

Tutorial n°1

I - Conceptual issues

A- Properties of the free energy

We discuss here some properties of the free energy in relation to the study of phase transitions.

- 1) Recall the definition of a convex-up (or simply concave) function and a convex-down (or simply convex) function.
- 2) Starting from the general form of a partition function Z(h, J, T) but taking as example that of the Ising model in a magnetic field h justify that the free energy F(h, J, T) is a concave function of its arguments.
- 3) Deduce from this property that:
 - -F is a continuous function of its arguments.
 - -F is differentiable almost everywhere.
 - $-\frac{dF}{dx}$ is monotonically non-increasing
- 4) Prove directly the concavity of F(T) by computing $\frac{\partial^2 F}{\partial T^2}$. Do the same for $\frac{\partial^2 F}{\partial h^2}$.

B- Spontaneous symmetry breaking and magnetization

We now study the properties of the magnetization. We start with a trivial lemma:

Lemma: For any function
$$f$$
 of the $\{S_i\}$ one has: $\sum_{\{S_i\}} f(\{S_i\}) = \sum_{\{S_i\}} f(\{-S_i\})$

1) Deduce, from the lemma, that, for the partition function Z(-h, J, T), one has:

$$Z(-h, J, T) = Z(h, J, T)$$

and F(-h, J, T) = F(h, J, T). Where does this property come from ?

- 2) Deduce from the previous question that, for F analytic of h, the magnetization at vanishing magnetic field should vanish: M(h=0)=0.
- 3) Consider the case where $F(h) = F(0) M|h| + O(h^{\sigma})$ with $\sigma > 1$ and show that, in this case, the magnetization at vanishing field does not vanish.

Clearly the previous behaviour relies on the non-commutativity of the limits $h \to 0$ and $N \to \infty$. A way to check this is to consider, at h = 0, and for a system with N spins, two configurations A and B related by \mathbb{Z}_2 symmetry. One thus has for the corresponding magnetizations $M_A = -M_B$.

- 4) Evaluate the ratio of the probabilities P_A and P_B to get the magnetization M_A and M_B respectively.
- **5)** Consider successively the limits $h \to 0^+, N \to \infty$ and then $h \to 0^-, N \to \infty$.

C- Spontaneous symmetry breaking and ergodicity breaking

Statistical mechanics is based on the principle that long time average should identify with ensemble average:

$$\langle A \rangle = \lim_{t \to \infty} \frac{1}{t} \int_0^t A\{X_i(t')\} \ dt' = \int \prod_i \ dX_i \ P_{eq}(\{X_i\}) A\{X_i\}$$

where the $\{X_i(t)\}$ correspond to the dynamical degrees of freedom (position and momentum for a fluid, spins in for magnetic systems, etc) and $P_{eq}(\{X_i\})$ the probability distribution at equilibrium.

The ergodic hypothesis states that when $t \to \infty$ the "trajectory" $\{X_i(t)\}$ should be arbitrarily close to every possible configuration of the $\{X_i\}$. As a consequence, even in a ferromagnetic phase, *i.e.* at $T < T_c$, two states of magnetization M_A and $M_B = -M_A$ should be equally sampled.

- 1) Consider the situation where the net positive magnetization is given by M_A . According to the ergodic hypothesis, after some time, a large cluster of spins down should form leading the magnetization to reverse. Using the Arrhenius law give the expression of typical time τ of this phenomenon to occur as a function of ΔF , the free energy difference between the two different configurations.
- 2) Evaluate ΔF as function of the number N involved in the cluster of spins that reverses, and the dimension D. Conclude.

II - Ising model with long-range interactions

In this exercise we study the possibility of domains in the Ising model in the presence of long-range interactions. One considers a system of N+1 spin interacting ferromagnetically with Hamiltonian:

$$H = -\sum_{i,j} J_{ij} S_i S_j$$

with J_{ij} of the form:

$$J_{ij} \sim \frac{J}{|i-j|^{1+\sigma}}$$

with J is a positive real number and σ a real number. One assumes that the system is ordered (e.g. the spins are all up) and that there exists a domain of p+1 spins down indexed by $i \in [0, p]$.

- 1) Write the increase of energy ΔE due to the presence of this domain of spins down as a double sum running on the position of the spins down belonging to the domain and on the position of the spins up.
- 2) Carry out a continuum limit on the double sum obtained in question 1) and show that ΔE is given by:

$$\Delta E = \frac{2J}{a^2 \sigma (1 - \sigma)} \left[(L - z)^{1 - \sigma} - L^{1 - \sigma} - a^{1 - \sigma} + (z + a)^{1 - \sigma} \right]$$

where z parametrizes the size of the domain of spins down, L is the size of the whole system, and a is the lattice space.

3) Consider a domain of size $z \gg a$ and get the simplified expression for ΔE :

$$\Delta E = \frac{2J}{a^2\sigma(1-\sigma)}z^{1-\sigma} \ .$$

2

4) Consider the possibility of a large domain of spins down according to the value of σ .



Tutorial n°2

Mean field approach: variational method

One considers a system of Hamiltonian H and of free energy F. Show the equality:

$$F = F_0 - k_B T \log \langle e^{-\beta(H - H_0)} \rangle_0$$

where H_0 is a Hamiltonian, F_0 the associated free energy and $\langle A \rangle_0$ the mean value of A in the canonical ensemble defined by H_0 . In what follows H_0 will be chosen in such a way that all quantities computed in this ensemble will be particularly simple.

2) Show that for any function f one has:

$$\langle e^f \rangle \ge e^{\langle f \rangle}$$

and deduce an upper bound, F_{var} , of the free energy F in terms of F_0 and $\langle H - H_0 \rangle_0$.

The idea of the method is to use this property to find the best approximation of the genuine free energy F for the Ising model in a uniform magnetic field h:

$$H = -J\sum_{\langle i,j\rangle} S_i S_j - h\sum_i S_i$$

considering, for H_0 , the Hamiltonian of a system of N free spins:

$$H_0 = -\lambda \sum_{i} S_i$$

where λ should be determined to optimize F_{var} , i.e. to find its lowest value.

- 3) Compute the partition function Z_0 associated to the Hamiltonian H_0 . Deduce the value of $\langle S_i \rangle_0$.
- 4) Use the result of the previous question to show that the mean value $\langle H H_0 \rangle_0$ is given by:

$$\langle H-H_0
angle_0=-rac{JNz}{2} anh^2eta\lambda+(\lambda-h)N anheta\lambda$$

- 5) Give the expression of F_{var} and find the optimal value λ_{min} of λ making F_{var} minimal.
- 6) Determine, from this value of F_{var} , the magnetization m and the equation that it obeys. Comment.
- 7) Give the expression of the Gibbs free energy $\Gamma(m)$ as a function of m. After some algebra show that:

$$\Gamma[m] = -Nk_BT\log 2 - \frac{JNz}{2}m^2 + \frac{Nk_BT}{2}[(1-m)\log(1-m) + (1+m)\log(1+m)]$$



Tutorial n°3

Ising model in one dimension: block-spin approach

One considers the Ising model in one dimension for N spins in presence of a magnetic field. The Hamiltonian is given by:

$$\beta H = -K \sum_{\langle i,j \rangle} S_i S_j - h \sum_i S_i$$

- 1) Write the expression of the partition function Z(N, K, h).
- 2) We shall perform the partial sum on the even-index spins in the partition function. To do that one divides the one dimensional lattice into a sublattice of odd-index spins S_i and a sublattice of even-index spins σ_i , see Fig.1.

Figure 1: The two sublattices of the one dimensional Ising model.

Show that the partition function reads:

$$Z = \sum_{[S_i]} e^{-\beta H[S_i]} \equiv \sum_{[S_i]}^{N} e^{\sum_{i=1}^{N} B(S_i, S_{i+1})} = \sum_{[S_i']}^{N/2} \sum_{[\sigma_i]}^{N/2} e^{\sum_{i=1}^{N/2} B(S_i', \sigma_i) + B(\sigma_i, S_{i+1}')}$$
(1)

where $S'_{i} = S_{2i-1}$, $\sigma_{i} = S_{2i}$ and $B(S_{i}, S_{i+1}) = g + \frac{h}{2}(S_{i} + S_{i+1}) + KS_{i}S_{i+1}$ where g is a constant.

3) One assumes that:

$$e^{-\beta H'[S_i']} \equiv \prod_{i=1}^{N/2} \left[\sum_{\sigma_i = \pm 1} e^{B(S_i', \sigma_i)} + B(\sigma_i, S_{i+1}') \right] \equiv e^{\sum_{i=1}^{N/2} B'(S_i', S_{i+1}')}$$

where $B'(S'_i, S'_{i+1})$ is supposed to be of the same form as $B(S_i, S_{i+1})$ but with parameters K', h' and g'.

Derive the relations between the sets of coupling constants $\{K', h', g'\}$ and $\{K, h, g\}$. It will be convenient to define the coupling constants:

$$\left\{ \begin{array}{l} x = e^{K} & , \ y = e^{h} & , \ z = e^{g} \\ \\ x' = e^{K'} & , \ y' = e^{h'} & , \ z' = e^{g'} \end{array} \right.$$

and show that the solution of the corresponding system is given by:

$$\left\{ \begin{array}{l} z'^4 = z^8 (x^2 y + x^{-2} y^{-1}) (x^{-2} y + x^2 y^{-1}) (y + y^{-1})^2 \\ \\ y'^2 = y^2 \; \frac{x^2 y + x^{-2} y^{-1}}{x^{-2} y + x^2 y^{-1}} \\ \\ x'^4 = \frac{(x^2 y + x^{-2} y^{-1}) (x^{-2} y + x^2 y^{-1})}{(y + y^{-1})^2} \; . \end{array} \right.$$

Finally using the change: $x \to \tilde{x} = x^{-4}$, $y \to \tilde{y} = y^{-2}$ show that the two last equations read:

$$\begin{cases}
\tilde{y}' = \frac{\tilde{y}(\tilde{x} + \tilde{y})}{1 + \tilde{x}\tilde{y}} \\
\tilde{x}' = \frac{\tilde{x}(1 + \tilde{y})^2}{(\tilde{x} + \tilde{y})(1 + \tilde{x}\tilde{y})}
\end{cases} (2)$$

Note that taking the logarithm of the solution of (2) one gets the RG flow equations for h and K:

$$\begin{cases} h' = h + \delta h(K, h) \\ K' = K + \delta K(K, h) \end{cases}$$
 (3)

- i) Consider the system (2) and show that the h=0 subspace is closed, *i.e.* starting with a vanishing magnetic field one gets a vanishing field after one RG step.
- ii) Show that there is a line of fixed points at $\tilde{x}=1, \ \forall \ \tilde{y}$. Interpret this in terms of the original variables h and K (or even better T). Analyze the structure of the RG flow near any fixed point $\tilde{x}^*=1$ and $\tilde{y}^*=y_0$. To do this write $x=x^*+\delta x$ and $y=y_0^*+\delta y$.
- iii) Consider the fixed point $\tilde{x}^* = 0$ and $\tilde{y}^* = 0$. What are the physical properties that characterize this fixed point? Analyze the renormalization group (RG) flow around this fixed point.
- iv) Show that there is a fixed point P_c at $\tilde{x}^* = 0$ and $\tilde{y}^* = 1$. What are the physical properties that characterize this fixed point? Analyze the structure of the RG flow near P_c .
 - v) Draw the RG flow diagram including all fixed points and the RG lines relating them.
- vi) Write the scaling law for the correlation length ξ in terms of the scaling variables K and h. Determine the form of $\xi(K,h)$.



Tutorial n°4

Low-temperature expansion of the O(N) model

One considers a lattice and a system of unitary N-components spins $S_i = (S_{i1}, \ldots, S_{iN})^T$ at each site i of the lattice. They are supposed to be at equilibrium at temperature $T = 1/\beta$. Note that one sets $k_B = 1$. The Hamiltonian of the system is assumed to have the O(N) symmetry and to favor the parallel alignment of neighboring spins:

$$H = -J \sum_{\langle i,j \rangle} S_i.S_j - \sum_i h.S_i$$

with J > 0.

One wants to study the system at low temperatures, where the spins are almost aligned, using a continuous description. One therefore considers a field S(r), with $r = (r_1, \ldots, r_D)^T$, such that $|S(r)|^2 = S_{\alpha}(r)S_{\alpha}(r) = 1$, $\forall r$, and one takes the simplest possible continuous Hamiltonian:

$$\mathcal{H}[S] = rac{c}{2} \int\! d^D x \, \left(\partial_i S_lpha
ight) \left(\partial_i S_lpha
ight) - h \int\! d^D x \, S_N ,$$

where Einstein's summation is assumed and h is a uniform external field aligned along the direction of the N^{th} -component of S in the spin space, and c > 0.

- 1. Why didn't one include a generic term quadratic in S of the form $A_{\alpha\beta}S_{\alpha}S_{\beta}$?
- 2. Justify, on symmetry grounds, the form of the term quadratic in the gradient of S(r).
- 3. Show that for h > 0 the ground state corresponds to $S(r) = (0, ..., 1)^T, \forall r$.
- 4. One considers small fluctuations spin-waves above the ground state. One writes $S = (\pi, \sigma)^T$, with $\pi = (S_1, \ldots, S_{N-1})^T$ and $\sigma = S_N$. As π is assumed to be small one can express σ in terms of π , i.e. $\sigma = \sqrt{1 \pi^2}$, so that it can be integrated out. Show first that

$$\delta\left(S^2-1\right) = \frac{1}{2\sqrt{1-\pi^2}} \,\delta\!\left(\sigma - \sqrt{1-\pi^2}\right).$$

5. Write the partition function

$$Z[h] = \int \! \mathcal{D} S \, e^{-eta \mathcal{H}[S]}$$

in term of fields π and σ .

6. Show then that the partition function can be transformed to

$$Z[h] = \int \mathcal{D}\pi \, e^{-\beta \mathcal{G}[\pi]} \tag{1}$$

with

$$\mathcal{G}[\pi] = \mathcal{H}\left[(\pi, \sqrt{1-\pi^2})^T
ight] + rac{
ho}{2} T \int\! d^D x \, \log(1-\pi^2) \, .$$

What is the relation between the constant ρ and the underlying lattice spacing a? What is domain of variation of π in Eq.(1)?

- 7. Write down explicitly $\mathcal{G}[\pi] \equiv \int d^D x \, g(\pi)$, in terms of π and h only.
- 8. One will keep in g only the terms up to fourth order in π . Show that $g = g_0 + g_1 + g_2 + \mathcal{O}(\pi^6)$ with

$$g_0(\pi) = \frac{c}{2} (\partial_i \pi_\alpha)(\partial_i \pi_\alpha) + \frac{h}{2} \pi_\alpha \pi_\alpha,$$

$$g_1(\pi) = \frac{c}{2} \pi_\alpha (\partial_i \pi_\alpha) \pi_\beta (\partial_i \pi_\beta) + \frac{h}{8} \pi_\alpha \pi_\alpha \pi_\beta \pi_\beta - T \frac{\rho}{2} \pi_\alpha \pi_\alpha,$$

$$g_2(\pi) = -T \frac{\rho}{4} \pi_\alpha \pi_\alpha \pi_\beta \pi_\beta,$$

where one has discarded a constant independent of π and grouped the terms for reasons to be made clear in the following.

9. Show that:

$$\langle \pi_{\alpha}(\mathbf{r})\pi_{\beta}(\mathbf{r})\rangle_{0} = T\delta_{\alpha\beta} \int_{0}^{\Lambda} \frac{d^{D}q}{(2\pi)^{D}} \frac{1}{h+cq^{2}},$$
 (2)

$$\langle \partial_j \pi_{\alpha}(\mathbf{r}) \pi_{\beta}(\mathbf{r}) \rangle_0 = 0,$$
 (3)

$$\langle \partial_j \pi_{\alpha}(\mathbf{r}) \partial_j \pi_{\beta}(\mathbf{r}) \rangle_0 = T \delta_{\alpha\beta} \int_0^{\Lambda} \frac{d^D q}{(2\pi)^D} \frac{q^2}{h + cq^2},$$
 (4)

where $\langle ... \rangle_0$ denotes the average under the statistical weight associated with the Gaussian Hamiltonian $\mathcal{G}_0 = \int d^D x \, g_0(\pi)$ and Λ is the upper-wavevector cutoff.

Remark: One has to make the assumption that the domain of variation of π_{α} can be safely extended from $-\infty$ to $+\infty$. This can be justified by the fact that the minimum of the Hamiltonian $\mathcal{G}[\pi]$ is given by $\pi=0$. Also one sees from Eqs.(2) and (4) that the main fluctuations satisfy $\pi \sim \sqrt{T}$. Also one can show that field configurations such that $|\pi| \sim 1$ give exponentially small contributions – of order $e^{-cte/T}$ – to the partition function that can be neglected within the perturbative approach. This allows to ignore the constraint $|\pi| \leq 1$.

- 10. Show that $\langle g_{11}\rangle_0 = O(T^2)$, $\langle g_{12}\rangle_0 = O(T^2)$, $\langle g_{13}\rangle_0 = O(T^2)$, where g_{11} , g_{12} and g_{13} are the three terms entering in the expression of g_1 . Show also that $\langle g_2\rangle_0 = O(T^3)$.
- 11. Since one is interested primarily in the low temperature behavior of the model, one will neglect completely the term $g_2(\pi)$ and consider $\mathcal{G}_1 = \int d^D x \, g_1(\pi)$ as a perturbation with respect to the Gaussian model with Hamiltonian \mathcal{G}_0 . One sets up a diagrammatic representation in which π_{α} and $\partial_i \pi_{\alpha}$ are represented by the field lines below.

Draw the 3 diagrams corresponding to the three terms of \mathcal{G}_1 , indicating as a weight their coefficients c/2, h/8 and $-T\rho/2$.

12. It is actually possible to avoid indicating α or (α, i) on the field lines if the following convention is adopted. Vertices with 4 fields, which are usually drawn as points, are splitted into two points joined by a small dotted line (figure below). The whole thing is a vertex. The convention is that on each side of a splitted vertex, the two fields have the same index,

e.g., π_{α} and π_{α} one one side, and π_{β} and π_{β} on the other side. As these indices are dummy they don't need to be specified. Likewise, on vertices with two field lines there is no need to indicate the indices. Give the expression of the diagrams below of \mathcal{G}_1 and indicate their weights, including h and c factors.



13. In order to perform a momentum-shell renormalization, one decomposes $\pi(r) = \pi_{<}(r) + \pi_{>}(r)$, where $\pi_{<}(r)$ contains the Fourier components of $\pi(r)$ in the interval $[0, \Lambda/s]$ and $\pi_{>}(r)$ all the remaining components in the interval $[\Lambda/s, \Lambda]$. Show that the coarse-grained effective Hamiltonian for $\pi_{<}$ can be expressed as

$$\mathcal{G}_{<}[\pi_{<}] = \mathcal{G}_{0}[\pi_{<}] + \langle \mathcal{G}_{1}[\pi_{<} + \pi_{>}] \rangle_{0} + O(T^{2}),$$

where constant terms have been discarded. What is the meaning of $\langle ... \rangle_0$ above?

- 14. How are the Eqs.(2-4) modified if π is replaced by π ?
- 15. By symmetry the coarse-grained Hamiltonian $\mathcal{G}_{<}$ will have the same form as \mathcal{G} , but with renormalized coefficients $c_{<} = c + \delta c$, $h_{<} = h + \delta h$ and $\rho_{<} = \rho + \delta \rho$. Write down $\mathcal{G}_{<}$.
- 16. Determine the non-vanishing diagrams arising from $\langle \int d^D x g_{11} \rangle_0$, with their weight, and show that they yield the contributions

$$\delta c_1 = Tc \int_{\Lambda/s}^{\Lambda} \frac{d^D q}{(2\pi)^D} \frac{1}{h + cq^2},$$

$$\delta h_1 = Tc \int_{\Lambda/s}^{\Lambda} \frac{d^D q}{(2\pi)^D} \frac{q^2}{h + cq^2},$$

to δc and δh .

- 17. Give the non-vanishing diagrams arising from the contribution $\langle \int d^D x g_{12} \rangle_0$ and determine their weights.
- 18. Their contributions to δh are noted δh_2 and δh_3 respectively. Calculate δh_2 and δh_3 .
- 19. The coefficient ρ can be expressed as

$$\rho = \int_0^\Lambda \frac{d^D q}{(2\pi)^D}.$$

What physical argument can you put forward to explain that?

20. By directly decomposing both ρ into $\rho_{<} + \rho_{>}$ and π into $\pi_{<} + \pi_{>}$ show that $\langle \int d^{D}x g_{13} \rangle_{0}$ yields a natural contribution to $\mathcal{G}_{<}$, and produces in addition a correction to h:

$$\delta h_4 = -T \int_{\Lambda/s}^{\Lambda} \frac{d^D q}{(2\pi)^D} \,.$$

21. Calculate $\delta h_1 + \delta h_3 + \delta h_4$.

22. One now defines the renormalized fields by the relation $\pi'(r') = \zeta^{-1}\pi_{<}(sr')$, i.e. one rescales the coarse-grained field by ζ and the lengths by s. Let $\mathcal{G}'[\pi']$ be the renormalized effective Hamiltonian associated to π' . Show that its coefficients are such that

$$c_s = c \left(1 + TA\right) s^{D-2} \zeta^2,$$

$$h_s = h \left(1 + \frac{N-1}{2} TA\right) s^D \zeta^2,$$

where

$$A = K_D \int_{\Lambda/s}^{\Lambda} dq \, \frac{q^{D-1}}{h + cq^2} \,,$$

 K_D being the area of the unit hypersphere in D dimensions divided by $(2\pi)^D$.

23. Let us now imagine that the field h acts in the direction of π_1 . Explain why in the renormalization procedure it transforms into $h' = hs^d\zeta$. Deduce that in order to preserve the rotational symmetry of the model one must require

$$\zeta = \left(1 + \frac{N-1}{2}TA\right)^{-1}.$$

24. One now sets $s = 1 + d\ell$. Show that at zero external field (h = 0) the renormalization flow for c is given by

$$rac{dc}{d\ell} = (D-2)c - (N-2)TK_D\Lambda^{D-2}$$
.

- 25. One assumes in the following D > 2 and N > 2. Determine the fixed point c^* . Determine the linearized flow equation in the vicinity of this fixed point.
- 26. How does c evolve at high temperature where $c < c^*$? To which phase corresponds the asymptotic fixed point reached?
- 27. How does c evolve at low temperatures where $c>c^{\star}$? To which phase corresponds the asymptotic fixed point reached?
- 28. Considering now that c is taken fixed, deduce the value of T_c in this model. In the vicinity of which critical dimension D^* should one place ourselves in order for this renormalization procedure to be coherent?
- 29. Deduce the Mermin-Wagner theorem.
- 30. Show that at the fixed point one has $h(\ell) = h \ell^{y_h}$ and calculate y_h . Using the general relation $\eta = 2 + D 2y_h$ deduce that

$$\eta \simeq rac{D-2}{N-2}$$
 .

in the vicinity of the critical dimension D^* .