beta zJm)\right)^{-1} \quad (56)$$

In the disordered phase ($m = 0$) one has

$$x(T, \Delta, J) = \left(1 + 2e^{-\beta\Delta}\right)^{-1} = \frac{\delta - 1}{\delta} \quad (57)$$

By combining this result with the order-disorder transition

$$a(T_c(\Delta)) = \frac{zJ}{2} \left(1 - \frac{zJ}{\delta k_B T_c}\right) = 0, \quad \left[\delta = \frac{zJ}{k_B T_c}\right] \quad (58)$$

one obtains (TO DO)

$$T_c(x) = T_c(0)(1 - x) \quad (59)$$

There is a dependence of the critical temperature λ on the He^3 concentration x .

The tricritical point is the one that satisfies the conditions

$$\begin{cases} a(T_t, \Delta_t) = 0 \\ b(T_t, \Delta_t) = 0 \end{cases} \Rightarrow \begin{cases} \delta_t = \frac{zJ}{k_B T_t} \\ \delta_t = 3 \end{cases} \quad (60)$$

$$x(T_t, \Delta_t) = \frac{\delta_t - 1}{\delta_t} = \frac{2}{3} \quad (61)$$

Remark. Experimental estimate of x_t is ~ 0.67 .

Exercise 1

Expand the free-energy per site

$$\frac{G}{N} = \frac{z}{2} J m^2 - \Delta - k_B T \ln A \quad (62)$$

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

$$x \equiv \beta z J m, \quad B \equiv 2e^{-\beta\Delta} \quad (63)$$

Since $\cosh x \simeq 1 + \frac{x^2}{2} + \frac{x^4}{24}$,

$$A = 1 + B \cosh x \simeq 1 + B \left(1 + \frac{x^2}{2} + \frac{x^4}{24} \right) \quad (64)$$

$$\begin{aligned} \ln A &= \ln \left(1 + B + \frac{Bx^2}{2} + \frac{Bx^4}{24} \right) \\ &\simeq \ln \left[(1 + B) \left(1 + \frac{B}{2(1+B)} x^2 + \frac{B}{24(1+B)} x^4 \right) \right] \\ &= \ln(1 + B) + \ln(1 + t) \end{aligned} \quad (65)$$

where

$$t \equiv \frac{B}{2(1+B)} x^2 + \frac{B}{24(1+B)} x^4 \quad (66)$$

Let us first consider the term

$$\frac{B}{1+B} = \frac{2e^{-\beta\Delta}}{1+2e^{-\beta\Delta}} = \frac{2}{2+e^{\beta\Delta}} = \delta^{-1} \quad (67)$$

$$\Rightarrow \ln A = \ln(1+B) + \frac{x^2}{2\delta} + \left(\frac{1}{24\delta} - \frac{1}{8\delta^2} \right) x^4 - \frac{1}{24\delta^2} x^6 \quad (68)$$

Remark. We have that $x \equiv \beta z J m$.

$$\begin{aligned} -\frac{\ln A}{B} + \frac{z}{2} J m^2 - \Delta &\simeq a_0(T, \Delta) + \left(\frac{z}{2} J - \frac{\beta z^2 J^2}{2\delta} \right) m^2 \\ &\quad + \left(\frac{1}{8\delta} - \frac{1}{24\delta} \right) \beta^3 z^4 J^4 m^4 + \frac{1}{24\delta^2} \beta^5 z^6 J^6 m^6 \end{aligned} \quad (69)$$

$$G(T, \Delta, J, m) = a_0(T, \Delta) + a(T, \Delta) m^2 + b(T, \Delta) m^4 + c(T, \Delta) m^6 \quad (70)$$

where

$$a(T, \Delta) = \frac{zJ}{2} \left(1 - \frac{\beta z J}{\delta} \right) \quad (71a)$$

$$b(T, \Delta) = \frac{\beta^3 z^4 J^4}{8\delta} \left(\frac{1}{\delta} - \frac{1}{3} \right) = \frac{\beta^3 z^4 J^4}{8\delta^2} \left(1 - \frac{\delta}{3} \right) \quad (71b)$$

$$c(T, \Delta) = \frac{\beta^5 z^6 J^6}{24\delta^2} > 0 \quad (71c)$$

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

$$F_{var} = \langle \mathcal{H} \rangle_{\rho_{TR}} + k_B T \langle \ln \rho_{TR} \rangle_{\rho_{TR}} \quad (72)$$

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

$$\rho_{TR} = \frac{e^{-\beta \mathcal{H}_{TR}}}{Z_{TR}} \quad (73)$$

with

$$Z_{TR} = e^{-\beta F_{TR}} = \sum_{\{\Phi_i\}} e^{-\beta \mathcal{H}_{TR}(\{\Phi_i\})} \quad (74)$$

If we are able to choose hamiltonian trial as here, we can do this sum, this is the idea. In principle, if we are able to find an Hamiltonian that we can solve without choosing a mean field it is ok.

Then, since

$$\ln \rho_{TR} = -\beta \mathcal{H}_{TR} - \ln Z_{TR} \quad (75)$$

we have

$$k_B T \langle \ln \rho_{TR} \rangle_{\rho_{TR}} = k_B T \left\langle \frac{-\mathcal{H}_{TR}}{k_B T} \right\rangle + k_B T \underbrace{\langle -\ln Z_{TR} \rangle}_{\beta F_{TR}} \quad (76)$$

$$k_B T \langle \ln \rho_{TR} \rangle_{\rho_{TR}} = \langle -\mathcal{H}_{TR} \rangle + F_{TR} \quad (77)$$

$$\Rightarrow F_{var} = \langle \mathcal{H} \rangle_{\rho_{TR}} - \langle \mathcal{H}_{TR} \rangle_{\rho_{TR}} + F_{TR} = \langle \mathcal{H} - \mathcal{H}_{TR} \rangle_{\rho_{TR}} + F_{TR} \quad (78)$$

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

$$\rho_{TR}^{MF}(\Phi_1, \dots, \Phi_N) = \prod_{i=1}^N \rho_{TR}^{(1)}(\Phi_i) \quad (79)$$

that in this case becomes

$$\prod_i \rho_{TR}^{(1)}(\Phi_i) = \frac{1}{Z_{TR}^{MF}} e^{-\beta \sum_i b_i \Phi_i} \quad (80)$$

and

$$Z_{TR} = \sum_{\{\Phi\}} e^{-\beta \sum_i b_i \Phi_i} \quad (81)$$

where b_i are the variational parameters.

$$\mathcal{H}_{TR} = - \sum_i b_i \Phi_i \quad (82)$$

If we consider again the Ising model

$$\mathcal{H} = -J \sum_{\langle ij \rangle} S_i S_j - H \sum_i S_i \quad (83)$$

$$\begin{aligned} F_{var} &= \langle \mathcal{H} - \mathcal{H}_{TR} \rangle_{\rho_{TR}} + F_{TR} \\ &= F_{TR} + \left\langle \left(-J \sum_{\langle ij \rangle} S_i S_j - H \sum_i S_i \right) - \left(- \sum_i b_i S_i \right) \right\rangle_{\rho_{TR}} \\ &= F_{TR} + \left\langle -J \sum_{\langle ij \rangle} S_i S_j + \sum_i (b_i - H) S_i \right\rangle_{\rho_{TR}} \\ &= F_{TR} - J \sum_{\langle ij \rangle} \langle S_i S_j \rangle_{\rho_{TR}} + \sum_i (b_i - H) \langle S_i \rangle_{\rho_{TR}} \end{aligned} \quad (84)$$

Since $\rho_{TR} = \prod_i \rho_i$,

$$\langle S_i S_j \rangle_{\rho_{TR}} = \langle S_i \rangle_{\rho_{TR}} \langle S_j \rangle_{\rho_{TR}} \quad (85)$$

$$F_{var} = F_{TR} - J \sum_{\langle ij \rangle} \langle S_i \rangle_{\rho_{TR}} \langle S_j \rangle_{\rho_{TR}} + \sum_i (b_i - H) \langle S_i \rangle_{\rho_{TR}} \quad (86)$$

$$\frac{\partial F_{var}}{\partial b_i} = 0, \quad \forall i \quad (87)$$

$$0 = \frac{\partial F_{var}}{\partial b_i} = \left[-J \sum_{j \text{ n.n. } i} \langle S_i \rangle_{\rho_{TR}} + b_i - H \right] \frac{\partial \langle S_i \rangle}{\partial b_i} \quad (88)$$

or

$$b_i = J \sum_{j \text{ n.n. } i} \langle S_j \rangle_{\rho_{TR}} + H \quad (89)$$

$$\begin{aligned} \langle S_i \rangle_{\rho_{TR}} &= \frac{1}{Z_{TR}} \sum_{\{S\}} S_i e^{\beta \sum_k S_k b_k} = \frac{\prod_k \sum_{S_k} S_k e^{\beta S_k b_k}}{\prod_k \sum_{S_k} e^{\beta S_k b_k}} \\ &= \frac{\sum_{S_i=\pm 1} S_i e^{\beta S_i b_i}}{\sum_{S_i=\pm 1} e^{\beta S_i b_i}} = \frac{\cosh(\beta b_i)}{\sinh(\beta b_i)} \\ &= \tanh(\beta b_i) \end{aligned} \quad (90)$$

$$b_i = J \sum_{j \text{ n.n. } i} \tanh(\beta b_j) + H \quad (91)$$

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. (lesson)

Exercise 2

Consider again the antiferromagnetic Ising model

$$\mathcal{H}[\{S\}] = -J \sum_{\langle \vec{r}_A \vec{r}_B \rangle} S(\vec{r}_A) S(\vec{r}_B) - H \sum_{\vec{r}_A} S(\vec{r}_A) + H \sum_{\vec{r}_B} S(\vec{r}_B) \quad (92)$$

where $J > 0$ and $H > 0$.

- \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

$$F \leq F_{var} = \langle \mathcal{H} \rangle_{\rho_{TR}} - \langle \mathcal{H}_{TR} \rangle_{\rho_{TR}} + F_{TR} = \langle \mathcal{H} - \mathcal{H}_{TR} \rangle_{\rho_{TR}} + F_{TR} \quad (93)$$

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

$$\mathcal{H}_{TR} = -H_A \sum_{r_A} S(r_A) - H_B \sum_{r_B} S(r_B) \quad (94)$$

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

$$\begin{aligned} F_{var} = & F_{TR}(\beta H_A, \beta H_B) - 4NJ \langle S_A \rangle_{\rho_{TR}} \langle S_B \rangle_{\rho_{TR}} \\ & - \frac{1}{2}NH \left(\langle S_A \rangle_{\rho_{TR}} - \langle S_B \rangle_{\rho_{TR}} \right) + \frac{1}{2}N \left(H_A \langle S_A \rangle_{\rho_{TR}} + \langle S_B \rangle_{\rho_{TR}} \right) \end{aligned} \quad (95)$$

where

$$\langle S_A \rangle_{\rho_{TR}} \equiv m_A + n \quad (96a)$$

$$\langle S_B \rangle_{\rho_{TR}} \equiv m_B - n \quad (96b)$$

with $m = m_A + m_B$, and

$$m_A = \tanh(\beta H - 4\beta J m_B) \quad (97a)$$

$$m_B = \tanh(\beta H - 4\beta J m_A) \quad (97b)$$

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

$$F_{var} = A + Bm^2 + cm^4 + O(m^6) \quad (98)$$

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