Lecture 13.
Wednesday 27th November, 2019.
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Using the constraints

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

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

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

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 This has the form of the original Hamiltonian where S_i have been replaced by their statistical averages.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

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

The total free energy becames:

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

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:

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

To solve it, remember that

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

Hence,

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

which implies

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

Defining

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

we get

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

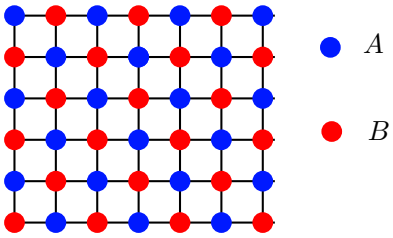
this is the Bragg-William approximation.

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

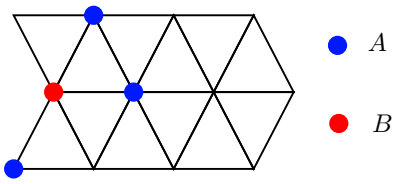
$$\mathcal{H} = + J \sum_{\langle ij \rangle} S_i S_j - H \sum_i S_i, \tag{19}$$

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

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

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

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

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

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

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

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 $\in B$.

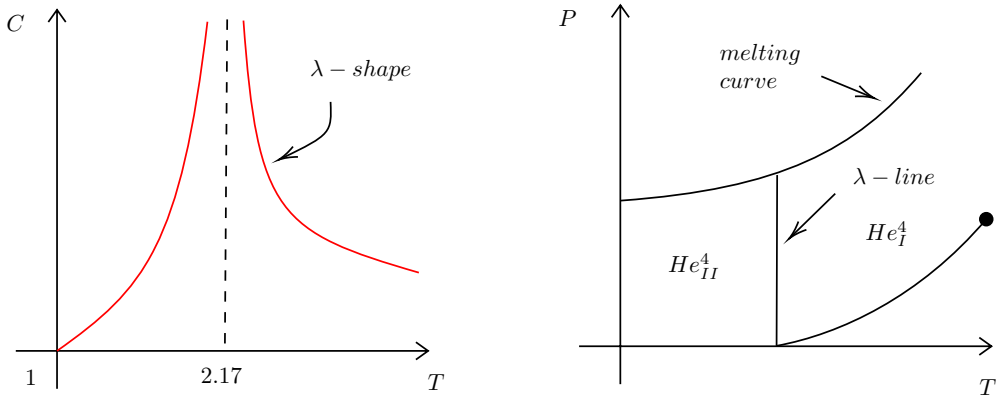
0.0.1 Second approach: Blume-Emery-Griffith model

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

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

where the first term can be written as

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

where

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

Hence,

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

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

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

Let us consider each term

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

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

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

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 $N k_B T$,

$$\ln \rho_i \equiv \ln \rho^{(1)}(S_i) = \tag{46}$$