

I.2. Mean field theory of the paramagnetic to ferromagnetic transition

We consider a model hamiltonian of interacting localized spins \vec{S}_i on a lattice in d dimensions. We restricted the orientation of spins along the z direction and the range of interaction to the nearest-neighbors sites only. This is the Ising model whose Hamiltonian reads:

$$H = - \sum_{\langle ij \rangle} J_{ij} S_i S_j$$



where for a ferromagnetic transition $J_{ij} > 0$. $S_i = S_i^z$ is the spin operator along z direction. Its eigenvalues are well known in the basis $|S_i\rangle$

$$S_i |S_i\rangle = \pm \frac{1}{2} |S_i\rangle$$

so that one can simply identify S_i in the hamiltonian as taking the values $\pm \frac{1}{2}$. Now it is useful to normalize the spins to ± 1 that is, one will consider

$$H = - \sum_{\langle ij \rangle} J'_{ij} S_i S_j$$

where $J'_{ij} = J_{ij}/4$. In the presence of a magnetic field the hamiltonian reads

$$H = - \sum_{\langle ij \rangle} J'_{ij} S_i S_j - \sum_i g \mu_B \frac{1}{2} B S_i \\ \equiv B' S_i$$

where we can define $B' = g \mu_B \frac{1}{2} B = \mu_B B$ ($g=2$).

The calculation of the partition function in the canonical ensemble

$$\mathcal{Z} = \text{Tr } e^{-\beta H}$$

can

exactly

only be achieved in 1D ($d=1$) and 2D ($d=2$, Onager). In 3D one has to resort to approximations. The mean field theory is the simplest approach to 2 and to the calculation of critical exponents.

We will use the so-called Variational Method to derive the mean field equations.

First recall the definition of statistical entropy for system described by the Hamiltonian H :

$$S(D) = -k_B \text{Tr}\{D \ln D\}$$

where $D = \frac{e^{-\beta H}}{Z}$ is the density operator for the canonical ensemble. Also, the trace Tr is defined

$$\text{Tr} \equiv \sum_{\{S_1, \dots, S_N\}} \langle S_1, \dots, S_N | \dots | S_1, \dots, S_N \rangle$$

where the N -Spin state $|S_1, \dots, S_N\rangle = |S_1\rangle \otimes \dots \otimes |S_N\rangle$, is a tensorial product of individual spin states.

Consider the identity

$$S(D) \leq -k_B \text{Tr} D \ln D'$$

where $D' \neq D$

Now if the exact $\{D\}$ ^{partition function} density operator ^{cannot be calculated} let us consider a trial, but simpler, ^{one-body} Hamiltonian for which Z can be calculated exactly:

$$H_E = -\sum_i x_i S_i$$

which is a one-body Hamiltonian, where x_i is a variational parameter. The corresponding density operator is

$$D_E = \frac{e^{-\beta H_E}}{Z_E}$$

where $Z_E = \text{Tr} e^{-\beta H_E}$ is the trial partition function. We thus have the following inequality

$$S(D_E) \leq -k_B \overline{\text{Tr}} D_E \ln D$$

Here the equality is obviously satisfied for $D_E = D$. Multiplying the expression by $-T$ one finds:

$$\begin{aligned} -TS(D_E) &\geq K_B T \text{Tr} \left\{ D_E \ln \left[e^{-\beta H} / Z \right] \right\} \\ &\geq K_B T \text{Tr} \left\{ D_E (-\beta H) - D_E \ln Z \right\} \\ &\geq \frac{-K_B T}{K_B T} \text{Tr} \left\{ D_E H \right\} - K_B T \underbrace{\text{Tr} D_E}_{\ln Z} \end{aligned}$$

Since the density ρ is normalized by the partition function

$$\text{Tr } D_E = 1$$

so that

$$-TS(D_E) \geq -\langle H \rangle_E - K_B T \ln Z.$$

$$\begin{aligned} \langle H_E \rangle_E - \langle H_E \rangle_E - TS(D_E) &= F_E - \langle H_E \rangle_E \geq \underbrace{-K_B T \ln Z}_{F} - \langle H \rangle_E \\ &\Rightarrow F_E \geq F + \langle H_E - H \rangle_E \end{aligned}$$

or

$$F \leq F_E + \langle H - H_E \rangle_E$$

which is known as the Bogoliubov identity. We define
(or Feynman variational principle)

$$F_{CM}[\beta, \{x_i\}] \equiv F_E[\beta, \{x_i\}] + \langle H - H_E \rangle_E$$

as the meanfield free energy that depends on β and x_i as natural variables. The variational method consists in the minimization of F_{CM} with respect to x_i in order to get the configurations $\{x_i^*\}$ that will lead to the best F_{CM} , that is closer to the exact F . Explicitly

$$\begin{cases} \delta F_{CM} = 0 \\ \delta x_i \Big|_{x_i = x^*} \end{cases}$$

the contributions to F_{CM} are :

$$\begin{aligned} Z_E &= \text{Tr } e^{+\beta \sum_i x_i s_i} \\ &= \prod_i \text{Tr}_{\{s_i\}} e^{\beta x_i s_i} \\ &= \prod_i \left[\sum_{s_i=\pm 1} e^{\beta x_i s_i} \right] \\ Z_E &= \prod_i [e^{\beta x_i} + e^{-\beta x_i}] = 2^N \cosh^N(\beta x_i); \end{aligned}$$

$$\langle H - H_E \rangle_E = \frac{1}{Z_E} \text{Tr} (H - H_E) e^{-\beta H_E}$$

dans l'hypothèse,
que nous ne faisons
pas tout de suite, où
tous les x_i sont identiques.

$$= - \sum_{\langle i,j \rangle} J_{ij}' \langle s_i s_j \rangle_E - \sum_i B_i' \langle s_i \rangle_E + \sum_i x_i \langle s_i \rangle_E$$

As H_E is a one-body Hamiltonian,

$$\langle s_i s_j \rangle_E = \langle s_i \rangle_E \langle s_j \rangle_E$$

which leads to

$$\langle H - H_E \rangle_E = - \sum_{\langle i,j \rangle} J_{ij}' \langle s_i \rangle_E \langle s_j \rangle_E - \sum_i (B_i' - x_i) \langle s_i \rangle_E$$

Now

$$\langle s_i \rangle_E = \frac{1}{Z_E} \text{Tr}_{\{s_i\}} s_i e^{\beta x_i s_i}$$

$$= \frac{1}{Z_E} (e^{\beta x_i} - e^{-\beta x_i})$$

$$\langle s_i \rangle_E = \frac{e^{\beta x_i} - e^{-\beta x_i}}{e^{\beta x_i} + e^{-\beta x_i}} = \tanh \beta x_i$$

it follows then

$$F_{CM} [\beta, \{x_i\}] = - \sum_{\langle i,j \rangle} J_{ij}' \tanh \beta x_i \tanh \beta x_j - \sum_i (B_i' - x_i) \tanh \beta x_i - \beta^{-1} \ln(2 \cosh p)$$

Variational condition :

$$\left. \frac{\delta F_{CM}}{\delta x_i} \right|_{x_i} = 0$$

$$\frac{\delta F_{CM}}{\delta x_i} = -\sum_j 2J_{ij}' \tanh \beta x_j \frac{\partial \tanh \beta x_i}{\partial x_i} - B_i' \frac{\partial \tanh \beta x_i}{\partial x_i} + \tanh \beta x_i + x_i \frac{\partial \tanh \beta x_i}{\partial x_i}$$

~~$\beta^{-1} \frac{\partial^2 \tanh \beta x_i}{\partial x_i^2}$~~

$$0 = -2 \sum_j J_{ij}' \tanh \beta x_j^* \frac{\partial \tanh \beta x_i^*}{\partial x_i^*} - B_i' \frac{\partial \tanh \beta x_i^*}{\partial x_i^*} + x_i \frac{\partial \tanh \beta x_i}{\partial x_i}$$

$$= \left[-2 \sum_j J_{ij}' \tanh \beta x_j^* - B_i' x_i^* \right] \frac{\partial \tanh \beta x_i^*}{\partial x_i^*} = 0$$

$$\Rightarrow \boxed{x_i^* = B_i' + 2 \sum_j J_{ij}' \tanh \beta x_j^*}$$

which can be considered as a self-consistent condition for the x_i^* 's

In the presence of a field B , the natural variables of F_{CM} are β , B and $\{x_i^*\}$. Both x_i^* and B are related through the self-consistent condition. In order to express the free energy in terms of the order parameter M , let's do a Legendre transform

$$F_{CM}[\beta, \{x_i^*\}(B), B] + \sum_i B_i' M_i = T_{CM}[\beta, M_i]$$

where the magnetisation M_i is the conjugate variable of B_i :

$$M_i = -\frac{\partial F_{CM}}{\partial B_i} \quad \text{or} \quad \bar{M}_i = -\frac{\partial F_{CM}}{\partial B_i'}$$

because $\bar{M}_i = -\frac{\partial F_{CM}}{\partial B_i'} - \underbrace{\frac{\partial F_{CM}}{\partial x_i^*} \frac{\partial x_i^*}{\partial B_i'}}_0$

$$\boxed{\bar{M}_i = -\frac{\partial F_{CM}}{\partial B_i'} = +\tanh \beta x_i^*}$$

and $\beta x_i^* = \text{Arg} \tanh \bar{M}_i = \frac{1}{2} \ln \left[\frac{1+\bar{M}_i}{1-\bar{M}_i} \right]; -1 \leq \bar{M}_i \leq 1$

$T_{CM}[\beta, \bar{M}_i]$ is called the Gibbs free energy, which will read

$$\Gamma_{CM}[\beta, \bar{M}] = -\sum_{\langle i,j \rangle} J_{ij}' \bar{M}_i \bar{M}_j - \sum_i B_i' \bar{M}_i + \sum_i (B_i' \bar{M}_i) \\ + \sum_i \frac{\bar{M}_i}{2\beta} \ln \left[\frac{1+\bar{M}_i}{1-\bar{M}_i} \right] - \beta^{-1} \sum_i \ln(2 \cosh \beta x_i^*)$$

if $\ln 2 \cosh \beta x_i^* = \ln 2 + \underbrace{\frac{1}{2} \ln \cosh^2 \beta x_i^*}_{-\frac{1}{2} \ln (1 - \tanh^2 \beta x_i^*)} - \underbrace{\frac{1}{2} \ln (1 - \bar{M}_i^2)}_{-\frac{1}{2} [\ln (1 - \bar{M}_i) + \ln (1 + \bar{M}_i)]}$

$$M_{CM}[\beta, \bar{M}_i] = \underbrace{M_0(\beta)}_{-Nk_B T \ln 2} - \sum_{\langle i,j \rangle} J_{ij}' \bar{M}_i \bar{M}_j + \frac{1}{\beta} \sum_i \left[\frac{(1+\bar{M}_i)}{2} \ln (1+\bar{M}_i) + \frac{(1-\bar{M}_i)}{2} \ln (1-\bar{M}_i) \right]$$

the first term $\sim \sum \bar{M}_i \bar{M}_j$ is the internal energy, whereas the last two terms stands as entropy term.

If we consider the situation close to T_c where \bar{M}_i is small ($\bar{M}_i \ll 1$). Observing that

$$\ln [1 + \bar{M}_i] \approx \bar{M}_i - \frac{\bar{M}_i^2}{2} + \frac{\bar{M}_i^3}{3} - \dots$$

one gets for the entropy term :

$$\left(\frac{1+\bar{M}_i}{2} \right) \ln (1+\bar{M}_i) + \left(\frac{1-\bar{M}_i}{2} \right) \ln (1-\bar{M}_i)$$

$$\simeq \left(\frac{1+\bar{M}_i}{2} \right) \left(\bar{M}_i - \frac{\bar{M}_i^2}{2} + \frac{\bar{M}_i^3}{3} - \frac{\bar{M}_i^4}{4} + \dots \right)$$

$$+ \left(\frac{1-\bar{M}_i}{2} \right) \left(-\bar{M}_i - \frac{\bar{M}_i^2}{2} - \frac{\bar{M}_i^3}{3} - \frac{\bar{M}_i^4}{4} - \dots \right)$$

$$= \bar{M}_i^2 \left(1 - \frac{1}{2} \right) + \bar{M}_i^4 \left(\frac{1}{6} \cdot 2 - \frac{1}{8} - \frac{1}{8} \right) + \dots = \frac{\bar{M}_i^2}{2} + \frac{1}{12} \bar{M}_i^4 + \dots$$

Γ_{CM}^0 to quartic order one finds:

$$\Gamma_{CM}^0 [\beta, \bar{M}_i] = \bar{M}_0 - \sum_{\langle i,j \rangle} J_{ij}' \bar{M}_i \bar{M}_j + \beta^{-1} \sum_i \left(\frac{\bar{M}_i^2}{2} + \frac{1}{12} \bar{M}_i^4 + \dots \right)$$

The Uniform Mean field Solution is obtained by neglecting spatial variation of the order parameter \bar{M}_i by taking $\bar{M}_i = \bar{M}$ for all sites i . One therefore gets:

$$-\bar{M} \sum_{\langle i,j \rangle} J_{ij}' ; z \text{ being the number n.n.}$$

$$\bar{\Gamma}_{CM}^0 [\beta, \bar{M}] = \frac{\Gamma_{CM}^0 [\beta, \bar{M}]}{N} = \bar{M}^0 - \underbrace{2J' \bar{M}^2}_{\frac{K_B}{2} (T - \frac{2\sum J'}{K_B})} + \frac{1}{\beta} \left(\frac{\bar{M}^2}{2} + \frac{1}{12} \bar{M}^4 + \dots \right)$$

$$= \bar{M}^0 + \frac{K_B}{2} \left(T - \frac{2\sum J'}{K_B} \right) \bar{M}^2 + b(T) \bar{M}^4 + \dots$$

$$= \bar{M}^0 + a(T) \bar{M}^2 + b(T) \bar{M}^4 + \dots$$

which is the Landau free energy (expansion in terms of the order parameter \bar{M}). The coefficients of the Landau theory are

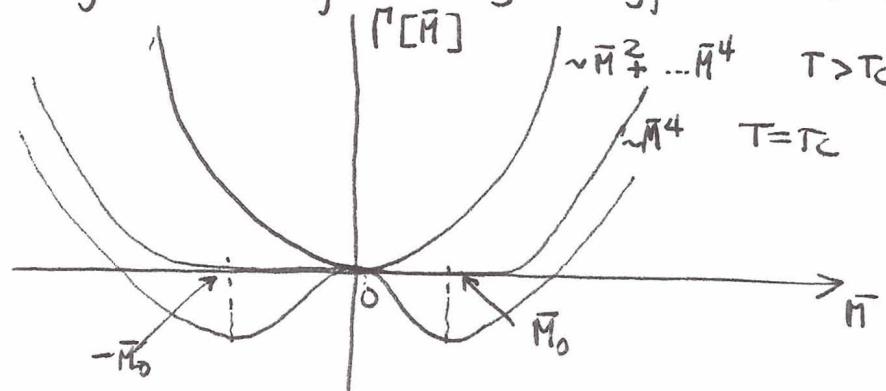
$$a(T) = \frac{K_B}{2} \left(T - \frac{2\sum J'}{K_B} \right)$$

$$b(T) \approx b(T_c) = \frac{K_B T_c}{12}$$

We introduce the ^{MF} critical temperature

$$T_c = \frac{2\sum J'}{K_B} = \frac{zJ}{2K_B} \quad (\text{comme dans la théorie de Weiss})$$

If we plot $\Gamma[\bar{M}]$ as a function of \bar{M} for different temperature



$$\frac{\partial \bar{M}}{\partial M} = B \Rightarrow \frac{\partial \bar{M}}{\partial \bar{M}} = B/\mu_B \quad \text{si} \quad \frac{\partial \bar{M}}{\partial M} = \frac{\partial \bar{M}}{\partial M/N} = \frac{\partial \bar{M}}{\mu_B \partial \bar{M}} = B$$

Comme

$$\bar{P}[\bar{M}] = \frac{M}{N}[\bar{M}] = \underbrace{a'(\tau - T_c)}_{\alpha(\tau)} \bar{M}^2 + \underbrace{\frac{k_B T_c}{12}}_{b(T_c)} \bar{M}^4 + \dots$$

Il s'ensuit

1) $\frac{\partial \bar{P}}{\partial \bar{M}} = B\mu_B = 2\alpha(\tau) \bar{M} + 4b(T_c) \bar{M}^3$

À $T=T_c$ $\alpha(\tau) = 0 \quad \therefore \quad \bar{M} = \sqrt[3]{\frac{B\mu_B}{4b(T_c)}} = \sqrt{3\beta_c \mu_B B^{\frac{1}{2}}} \quad S=3$

isotherme critique

$S=3$: exposant critique.

2) à $B=0$, T donnée :

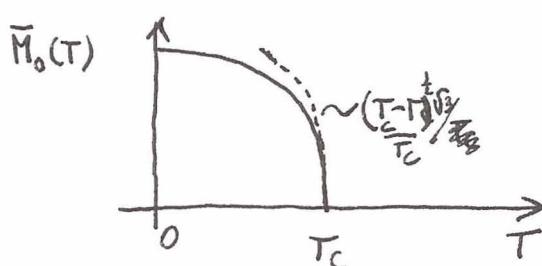
$$\frac{\partial \bar{P}}{\partial \bar{M}} = 0 = 2\bar{M}\alpha(\tau) + 4b(T_c) \bar{M}^3$$

$$\bar{M}(\alpha(\tau) + 2b(T_c) \bar{M}^2) = 0 \Rightarrow \bar{M} = 0 \quad (\text{solutions triviales})$$

ou

$$\bar{M}^2 \rightarrow \bar{M}_0^2 = -\frac{\alpha(\tau)}{2b(T_c)} = \frac{k_B}{4\beta_c T_c} (\frac{T_c - T}{T_c})$$

$\alpha(\tau) < 0$ condition nécessaire :



$$\begin{aligned} \bar{M}_0 &= \sqrt{3(\frac{T_c - T}{T_c})} \\ &= \sqrt{3} \left(\frac{T_c - T}{T_c} \right)^{\frac{1}{2}} \end{aligned}$$

$\beta = \frac{1}{2}$

Exp. critique d'Antoine

Suscéptibilité magnétique

3) On revient à

$$\frac{\partial \bar{M}}{\partial \bar{M}} = \mu_B B$$

$$\frac{\partial^2 \bar{M}}{\partial \bar{M} \partial \bar{M}} = \mu_B \frac{\partial B}{\partial M} = \mu_B \chi^{-1} \quad (\text{Note } \left(\frac{\partial M}{\partial B} \right)_B = \chi)$$

$$\frac{\partial^2 \bar{M}}{\partial \bar{M}^2} = \mu_B^2 N \frac{\partial B}{\partial M} = \mu_B^2 N \chi^{-1}$$

$$\begin{aligned} \frac{\partial}{\partial \bar{M}} \frac{\partial \bar{M}}{\partial \bar{M}} &= \frac{\partial}{\partial \bar{M}} [2a(\tau) \bar{M} + 4b(\tau_c) \bar{M}^3] \\ &= 2a(\tau) + 12b(\tau_c) \bar{M}^2 = \mu_B^2 N \chi^{-1} \end{aligned}$$

$$\Rightarrow \chi(\tau) = \frac{\mu_B^2 N}{2a(\tau) + 12b(\tau_c) \bar{M}_0^2}$$

$$\left. \begin{array}{l} T > T_c \\ \bar{M}_0 = 0 \end{array} \right\} = \frac{\mu_B^2 N}{2a(\tau)} = \frac{\mu_B^2 N / k_B}{T - T_c} = \frac{C}{(T - T_c)^\gamma}$$

$$\gamma = 1$$

exposant critique

$$\begin{aligned} \bar{M}_0^2 &= 3 \left(\frac{T_c - T}{T_c} \right) \quad \chi(T \rightarrow T_c^-) = \frac{\mu_B^2 N}{k_B(T - T_c) + \frac{1}{2} K_B T_c^2 3 \left(\frac{T_c - T}{T_c} \right)} \\ &= \frac{\mu_B^2 N / k_B}{2(T_c - T)} = \frac{C/2}{(T_c - T)^{\gamma'}} \quad \gamma' = \gamma = 1 \end{aligned}$$

1) Chaleur spécifique (Champ nul)

$$C = \left. \frac{\partial E}{\partial T} \right|_{B=0} = -T \frac{\partial^2 \bar{M}}{\partial T^2}_{eq.}$$

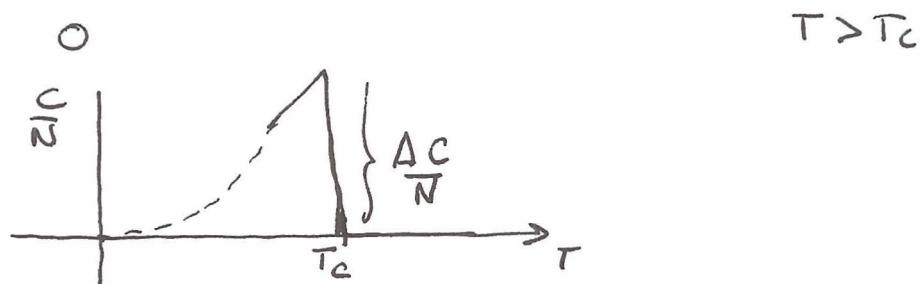
$$\bar{M}_q[\bar{M}_0] = \underbrace{\frac{k_B}{2} (T - T_c) \cdot \bar{M}_0^2}_{\propto (T)} + b(T_c) \bar{M}_0^4 + \underbrace{\bar{M}_0}_{\sim -K_B T^{3/2}}$$

$$\bar{M}_{eq}[\bar{M}_0] = a(\tau) \bar{M}_0^2 + b(\tau_c) \bar{M}_0^4$$

$$= a(\tau) \left(-a(\tau) \right) + b(\tau_c) \cdot \frac{a^2(\tau)}{4b^2(\tau_c)}$$

$$\bar{M}_{eq}[\bar{M}_0] = -\frac{a^2(\tau)}{4b(\tau_c)} = -\frac{a'^2(\tau-\tau_c)^2}{4b(\tau_c)}$$

$$-T \frac{\partial^2 \bar{M}_{eq}}{\partial T^2} = \frac{C}{N} = T a'^2 / 2b(\tau_c) \equiv \frac{\Delta C}{N} \quad T < \tau_c$$



$$\text{Si } \frac{C}{N} \sim |T - T_c|^{-\alpha'}$$

$\alpha' = \alpha = 0$ comme exp. de
chaleur spécifique

discontinuité en th. des champs
Mayen.

Spatial correlations

Within mean field theory, the uniform solution $\bar{M}_i = \bar{M}$, corresponds to the Landau theory near T_c :

$$M[\bar{M}] = M^0 - \sum_{\langle ij \rangle} J_{ij} \bar{M}^2 + \frac{N}{\beta} \left[\frac{1}{2} \bar{M}^2 + \frac{1}{12} \bar{M}^4 + \dots \right]$$

Now if we relax the uniform constraint and develop the Gibbs potential we get

$$F[\bar{M}] = F^0 - \sum_{\langle ij \rangle} J_{ij} \bar{M}_i \bar{M}_j + \frac{1}{\beta} \sum_i \left[\frac{1}{2} \bar{M}_i^2 + \frac{1}{12} \bar{M}_i^4 + \dots \right]$$

Since \bar{M}_i is now a function of the site position i , it is possible to get the correlation length ξ in "mean field" theory and also the momentum dependence of $G(G)$, the Fourier transform of the correlation function and in turn to get the exponent η .

the

By definition the correlation function is

$$(G)_{ij} = \left(\frac{\partial M_i}{\partial B_j} \right)_{B=0}$$

which is the response of the order parameter at site i due to a variation of the magnetic field at site j . $(G)_{ij}$ can then be viewed as a matrix so that the inverse

$$(G)_{ij}^{-1} = \left(\frac{\partial B_j}{\partial M_i} \right)_{B=0}$$

Can be related to the Gibbs potential that is

$$B_j = \frac{\partial M}{\partial M_j} = \frac{\partial F}{\mu_B \partial \bar{M}_j}$$

$$\mu_B B_j = B'_j = \frac{\partial M}{\partial \bar{M}_j}; \quad \frac{\partial B'_j}{\partial M_i} = \frac{\partial^2 F}{\partial M_i \partial \bar{M}_j} = \frac{\partial^2 F}{\mu_B \partial \bar{M}_i \partial \bar{M}_j}$$

$$\text{or} \quad \boxed{\frac{1}{\mu_B^2} \frac{\partial^2 \Pi}{\partial M_i \partial M_j} = \frac{\partial G_{ij}}{\partial M_j} = (G)_{ij}^{-1}}$$

From the expression of the Gibbs potential, we have

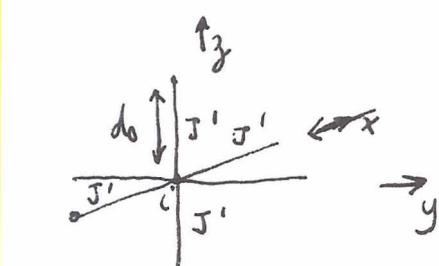
$$(G)_{ij}^{-1} = \frac{1}{\mu_B^2} \left\{ -2J'_{ij} + \frac{1}{\beta} \delta_{ij} \left[1 + \frac{12}{12} \bar{M}_i^2 + \dots \right]_{B=0} \right\}$$

Going in Fourier space using

$$\begin{aligned} G^{-1}(\vec{q}) &= \sum_j (G)_{ij}^{-1} e^{i\vec{q} \cdot (\vec{r}_i - \vec{r}_j)} \\ &= \frac{1}{\mu_B^2} \left[-2J'(\vec{q}) + \frac{1}{\beta} (1 + \bar{M}_0^2(T) + \dots) \right] \end{aligned}$$

with the Fourier transform of the exchange

$$\begin{aligned} J'(\vec{q}) &= \sum_j J'_{ij} e^{i\vec{q} \cdot (\vec{r}_i - \vec{r}_j)} \\ &= J' \sum e^{i\vec{q} \cdot (\vec{r}_i - \vec{r}_j)} \\ &\stackrel{GL}{=} J' \left\{ (e^{iq_x d_0} + e^{-iq_x d_0}) + (e^{iq_y d_0} + e^{-iq_y d_0}) \right. \\ &\quad \left. + (e^{iq_z d_0} + e^{-iq_z d_0}) \right\} \\ &= 2J' (\cos q_x d_0 + \cos q_y d_0 + \cos q_z d_0) \end{aligned}$$



Note that at $\vec{q}=0$, $J'(\vec{q}=0) = J'G = \frac{2}{z} J'$
where z is the number of nearest-neighbors for each site.
We can write:

$$\boxed{G(\vec{q}) = \frac{\mu_B^2}{2(J'(0) - J'(\vec{q})) + \left(\frac{1}{\beta} - 2J'(0) \right) + \frac{1}{\beta} \bar{M}_0^2}}$$

At $T > T_C$, we have $M_0 = 0$ and for small (relevant) wave-vector \vec{q}
namely $qd_0 \ll 1$, we get

$$J'(0) - J'(\vec{q}) \approx \frac{2J'}{21} (q_x^2 + q_y^2 + q_z^2) d_0^2 = J' d_0^2 q^2$$

also $\frac{1}{\beta} - 2J'(0) = K_B T - 2J'(0) = K_B \left(T - \frac{2J'(0)}{K_B} \right)$

we define the characteristic temperature

$$\frac{2J'(0)}{K_B} = T_c$$

$$T_c = \frac{22J'}{K_B}$$

as obtained earlier. therefore we have at small q and $T > T_c$:

$$G(\vec{q}) = \frac{\mu_B^2 (K_B T_c)^{-1}}{\underbrace{\frac{2J' d_0^2}{K_B T_c} q^2}_{\equiv \xi_0^2} + \underbrace{\left(\frac{T-T_c}{T_c} \right)}_{\equiv \varepsilon}}$$

or

$$G(\vec{q}) = \frac{\mu_B^2 (K_B T_c)^{-1} \varepsilon^{-1}}{1 + \xi(T)^2 q^2}$$

where

$$\xi(T) = \xi_0^+ \left(\frac{T-T_c}{T_c} \right)^{-\nu} \quad \nu = \frac{1}{2}$$

is the correlation length and $\nu = \frac{1}{2}$ is the exponent in this meanfield approach. $G(\vec{q})$ has therefore a Lorentzian form. At T_c , $\xi^2 q^2 \rightarrow \infty$ for q finite, $G(\vec{q})$ goes as:

$$G(\vec{q}) \sim \frac{1}{q^2}$$

which implies that

$$\xi = 0$$

In this small q limit, we can Fourier transform the correlation function

$$= \frac{1}{N} \sum_{\vec{q}} G(\vec{q}) e^{i\vec{q} \cdot (\vec{r}_i - \vec{r}_j)}$$

$$(G)_{ij} \rightarrow G(r = |\vec{r}_i - \vec{r}_j|) = \frac{d}{(k_B T_C)}^{-1} \mu_B^2 \varepsilon^{-1} \int \frac{d^d q}{(2\pi)^d} \frac{e^{i\vec{q} \cdot \vec{r}}}{\xi^2 q^2 + 1}$$

$$= \frac{\mu_B^2 d_0^3 (k_B T_C)^{-1}}{4\pi^2} \int_0^{q_0} q^2 dq \underbrace{\int_{-1}^1 \frac{d(\cos \theta) e^{iq r \cos \theta}}{(\xi^2 q^2 + 1)}}_{\frac{2i \sin qr}{\xi^2 q^2 + 1}}$$

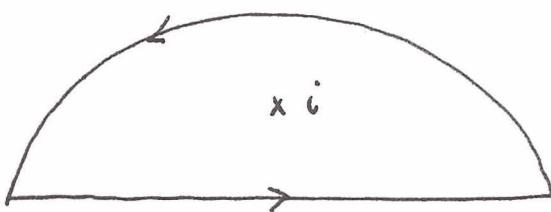
$d=3$

Here $q_0 \sim 1/d_0$ is a cut-off, which is chosen consistently with the small q expansion described before. We can rewrite the expression as (parity of the integrand)

$$G(r) = \frac{\mu_B^2 d_0^3 (k_B T_C)^{-1}}{4\pi^2} \frac{\varepsilon^{-1}}{r} \text{Im} \int_{-q_0}^{+q_0} \frac{q^{2-1} dq}{(\xi^2 q^2 + 1)} e^{iqr}$$

$$\xi^{-2} \underbrace{\int_{-q_0\xi}^{+\xi q_0 \rightarrow \infty} \frac{q' dq' e^{iq'r/\xi}}{(q'^2 + 1)}}_{q\xi = q'}$$

in the complex plane, the integral can be done easily



Using indeed the Cauchy integral formula for the upper half plane we get

$$G(r) = \frac{\mu_B^2 d_0^3 (k_B T_C)^{-1}}{4\pi^2} \frac{\varepsilon^+}{\xi^{+2} \varepsilon^-} \text{Im} \left[\frac{2\pi i \cdot i e^{-r/\xi}}{x i} \right]$$

$$G(r) = \frac{\mu_B^2 d_0^3 (k_B T_C)^{-1}}{4\pi} \frac{e^{-r/\xi}}{r}$$

which is consistent with the form:

$$G(r) = \frac{\mu_B^2 d_0^3 (k_B T_C)^{-1}}{4\pi \xi_0^{d+2}} \frac{e^{-r/\xi}}{r^{d-2+\gamma}}$$

or once again $\gamma=0$. Note that $G(r) \sim \frac{1}{r}$ for $r \ll \xi$, which is homogeneous and indicates already "scaling" and self-similarity. This self-similarity property breaks down at large distance $r \gg \xi$ where the exponential form $e^{-r/\xi}$ dominates the decay of $G(r)$.

At $T < T_C$, $M_0 = \sqrt{3} \left(\frac{T_C - T}{T_C} \right)^{\frac{1}{2}}$ is finite and $G(\vec{q})$ becomes.

$$G(\vec{q}) = \frac{\mu_B^2 (k_B T_C)^{-1}}{\frac{25 d_0^2 q^2}{k_B T_C} + \left(\frac{T_C - T}{T_C} \right) + 3 \left(\frac{T_C - T}{T_C} \right)}$$

$\underbrace{2 \left(\frac{T_C - T}{T_C} \right)}_{2\varepsilon^-}$

$$G(\vec{q}) = \frac{\frac{1}{2} \mu_B^2 (k_B T_C)^{-1}}{\xi_0^{-2} q^2 + \varepsilon^-}$$

which is also a Lorentzian and then we can define at $T \rightarrow T_C^-$

$$G(q) \sim \frac{1}{q^{2-\gamma'}}$$

with $\gamma' = \gamma = 0$. The Fourier transform proceeds similarly.

Here $(\frac{\partial f}{\partial \sigma})^2 = \frac{J^2 d_0^2 q^2}{k_B T_c}$, and we have

$$G(r) = \frac{\frac{1}{2} \mu_B^2 d_0^3 (k_B T_c)^{-1}}{\left(\frac{\xi_0}{2}\right)^2 4\pi} \frac{e^{-r/\xi}}{r} - \bar{M}_0^2$$

where ξ is the correlation length below T_c

$$\xi = \xi_0 \left(\frac{T - T_c}{T_c} \right)^{-\frac{1}{n}}$$

it follows that

$$\nu' = \nu = \frac{1}{2}$$

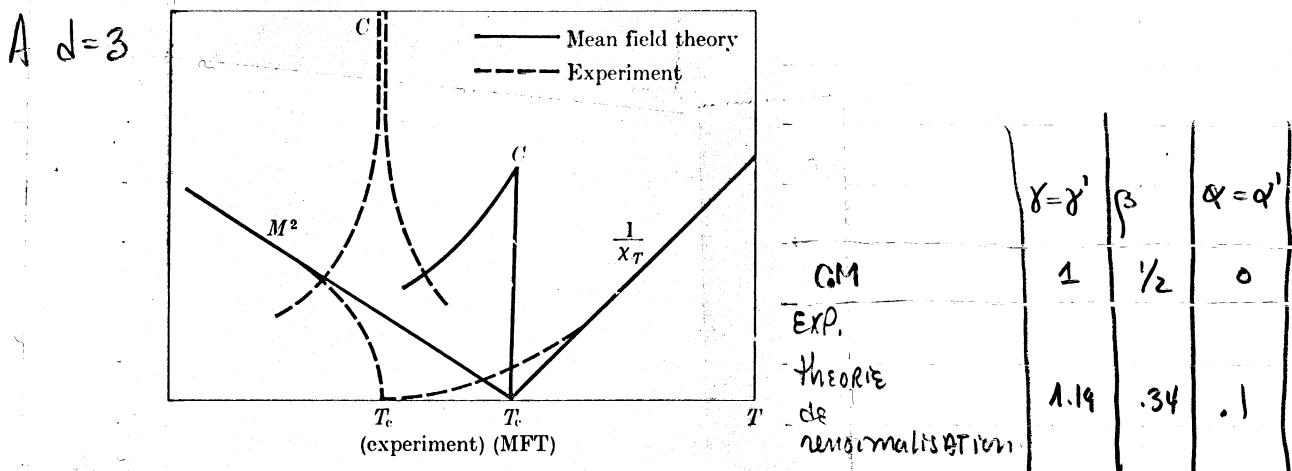


FIG. 6.6. Schematic comparison of typical experimental measurements on a Heisenberg ferromagnet (such as EuS) with the predictions of the molecular field theory (cf. Fig. 3.3). Note that the curve for $1/\chi_T$ is shown only for $T > T_c$.

les écarts P/r aux résultats expérimentaux sont énormes ! non seulement pour les exposants mais aussi pour le T_c : $T_{c\text{exp}} \ll T_{c\text{M}}$

$$\left(\text{Exemple : } T_c \Big|_{\text{Fe, Eu C.M.}} \approx 20,000 \text{ K} \right)$$

$$\left. T_c \right|_{\text{Exp.}} \approx 1000 \text{ K} !$$

* le champ moyen ne se soucie guère de la dimensionnalité du système pour les exposants $\{\gamma, \delta, \beta, \alpha, \text{etc}\}$ qui sont indépendants de d . En fait seul T_c dépend du nombre de coordination z du réseau.

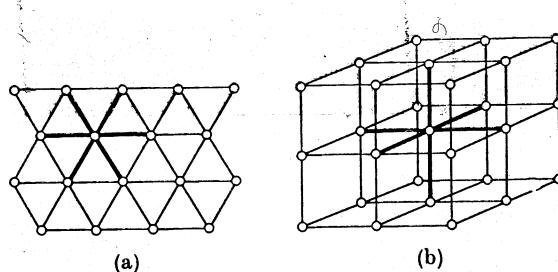


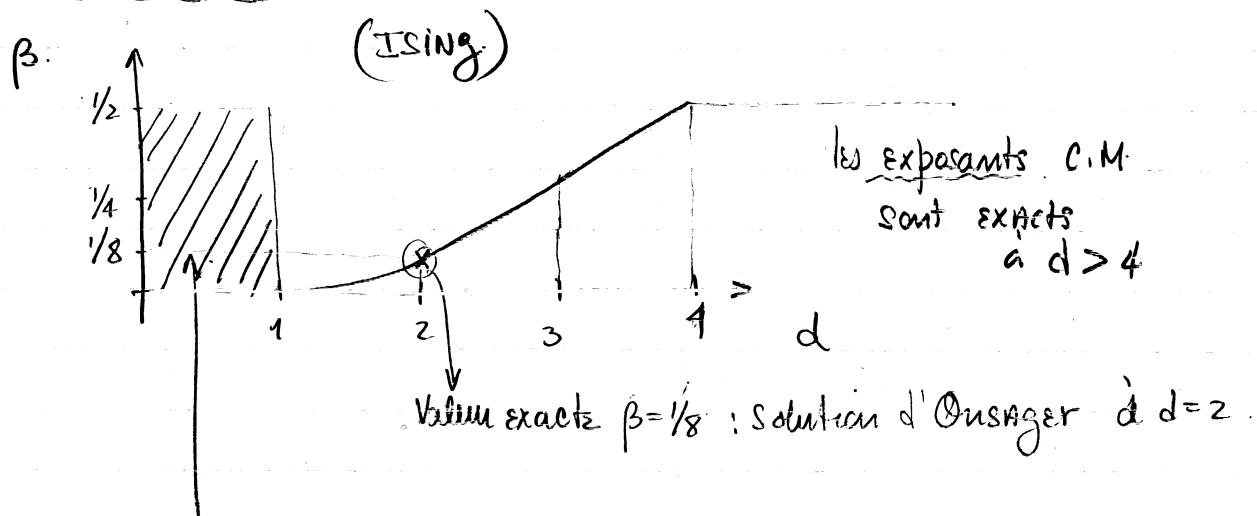
FIG. 6.7. (a) The plane triangular lattice, and (b) the simple cubic lattice. The fact that both lattices have the same coordination number ($q = 6$) means that within the mean field approximation they are predicted to have the same critical temperature (cf. (6.51)). This prediction is at odds with the more accurate approximation procedures to be discussed in Chapter 9, and it is currently believed that the critical temperature depends rather strongly upon lattice dimensionality. After Ziman (1964).

Pour un modèle d'Ising :

$$\hat{H} = -J \sum_{ij} \hat{S}_i^z \hat{S}_j^z \quad (M=1 \text{ composante}).$$

* l'existence d'un ordre à longue distance à $T \neq 0$ est fortement fonction de la dimensionnalité du système et du nombre de composantes

du paramètre d'ordre



Phase transition de phase à $d < 1$ ($M=1$).

* Note à $d \rightarrow \infty$ (équivalent aux interactions de longue portée)

$$T_c \Big|_{\text{EXACT}} = T_{c,\text{eff}}, + \{ \gamma, \alpha, \beta, \delta, \dots \} = \{ \gamma_{\text{eff}}, \dots \}$$

* La dimension 4 pour une transition ferromagnétique est critique

=> Souvent appelée dimension critique supérieure
dimension 2: dimension critique inférieure,
Pour C.M. (à $d < 2$ non définie !)