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0.0.1 Mean field critical exponents

Let us consider

$$f(m,T,0) \approx const + \frac{A}{2}m^2 + \frac{B}{4}m^4 + O(m^6) \tag{1}$$

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

$$\frac{\partial f}{\partial m} = 0 \tag{2}$$

which implies

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

Since $T_c = \frac{\hat{J}z}{k_B}$:

$$0 = \frac{k_B T_c}{T}(T-T_c)m_0 + Bm_0^3 \tag{4}$$

The solution are $m_0 = 0$ and

$$m_0 \simeq (T_c - T)^{1/2} \tag{5}$$

The mean field value is so $\beta = 1/2$.

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

$$m = \tanh\Big(\beta(\hat{J}zm + H)\Big) \tag{6}$$

Inverting it

$$\beta(\hat{J}zm + H) = \tanh^{-1} m \tag{7}$$

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

$$\tanh^{-1} m \simeq m + \frac{m^3}{3} + \frac{m^5}{5} + \dots \tag{8}$$

Therefore, by substituting

$$\begin{aligned} H = k_B T\left(m + \frac{m^3}{3} + \dots\right) - \hat{J}zm &= \left(k_B T - \hat{J}z\right)m + k_B T\frac{m^3}{3} + \dots \\ &\simeq k_B(T-T_c)m + \frac{k_B T}{3}m^3 \end{aligned} \tag{9}$$

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

$$H \sim k_B T_c \frac{m^3}{3} \tag{10}$$

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

α exponent

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

$$f(m, H) = \frac{\hat{J}zm^2}{2} - \frac{1}{\beta}\ln\Big(2\cosh\Big(\beta(\hat{J}zm + H)\Big)\Big) \tag{11}$$

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

$$f = -k_B T \ln 2 \tag{12}$$

therefore

$$c_H = -T\left(\frac{\partial^2 f}{\partial T^2}\right) = 0 \tag{13}$$

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.

$$m_0 = \pm\sqrt{-\frac{\hat{J}z}{2T_c}(T - T_c)} \tag{14}$$

γ exponent

Now we consider the γ exponent, for $H = 0$, $\chi \sim t^{-\gamma}$. Starting again from equation (6):

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

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

$$H = mk_B(T - T_c) + \frac{k_B T}{3}m^3 \tag{15}$$

$$\Rightarrow \chi_T = \frac{\partial m}{\partial H} = \frac{1}{\frac{\partial H}{\partial m}} \tag{16}$$

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

$$\chi \sim (T - T_c)^{-1} \tag{17}$$

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

Summary

The mean field critical exponents are

$$\beta = \frac{1}{2}, \quad \gamma = 1, \quad \delta = 3, \quad \alpha = 0 \tag{18}$$

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!

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 negleting correlation. How we can compute the correlation function within the meanfield theory with thermal fluctuations? We look at the response of the system. Esperimentally 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 happend 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 flexibile to deal with complex systems.

The method is similar to the one used in quantum mechanics, namely it is based on the following inequality

$$E_\alpha = \langle\psi_\alpha|\,\hat{H}\,|\psi_\alpha\rangle \geq E_0 \tag{19}$$

valid for all trial function ψ_α.

Remark. E_0 is the ground state energy.

Example 1. In many mody problem we have Hartee and Hartree-Fock.

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
   $$\langle f(\Phi)\rangle_p \equiv \mathrm{Tr}(p(\Phi)f(\Phi)) \tag{20}$$
   If we consider the function
   $$f(\Phi) = \exp[-\lambda\Phi] \tag{21}$$
   it is possible to show the inequality
   $$\left\langle e^{-\lambda\Phi}\right\rangle_p \geq e^{-\lambda\langle\Phi\rangle_p}, \quad \forall p \tag{22}$$

   Proof. $\forall\Phi\in\mathbb{R}$, $e^\Phi \geq 1+\Phi$. 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
   $$\rightarrow \left\langle e^{-\lambda\Phi}\right\rangle_p \geq \left\langle(1-\lambda(\Phi-\langle\Phi\rangle))e^{-\lambda\langle\Phi\rangle}\right\rangle_p = e^{-\lambda\langle\Phi\rangle_p}$$
   $\square$

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

$$\mathrm{Tr}(\rho(\Phi)) = 1 \quad \rho(\Phi) \geq 0 \quad \forall\Phi \tag{23}$$

Hence,

$$e^{-\beta F_N} = Z_N = \mathrm{Tr}_{\{\Phi\}}\, e^{-\beta\mathcal{H}[\{\Phi\}]} = \mathrm{Tr}_{\{\Phi\}}\, \rho e^{-\beta\mathcal{H}-\ln\rho} = \left\langle e^{-\beta\mathcal{H}-\ln\rho}\right\rangle_\rho \tag{24}$$

From the inequality (22),

$$e^{-\beta F_N} = \left\langle e^{-\beta\mathcal{H}-\ln\rho}\right\rangle_\rho \geq e^{-\beta\langle\mathcal{H}\rangle_\rho - \langle\ln\rho\rangle_\rho} \tag{25}$$

Taking the logs one has

$$F \leq \langle\mathcal{H}\rangle_\rho + k_B T\,\langle\ln\rho\rangle_\rho = \mathrm{Tr}(\rho\mathcal{H}) + k_B T\,\mathrm{Tr}(\rho\ln\rho) \equiv F_\rho \tag{26}$$

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

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

$$\boxed{\bar{\rho} = \rho_{eq} = \frac{1}{Z}e^{-\beta\mathcal{H}}} \tag{27}$$

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 to the inequality (26). Up to now everithing 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):

$$\rho = \rho(\Phi_1, \ldots, \Phi_N) \tag{28}$$

it is a $N-$body problem. The 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 when we have:

$$\psi_\alpha(\vec{\mathbf{r}}_1, \vec{\mathbf{P}}_1, \ldots, \vec{\mathbf{r}}_N, \vec{\mathbf{P}}_N) \tag{29}$$

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

$$\boxed{\rho(\Phi_1, \ldots, \Phi_N) \overset{MF}{\simeq} \prod_{\alpha=1}^{N} \rho^{(1)}(\Phi_\alpha) \equiv \prod_{\alpha=1}^{N} \rho_\alpha} \tag{30}$$

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

Remark. Approximation (30) is equivalent to assume statistical indipendence between particles (or more generally between different degrees of freedom). The indipendence 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, $\rho = \rho(S_1, S_2, \dots, S_N)$ and (30) becomes

$$\rho \overset{MF}{\simeq} \prod_{i=1}^{N} \rho^{(1)}(S_i) \equiv \prod_{i=1}^{N} \rho_i \tag{31}$$

With (30) and $\mathrm{Tr}(\rho_\alpha) = 1$, we compute the two averages in the (26) given the field. We have:

$$\mathrm{Tr}_{\{\Phi\}}(\rho \ln \rho) = \mathrm{Tr}\left(\prod_\alpha \rho_\alpha \left(\sum_\alpha \ln \rho_\alpha\right)\right) \overset{\text{to do}}{=} \sum_\alpha \mathrm{Tr}^{(\alpha)}(\rho_\alpha \ln \rho_\alpha) \tag{32}$$

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

Remark. We have $\mathrm{Tr}^{(\alpha)} \rho_\alpha = 1$.

We end up that

$$F_{\rho_{MF}} = \langle \mathcal{H} \rangle_{\rho_{MF}} + k_B T \sum_\alpha \mathrm{Tr}^{(\alpha)}(\rho_\alpha \ln \rho_\alpha) \tag{33}$$

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

How can we parametrixe 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:

   $$\mathrm{Tr}^{(\alpha)} \rho_\alpha = 1, \quad \mathrm{Tr}^{(\alpha)}(\rho_\alpha \Phi_\alpha) = \langle \Phi_\alpha \rangle \tag{34}$$

   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:

$$\mathcal{H}[\{S\}] = -J \sum_{\langle ij \rangle} S_i S_j - \sum_i H_i S_i \tag{35}$$

it means that

$$\Phi_\alpha \to S_i = \pm 1 \tag{36}$$

and that the order parameter (variational parameter) becomes

$$\langle \Phi_\alpha \rangle \to \langle S_i \rangle \equiv m_i \tag{37}$$

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

$$\rho^{(1)} \equiv \rho^{(1)}(S_i) \to \begin{cases} \mathrm{Tr}\, \rho_i^{(1)} = 1 \\ \mathrm{Tr}\, \rho_i^{(1)} S_i = m_i \end{cases} \tag{38}$$

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

- a: stastistical 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

$$\rho_i \equiv \rho^{(1)}(S_i) = a(1 - \delta_{S_i,1}) + b\delta_{S_i,1} \tag{39}$$