Using the constraints

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

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:

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

Hence,

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

In matrix form

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

Mean-field energy term

Let us consider the Hamiltonian

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

Since

$$
\rho_{MF} = \prod_{i=1}^{N} \rho_i
\tag{6}
$$

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

$$
\langle S_i S_j \rangle_{\rho_{MF}} = \langle S_i \rangle_{\rho_{MF}} \langle S_j \rangle_{\rho_{MF}}
\tag{7}
$$

Moreover, for all function g of S_i we can write

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

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

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

as expected.

Hence,

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

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 This has the form of the original Hamiltonian where S_i have been replaced by their statistical averages.

The entropy term is:

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

$$= \sum_i \left[\frac{1+m_i}{2} \ln \frac{1+m_i}{2} + \frac{1-m_i}{2} \ln \frac{1-m_i}{2} \right] \tag{10}$$

The total free energy becames:

$$F_{\rho_{MF}} = \langle \mathcal{H} \rangle_{\rho_{MF}} + k_B T \langle \ln \rho \rangle_{\rho_{MF}}$$

$$= -J \sum_{\langle ij \rangle} m_i m_j - \sum_i H_i m_i + k_B T \sum_i \left[\frac{1+m_i}{2} \ln \frac{1+m_i}{2} + \frac{1-m_i}{2} \ln \frac{1-m_i}{2} \right] \tag{11}$$

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

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

This gives:

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

To solve it, remember that

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

Hence,

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

which implies

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

Defining

$$z \bar{m}_i \equiv \sum_{j \in \, n.n. \, \text{of} \, i} \bar{m}_j \tag{17}$$

we get

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

this is the Bragg-William approximation.

Example 1 (Ising antiferromagnet in an external field)**.** Consider the model

$$\mathcal{H} = \boxed{+} J \sum_{\langle ij \rangle} S_i S_j - H \sum_i S_i, \tag{19}$$

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.
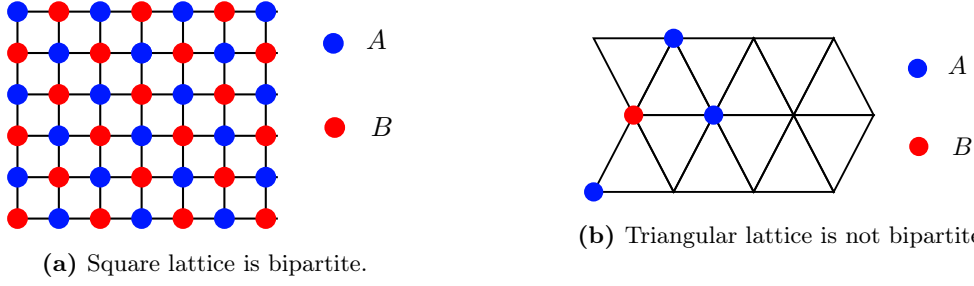
(a) Square lattice is bipartite.

(b) Triangular lattice is not bipartite.

Figure 1

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

If the lattic 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

$$S_j' \begin{cases} +S_j & j \in A \\ -S_j & j \in B \end{cases} \tag{20}$$

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

$$\mathcal{H}^* = -J\sum_{\langle ij \rangle} S_i'S_j' \tag{21}$$

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 $H_B = -H$.

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

The average magnetization per spin is

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

while

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

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

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

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

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

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

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

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

where the entropy is given by

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

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

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

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

As before, since

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

these self-consisten equations can be written as

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

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 $He^3 - He^4$ 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 $\lambda-$transition since at $T \sim T_\lambda$ the specific heat $C(T)$ behaves as in Figure 2a.

Remark. The $\lambda-$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.
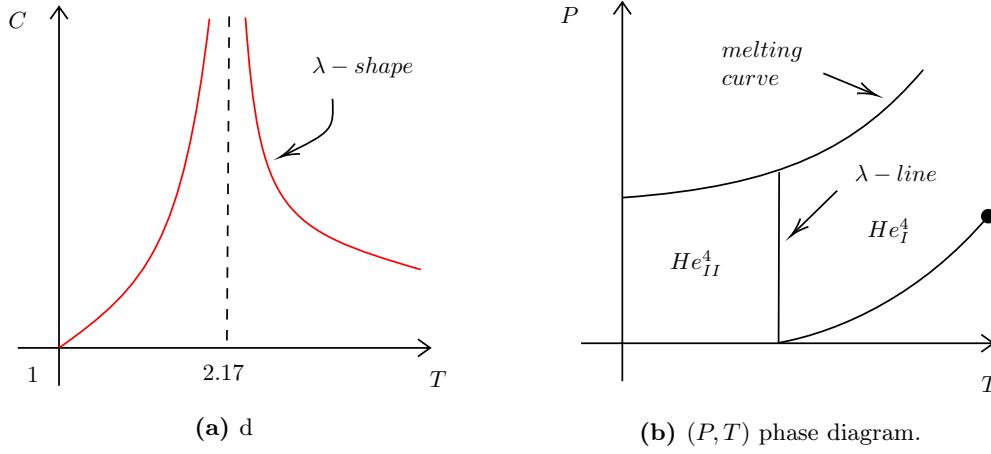
(a) d

(b) (P, T) phase diagram.

Figure 2

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

$$T_\lambda = T_\lambda(x) \tag{33}$$

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

$$x > x_t = \frac{n_3}{n_3 + n_4} \sim 0.67 \tag{34}$$

the fluid-superfluid transition becames first order! It is accompained 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 diluited 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

$$x \equiv 1 - \langle S_i^2 \rangle \tag{35}$$

The chemical potentials difference is

$$\Delta \propto \mu_3 - \mu_4 \tag{36}$$

and controls the number of He^3 atoms.

If:

- $\Delta \to -\infty \quad \Rightarrow x \to 0.$

- $\Delta \to +\infty \quad \Rightarrow x \to 1.$

and the order parameter for the $\lambda-$transition becomes

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

The minimal version of the model is:

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

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

Variational mean field approach to BEG

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

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

where the first term can be written as

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

where

$$\langle S_i \rangle = \langle S_j \rangle \equiv m \tag{41}$$

Hence,

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

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

$$\frac{\mathrm{d}G}{\mathrm{d}\rho_i} = 0 \tag{43}$$

Let us consider each term

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

$$\frac{\mathrm{d}}{\mathrm{d}p_i}\left(\text{Tr}(\rho_i S_i^2)\right) = S_i^2 \tag{44b}$$

$$\frac{\mathrm{d}}{\mathrm{d}p_i}(\text{Tr}(\rho_i \ln \rho_i)) = \ln \rho_i + 1 \tag{44c}$$

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

$$0 = -JNzmS_i + \Delta N S_i^2 + N k_B T \ln \rho_i + N k_B T \tag{45}$$

Dividing by $N k_B T$,

$$\ln \rho_i \equiv \ln \rho^{(1)}(S_i) = \beta J z m S_i - \beta \Delta S_i^2 - 1 \tag{46}$$

which implies

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

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

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

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

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

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

and

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

Hence,

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

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

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

(TO DO)

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

where

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

and the parameter

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

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

Since

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

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

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

By combining this result with the order-disorder transition

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

one obtains (TO DO)

$$T_c(x) = T_c(0)(1 - x) \tag{59}$$

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

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

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

Remark. Experimental estimate of x_t is ~ 0.67.

Exercise 1. Expand the free-energy per site

$$\frac{G}{N} = \frac{z}{2}Jm^2 - \Delta - k_B T \ln A \tag{62}$$

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

$$x \equiv \beta z Jm, \quad B \equiv 2e^{-\beta\Delta} \tag{63}$$

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

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

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

where

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

Let us first consider the term

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

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

Remark. We have that $x \equiv \beta z Jm$.

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

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

where

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

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

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

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

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

If one assumes that the family of trial distribution is of the Gibbs-Boltzmann form

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

with

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

then, since

$$\ln \rho_{TR} = -\beta \mathcal{H}_{TR} - \ln Z_{TR} \tag{75}$$

we have

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

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

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

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

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

that in this case becomes

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

and

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

where b_i are the variational parameters.

$$\mathcal{H}_{TR} = -\sum_i b_i \Phi_i \tag{82}$$

If we consider again the Ising model

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

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

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

$$\langle S_i S_j \rangle_{\rho_{TR}} = \langle S_i \rangle_{\rho_{TR}} \langle S_j \rangle_{\rho_{TR}} \tag{85}$$

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

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

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

or

$$b_i = J \sum_{j\,n.n.\,i} \langle S_j \rangle_{\rho_{TR}} + H \tag{89}$$

$$\langle S_i \rangle_{\rho_{TR}} = \frac{1}{Z_{TR}} \sum_{\{S\}} S_i e^{\beta \sum_k S_k b_k} = \frac{\prod_k \sum_{S_k} S_i e^{\beta S_k b_k}}{\prod_k \sum_{S_k} e^{\beta S_k b_k}}$$

$$= \frac{\sum_{S_i} S_i e^{\beta S_i b_i}}{\sum_{S_i = \pm 1} e^{\beta S_i b_i}} = \frac{\cosh(\beta b_i)}{\sinh(\beta b_i)} \tag{90}$$

$$= \tanh(\beta b_i)$$

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

Exercise 2. Consider again the antiferromagnetic Ising model

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

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

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

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

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

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

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

where

$$\langle S_A \rangle_{\rho_{TR}} \equiv m_A + n \tag{96a}$$
$$\langle S_B \rangle_{\rho_{TR}} \equiv m_B - n \tag{96b}$$

with $m = m_A + m_B$, and

$$m_A = \tanh(\beta H - 4\beta J m_B) \tag{97a}$$
$$m_B = \tanh(\beta H - 4\beta J m_A) \tag{97b}$$

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

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

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

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