0.0.1 Mean field critical exponents

Let us consider the equation

$$f(m, T, 0) \approx const + \frac{A}{2}m^2 + \frac{B}{4}m^4 + O(m^6)$$

with $B > 0$, so we do not need more term to find the minima of the solution. This is called stabilization. What is most important is the coefficient $A = \hat{J}z(1 - \beta\hat{J}z)$, that means that A can change sign.

β exponent

The β exponential observe the order parameter. Consider $H = 0$, $t \equiv \frac{T-T_c}{T_c}$ and $m \overset{t \to 0^-}{\sim} -t^\beta$. The condition of equilibrium is

$$\frac{\partial f}{\partial m} = 0$$

which implies

$$\frac{\partial f}{\partial m}\bigg|_{m=m_0} = Am_0 + Bm_0^3 = \left[\hat{J}z(1 - \beta\hat{J}z) + Bm_0^2\right]m_0 = 0$$

Since at the critical point we have $T_c = \frac{\hat{J}z}{k_B}$:

$$0 = \frac{k_B T_c}{T}(T - T_c)m_0 + Bm_0^3$$

The solution are $m_0 = 0$ and

$$m_0 \simeq (T_c - T)^{1/2} \tag{1}$$

Hence, the mean field value is $\beta = 1/2$.

δ exponent

Now, let us concentrate in the δ exponent. We are in the only case in which we are in $T = T_c$ and we want to see how the magnetization decrease: $H \sim m^\delta$.

Starting from the self-consistent equation, we have

$$m = \tanh\left(\beta(\hat{J}zm + H)\right) \tag{2}$$

Inverting it

$$\beta(\hat{J}zm + H) = \tanh^{-1}m$$

On the other hand, for $m \sim 0$

$$\tanh^{-1}m \simeq m + \frac{m^3}{3} + \frac{m^5}{5} + \dots$$

Therefore, by substituting

$$H = k_B T\left(m + \frac{m^3}{3} + \dots\right) - \hat{J}zm = \left(k_B T - \hat{J}z\right)m + k_B T\frac{m^3}{3} + \dots$$

$$\simeq k_B(T - T_c)m + \frac{k_B T}{3}m^3$$

At $T = T_c = \frac{\hat{J}z}{k_B}$, we have

$$H \sim k_B T_c \frac{m^3}{3} \tag{3}$$

The mean field value is $\delta = 3$.

α exponent

Consider the α exponent, for $H = 0$, $c_H \sim t^{-\alpha}$ and $t = (T - T_c)/T_c$. Compute the specific heat at $H = 0$. Consider first $T > T_c$, where $m_0 = 0$,

$$f(m, H) = \frac{\hat{J}zm^2}{2} - \frac{1}{\beta} \ln\left(2\cosh\left(\beta(\hat{J}zm + H)\right)\right) - k_B T \ln 2$$

If $m = 0$, $\cosh 0 = 1$ and

$$f = -k_B T \ln 2$$

it is called paramagnetic phase. Indeed,

$$c_H = -T\left(\frac{\partial^2 f}{\partial T^2}\right) = 0 \tag{4}$$

The mean field value is $\alpha = 0$.

Remark. For $T < T_c$, $m = m_0 \neq 0$. This implies that $c_H \neq 0$, but still $f = -k_B T \ln A$ with $A = const$. We obtain $\alpha = 0$ also in this case.

$$m_0 = \pm\sqrt{-\frac{\hat{J}z}{2T_c}(T - T_c)}$$

γ exponent

Now we consider the γ exponent, for $H = 0$, $\chi \sim t^{-\gamma}$. Starting again from equation (2):

$$m = \tanh\left(\beta(\hat{J}zm + H)\right)$$

and developing it around $m \simeq 0$, as shown before we get

$$H = mk_B(T - T_c) + \frac{k_B T}{3}m^3$$

$$\Rightarrow \chi_T = \frac{\partial m}{\partial H} = \frac{1}{\frac{\partial H}{\partial m}}$$

Since $\frac{\partial H}{\partial m} \simeq k_B(T - T_c) + K_B T m^2$, as $m \to 0$

$$\chi \sim (T - T_c)^{-1} \tag{5}$$

The mean field value is $\gamma = 1$.

Summary

The mean field critical exponents are

$$\beta = \frac{1}{2}, \quad \gamma = 1, \quad \delta = 3, \quad \alpha = 0 \tag{6}$$

We can immediately note that these exponents are different from those found by Onsager for the Ising model in two dimensions, so the mean field theory is giving us wrong predictions. This is because mean field theories are good approximations only if the system has a high enough dimensionality (and $d = 2$ is still too low for the Ising model, see Coarse graining procedure for the Ising model).

Remark. In the mean field critical exponents the dimension d does not appear. T_c instead depends on the number of z of neirest neighbours and hence on the embedding lattice (on the dimension)!

Remark. (lesson) The ν exponent define the divergence of the correlation lengths. In order to do that, in principle we should compute the correlation function, but which are the correlation we are talking about? The correlation or the fluctuation with to respect the average? In the ferromagnetic we have infinite correlation lengths, but it is not true, because instead of that we consider the variation correlated! Which is the problem here? In mean field we were neglecting correlation between fluctuation. We thought: let us compute neglecting correlation. How we can compute the correlation function within the mean field theory with thermal fluctuations? We look at the response of the system. Experimentally what can we do? It is a magnetic field, but we cannot use homogeneous magnetic field. Another way to compute the correlation function without looking at thermal fluctuation it is by considering a non homogeneous magnetic field. If we make a variation in H_i in the system, what happened in the H_j? This is an important point.

0.1 Mean field variational method

The mean field variational method is a general approach to derive a mean field theory. The method is valid for all T and is sufficiently flexible to deal with complex systems. The method is similar to the one used in quantum mechanics, namely it is based on the following inequality

$$E_\alpha = \langle \psi_\alpha | \hat{H} | \psi_\alpha \rangle \geq E_0 \tag{7}$$

valid for all trial function ψ_α.

Remark. E_0 is the ground state energy.

> **Example 1**
>
> In many body problem we have Hartree and Hartree-Fock variational methods.

The closest bound to E_0 is the one that is obtained by minimizing E_α, i.e. $\langle \psi_\alpha | \hat{H} | \psi_\alpha \rangle$ over $| \psi_\alpha \rangle$, where the $| \psi_\alpha \rangle$ are functions to be parametrized in some convenient way.

The method is based on the following inequalities

1. Let Φ be a random variable (either discrete or continuous) and let $f(\Phi)$ be a function of it.

   For all function f of Φ, the mean value with respect to a distribution function $p(\Phi)$ is given by
   $$\langle f(\Phi) \rangle_p \equiv \mathrm{Tr}(p(\Phi)f(\Phi)) \tag{8}$$

   If we consider the function

   $$f(\Phi) = \exp[-\lambda\Phi] \tag{9}$$

   it is possible to show the inequality

   $$\left\langle e^{-\lambda\Phi} \right\rangle_p \geq e^{-\lambda\langle\Phi\rangle_p}, \quad \forall p \tag{10}$$

   Proof of inequality (10). $\forall \Phi \in \mathbb{R}$, $e^\Phi \geq 1 + \Phi$. Hence,

   $$e^{-\lambda\Phi} = e^{-\lambda\langle\Phi\rangle}e^{-\lambda[\Phi-\langle\Phi\rangle]} \geq e^{-\lambda\langle\Phi\rangle}(1 - \lambda(\Phi - \langle\Phi\rangle))$$

Taking the average of both sides, we get

$$\rightarrow \left\langle e^{-\lambda\Phi} \right\rangle_p \geq \left\langle (1 - \lambda(\Phi - \langle\Phi\rangle))e^{-\lambda\langle\Phi\rangle} \right\rangle_p = e^{-\lambda\langle\Phi\rangle_p}$$

∎

2. The second inequality refers to the free energy. Let $\rho(\Phi)$ be a probability distribution, i.e. such that

$$\text{Tr}(\rho(\Phi)) = 1, \quad \rho(\Phi) \geq 0 \quad \forall\Phi \tag{11}$$

Hence,

$$e^{-\beta F_N} = Z_N = \text{Tr}_{\{\Phi\}}\, e^{-\beta\mathcal{H}[\{\Phi\}]} = \text{Tr}_{\{\Phi\}}\, \rho e^{-\beta\mathcal{H} - \ln\rho} = \left\langle e^{-\beta\mathcal{H} - \ln\rho} \right\rangle_\rho$$

From the inequality (10),

$$e^{-\beta F_N} = \left\langle e^{-\beta\mathcal{H} - \ln\rho} \right\rangle_\rho \geq e^{-\beta\langle\mathcal{H}\rangle_\rho - \langle\ln\rho\rangle_\rho}$$

Taking the logs one has

$$F \leq \langle\mathcal{H}\rangle_\rho + k_B T \langle\ln\rho\rangle_\rho = \text{Tr}(\rho\mathcal{H}) + k_B T\,\text{Tr}(\rho\ln\rho) \equiv F_\rho \tag{12}$$

Whenever we are able to write the last equation by using a ρ, then we will minimize it. This is the variational approach of statistical mechanics. The question is: which is the ρ that minimizes?

The functional F_ρ will reach its minimum value with respect to the variation of ρ with the constraint $\text{Tr}(\rho) = 1$, when

$$\bar{\rho} = \rho_{eq} = \frac{1}{Z} e^{-\beta\mathcal{H}} \tag{13}$$

So far so good but not very useful, since we are back to the known result that the distribution that best approximately the free energy of the canonical ensemble is given by the Gibbs-Boltzmann distribution. To compute ρ_{eq}, we need some approximation!

0.1.1 Mean field approximation for the variational approach

Let us now try to compute the Z by starting from the inequality (12). Up to now everything is exact. The idea is to choose a functional form of ρ and then minimize F_ρ with respect to ρ. Note that ρ is the $N-$point probability density function (it is a function of all the degrees of freedom):

$$\rho = \rho(\Phi_1, \ldots, \Phi_N)$$

it is a $N-$body problem, where Φ_α is the random variables associated to the $\alpha-$esim degree of freedom. This is in general a very difficult distribution to deal with. This is equivalent exactly at

$$\psi_\alpha(\vec{r}_1, \vec{P}_1, \ldots, \vec{r}_N, \vec{P}_N)$$

The mean-field approximation consists in factorising ρ into a product of $1-$point distribution function:

$$\rho(\Phi_1, \ldots, \Phi_N) \overset{MF}{\simeq} \prod_{\alpha=1}^{N} \rho^{(1)}(\Phi_\alpha) \equiv \prod_{\alpha=1}^{N} \rho_\alpha \tag{14}$$

where we have used the short-hand notation $\rho^{(1)}(\Phi_\alpha) \rightarrow \rho_\alpha$.

Remark. Approximation (14) is equivalent to assume statistical independence between particles (or more generally between different degrees of freedom). The independence of the degree of freedom is a very strong assumption!

Example 2

Let us consider the spin model on a lattice; what is the Φ_α? We have:

$$\Phi_\alpha \to S_i$$

Hence, $\rho = \rho(S_1, S_2, \ldots, S_N)$ and (14) becomes

$$\rho \overset{MF}{\simeq} \prod_{i=1}^{N} \rho^{(1)}(S_i) \equiv \prod_{i=1}^{N} \rho_i$$

With Eq.(14) and the condition $\text{Tr}(\rho_\alpha) = 1$, we compute the two averages in the Eq.(12) given the field. We have:

$$\text{Tr}_{\{\Phi\}}(\rho \ln \rho) = \text{Tr}\left(\prod_\alpha \rho_\alpha \left(\sum_\alpha \ln \rho_\alpha\right)\right) \overset{\text{to do}}{=} \sum_\alpha \text{Tr}^{(\alpha)}(\rho_\alpha \ln \rho_\alpha) \tag{15}$$

where $\text{Tr}^{(\alpha)}$ means sum over all possible values of the random variable Φ_α (with α fixed and $\text{Tr}^{(\alpha)} \rho_\alpha = 1$).

We end up that

$$F_{\rho_{MF}} = \langle \mathcal{H} \rangle_{\rho_{MF}} + k_B T \sum_\alpha \text{Tr}^{(\alpha)}(\rho_\alpha \ln \rho_\alpha) \tag{16}$$

Remark. $F_{\rho_{MF}} = F(\{\rho_\alpha\})$ and we have to minimize it with respect to ρ_α.

How can we parametrize ρ_α? There are two approaches that are mostly used:

1. Parametrize $\rho_\alpha \equiv \rho^{(1)}(\Phi_\alpha)$ by the average of Φ_α with respect to ρ_α, $\langle \Phi_\alpha \rangle_{\rho_\alpha}$ (in general is the local order parameter):

$$\rho_\alpha = \rho^{(1)}(\Phi_\alpha) \to \langle \Phi_\alpha \rangle_{\rho_\alpha}$$

   This means that there are two constraints in the minimization procedure:

$$\text{Tr}^{(\alpha)} \rho_\alpha = 1, \quad \text{Tr}^{(\alpha)}(\rho_\alpha \Phi_\alpha) = \langle \Phi_\alpha \rangle$$

   where the second is the self-consistent equation.

   Remark. In this case the variational parameter coincides with the order parameter.

2. In the second approach is ρ_α itself the variational parameter. $F_{\rho_{MF}}$ is minimized by varying ρ_α. It is a more general approach, that involves functional minimization.

0.1.2 First approach: Bragg-Williams approximation

We apply this approach to the Ising model with non uniform magnetic field. The Hamiltonian of such a system is

$$\mathcal{H}[\{S\}] = -J \sum_{\langle ij \rangle} S_i S_j - \sum_i H_i S_i \tag{17}$$

It means that
$$\Phi_\alpha \to S_i = \pm 1$$

and that the variational parameter becomes the order parameter

$$\langle \Phi_\alpha \rangle \to \langle S_i \rangle \equiv m_i$$

Remark. Note that this time $H \to H_i$ (non-uniform), hence m_i depends on the site i.

We have to define a $1-$particle probability density distribution $\rho_i \equiv \rho^{(1)}(S_i)$ such that

$$\rho_i \equiv \rho^{(1)}(S_i) \to \begin{cases} \operatorname{Tr} \rho_i = 1 \\ \operatorname{Tr} \rho_i S_i = m_i \end{cases} \tag{18}$$

Since we have to satisfy these two constraints, we need two free parameters. A linear functional form is sufficient. Denoting by:

- a: statistical weight associated to the value $S_i = -1$.

- b: statistical weight associated to all the remaining possible values of S_i (for an Ising only one value remains, i.e. $S_i = +1$).

The simplest function form with two parameters is the linear function, namely

$$\rho_i \equiv \rho^{(1)}(S_i) = a(1 - \delta_{S_i,1}) + b\delta_{S_i,1} \tag{19}$$