

exam 2019-2020

The Potts model - correction

A. Warming up

- 1) When T is large, all q states are equally populated.
- 2) When all fields $h_\mu = 0$ ($\mu = 1, \dots, q$), all spins align to the same value; the ground state is q -fold degenerate.
- 3) If all fields $h_\mu \neq 0$, we have to find the largest, that will “pin” the system, and lead to a unique ground state.
- 4) Here $h_1 > 0$ while all other fields vanish. When $h_1 \rightarrow 0$, we have $\langle x \rangle \rightarrow 1/q$, while when h_1 becomes large, we will get $\langle x \rangle \rightarrow 1$. We therefore propose the order parameter

$$m = \frac{q\langle x \rangle - 1}{q - 1}. \quad (1)$$

- 5) When $q = 2$, one can associate states $\sigma^{(1)} = +1$ to $\sigma = 1$ and $\sigma^{(1)} = -1$ to $\sigma = 2$. Making use of the identities

$$\delta_{\sigma_i^{(1)}, \sigma_j^{(1)}} = \frac{1 + \sigma_i^{(1)} \sigma_j^{(1)}}{2}, \quad \delta_{\sigma_i^{(1)}, +1} = \frac{1 + \sigma_i^{(1)}}{2}, \quad \delta_{\sigma_i^{(1)}, -1} = \frac{1 - \sigma_i^{(1)}}{2} \quad (2)$$

we get

$$H = - \sum_{i,j=1}^N J_{i,j} \frac{1 + \sigma_i^{(1)} \sigma_j^{(1)}}{2} - h_1 \sum_{i=1}^N \frac{1 + \sigma_i^{(1)}}{2} - h_2 \sum_{i=1}^N \frac{1 - \sigma_i^{(1)}}{2} \quad (3)$$

$$= - \sum_{i,j=1}^N \frac{J_{i,j}}{2} \sigma_i^{(1)} \sigma_j^{(1)} - \frac{h_1 - h_2}{2} \sum_{i=1}^N \sigma_i^{(1)} - \left[\frac{1}{2} \sum_{i,j=1}^N J_{i,j} + N \frac{h_1 + h_2}{2} \right]. \quad (4)$$

By identification :

$$H(\sigma_1^{(1)}, \dots, \sigma_N^{(1)}) = - \sum_{i,j=1}^N J_{i,j}^{(1)} \sigma_i^{(1)} \sigma_j^{(1)} - h^{(1)} \sum_{i=1}^N \sigma_i^{(1)} \quad \text{with} \quad \boxed{J_{i,j}^{(1)} = \frac{J_{i,j}}{2} \quad \text{and} \quad h^{(1)} = \frac{h_1 - h_2}{2}} \quad (5)$$

The square bracket in (4) is an immaterial constant.

- 6) For $q = 2$ we thus expect a second order phase transition.

B. The Curie-Weis approach, with a hint of Landau

- 7) With a d -dimensional hyper-cubic lattice, we have $2d$ neighbors for each spin (discarding possible edge effects, that we can get rid of invoking periodic boundaries).
- 8) With $J = 0$, $h_2 = h_3 = \dots = h_q$ and h_1 that may differ from the other fields, the mean fraction of spins in state 1 reads

$$\langle x \rangle = \frac{e^{\beta h_1}}{e^{\beta h_1} + (q - 1)e^{\beta h_2}}. \quad (6)$$

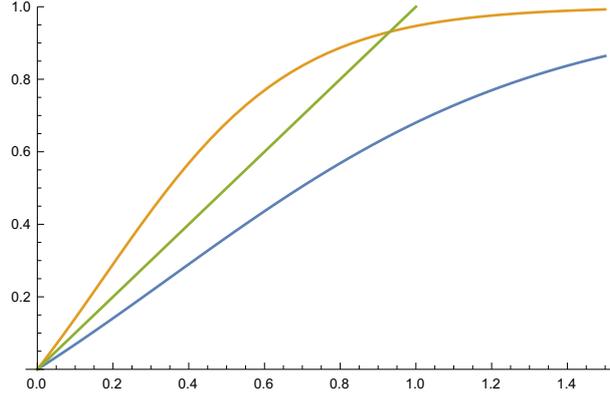


FIGURE 1 – The function $m \rightarrow \varphi(m)$ defined in (9). Here $q = 3$, with either $K = 2$ (“large” T , blue curve) or $K = 4$ (“small” T , yellow curve). The first bisectrix is also shown (green line).

- 9) The molecular field felt by any tagged spin does not stem from an external field $h_1, h_2 \dots$ but from the presence of neighbors interacting with the tagged spin.
- 10) A spin of type 1 interacts only with like spins. There is a fraction x of such spins, so that the molecular field is $h_1^m = 2dJx$. The fraction of spins of type different from one is $(1 - x)/(q - 1)$. The molecular field on say spins of type $\mu \neq 1$ is thus $h_\mu^m = 2dJ(1 - x)/(q - 1)$.
- 11) We now make use of relation (6) replacing h_1 and h_2 by the mean molecular fields :

$$\langle x \rangle = \frac{\exp[2dK\langle x \rangle]}{\exp[2dK\langle x \rangle] + (q - 1) \exp[2dK(1 - \langle x \rangle)/(q - 1)]} \quad (7)$$

where $K = \beta J$.

- 12) From $\langle x \rangle$, we compute

$$m = \frac{q\langle x \rangle - 1}{q - 1} \quad (8)$$

which gives

$$m = \varphi(m) = \frac{e^{2dKm} - 1}{e^{2dKm} + q - 1}. \quad (9)$$

Note that this also means

$$\langle x \rangle = \frac{e^{2dKm}}{e^{2dKm} + q - 1}. \quad (10)$$

- 13) The function above is sketched in Fig. 1. The self-consistent order parameter is found by looking for the intersection with the first bisectrix. We see that the system can either exhibit a spontaneous magnetization (curve with $K = 4$), or none (curve with $K = 2$). Not surprisingly, order can be sustained at small temperature, but not at large T .

- 14) We have

$$m = \frac{T^*}{T} m + \mathcal{C}_2 (q - 2) m^2 + \mathcal{C}_3 m^3 + \mathcal{O}(m^4), \quad (11)$$

where $\boxed{k_B T^* = 2dJ/q}$.

- 15) We start from

$$\frac{\partial \mathcal{R}(m)}{\partial m} = a_2 m + a_3 m^2 + a_4 m^3 + \dots \quad (12)$$

which has to vanish at equilibrium in absence of an external field. Thus, either $m = 0$, or

$$\tilde{a}_2 (T - T^*) + a_3 m + a_4 m^2 = 0 \quad (13)$$

Back to Eq. (11), we linearize the term in T^*/T close to T^* :

$$0 = \frac{T - T^*}{T^*} m - \mathcal{C}_2 (q - 2) m^2 - \mathcal{C}_3 m^3 + \mathcal{O}(m^4). \quad (14)$$

Comparing to Eq. (13), we get, up to a positive constant in all cases (since $\tilde{a}_2 > 0$)

$$a_3 = -\mathcal{C}_2(q - 2) \quad \text{and} \quad a_4 = -\mathcal{C}_3. \quad (15)$$

Hence, a_3 is of the sign of $2 - q$.

16) Since the admissible values of m can only be positive,

$$\boxed{\text{the phase transition is second order for } a_3 > 0, \text{ i.e. } q < 2; \text{ it is first order for } q > 2}. \quad (16)$$

17) The Ising model corresponds to $q = 2$ with a second order transition. This does not contradict our analysis. It is even compatible : for $q = 4$, we have a standard m^2/m^4 Landau theory, of second order type.

18) The Potts model with $q \rightarrow 1$ is expected to exhibit a second order transition.

C. The one-dimensional setting : transfer matrix and renormalization

19) With

$$H(\sigma_1, \dots, \sigma_N) = -J \sum_{i=1}^N \delta_{\sigma_i, \sigma_{i+1}} \quad (17)$$

the partition function is

$$Z = \sum_{\sigma_1, \sigma_2, \dots, \sigma_N} \prod_{i=1}^N \exp(\beta J \delta_{\sigma_i, \sigma_{i+1}}) \quad (18)$$

20) Introducing the $q \times q$ transfer matrix \mathbb{T} such that

$$\mathbb{T}(\sigma_i, \sigma_j) = \exp(\beta J \delta_{\sigma_i, \sigma_j}) \quad (19)$$

we can write

$$Z = \text{Tr}(\mathbb{T}^N) \quad (20)$$

For the case $q = 3$, this gives :

$$\mathbb{T} = \begin{pmatrix} e^{\beta J} & 1 & 1 \\ 1 & e^{\beta J} & 1 \\ 1 & 1 & e^{\beta J} \end{pmatrix} \quad (21)$$

For $q > 3$, the structure is the same, with exponential terms on the diagonal, and 1 on every non-diagonal entry.

21) \mathbb{T} is a circulant matrix, and therefore simple to diagonalize. We follow a more direct route than the Fourier transform method. It is seen that \mathbb{T} admits the eigenvector $|+\rangle = {}^t(1, 1, 1)$, with eigenvalue $t_+ = e^{\beta J} + 2$. The other eigenvalue is two-fold degenerate. Since we know the trace, we readily find that its value is $t_- = e^{\beta J} - 1$. The two associated eigenvectors, which have to be perpendicular to $|+\rangle$ are ${}^t(1, -1/2, -1/2)$ and ${}^t(-1/2, 1, -1/2)$. Note that $t_- < t_+$. Another possibly more convenient choice is to take these eigenvectors as ${}^t(0, 1, -1)/\sqrt{2}$ and ${}^t(0, -1, 1)/\sqrt{2}$.

In the general case,

$$\boxed{t_+ = e^{\beta J} + q - 1 \quad , \quad t_- = e^{\beta J} - 1}. \quad (22)$$

22) The eigenvalues being known, the trace of \mathbb{T}^N follows :

$$Z = t_+^N + 2t_-^N = \left(e^{\beta J} + 2\right)^N + 2 \left(e^{\beta J} - 1\right)^N \quad (23)$$

23) In the thermodynamic limit, the free energy per spin is

$$\beta f = -\log\left(e^{\beta J} + 2.\right) \quad (24)$$

This expression is analytic in T ; there is no phase transition, which is expected (one dimensional model with short range interactions).

24) The results generalize to arbitrary q :

$$t_+ = e^{\beta J} + q - 1, \quad t_- = e^{\beta J} - 1, \quad \boxed{Z = \left(e^{\beta J} + q - 1\right)^N + (q - 1) \left(e^{\beta J} - 1\right)^N}. \quad (25)$$

25) We integrate over every second spin, to get

$$Z(K, N, a) = A^{N'} Z(K', N', b) \quad \text{with } N' = N/2 \quad \text{and } b = 2a. \quad (26)$$

26) We start from

$$\sum_{\sigma'=1,\dots,q} \exp(K\delta_{\sigma,\sigma'} + K\delta_{\sigma',\sigma''}) = A \exp(K'\delta_{\sigma,\sigma''}) \quad (27)$$

and we distinguish the cases $\sigma = \sigma''$ from $\sigma \neq \sigma''$. They respectively lead to

$$e^{2K} + q - 1 = A e^{K'}; \quad 2e^K + q - 2 = A, \quad (28)$$

from which we get

$$\boxed{e^{K'} = \frac{e^{2K} + q - 1}{2e^K + q - 2}}. \quad (29)$$

The only two fixed points are the trivial small temperature (“ $K = \infty$ ”) and high temperature ($K = 0$) fixed points. For $K \rightarrow \infty$, we have $e^{K'} \sim e^K/2$, and the corresponding fixed point is unstable. For $K \rightarrow 0$, we have $K' \sim K^2/q$ and the corresponding fixed point is stable.

Note that resorting to the transfer matrix yields interesting information. The relation

$$\sum_{\sigma'=1,\dots,q} \exp(K\delta_{\sigma,\sigma'} + K\delta_{\sigma',\sigma''}) = A \exp(K'\delta_{\sigma,\sigma''}) \quad (30)$$

can be viewed as a matrix equality :

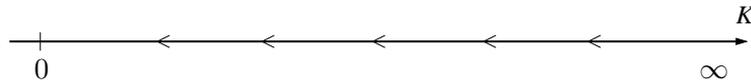
$$(\mathbb{T}_K)^2 = A \mathbb{T}_{K'}, \quad (31)$$

which translates into the following identity for eigenvalues

$$(e^K + q - 1)^2 = A (e^{K'} + q - 1), \quad (e^K - 1)^2 = A (e^{K'} - 1). \quad (32)$$

These relations directly imply Eq. (35) below.

27) The “renormalization flow” diagram goes as follows :



To show that the two fixed points are trivial, we can prove that $K' < K$. Indeed

$$e^{K'} < e^K \iff e^{2K} + (q - 2)e^K + 1 - q > 0. \quad (33)$$

The roots of $X^2 + (q - 2)X + 1 - q$ are 1 and $1 - q < 1$. Thus, (33) means that $e^K > 1$, which is true. consequently, $K' < K$ and there is no non-trivial fixed point.

28) There is no non-trivial fixed point ; no phase transition ; no surprise (see above).

29) Since $\xi(K) = \xi'(K')$, we have

$$\tilde{\xi}(K') = \frac{1}{2} \tilde{\xi}(K) \quad (34)$$

30) We obtain

$$\frac{e^{K'} + q - 1}{e^{K'} - 1} = \left(\frac{e^K + q - 1}{e^K - 1} \right)^2. \quad (35)$$

Therefore, $\log [(e^K + q - 1)/(e^K - 1)]$ transforms as $1/\xi$, so that the only admissible connection between both is

$$\tilde{\xi} \propto \frac{1}{\log [1 + q/(e^K - 1)]}. \quad (36)$$

Interestingly, this can be rewritten in terms of the eigenvalues of the transfer matrix as $\tilde{\xi} \propto 1/\log(t_+/t_-)$, This is the very same structure as for Ising model.

D. Mean-field analysis - take 2

31) Due to the coupling with all neighbors, every spin is subject to the same (mean) field. The notion of distance between spins becomes immaterial; the nature and dimension of the underlying lattice are irrelevant.

For a given configuration $\mathcal{C} = (\sigma_1, \dots, \sigma_N)$, we define $x_\sigma(\mathcal{C}) = (\sum_{i=1}^N \delta_{\sigma_i, \sigma})/N$ as the fraction of spins in state σ . By definition, $\sum_\sigma x_\sigma = 1$. The energy of a configuration can be written as $H(\mathcal{C}) = Ne(x_1(\mathcal{C}), \dots, x_q(\mathcal{C}))$, with the function $e(x_1, \dots, x_q)$ defined in the main text. Besides, the number of configurations for which $N_1 = Nx_1$ spins are in state 1, $N_2 = Nx_2$ in state 2, ..., $N_q = Nx_q$ in state q is the multinomial factor

$$\mathcal{N}_{x_1, \dots, x_q}^N = \binom{N}{N_1, N_2, \dots, N_q} = \frac{N!}{N_1! N_2! \dots N_q!} = \frac{N!}{(Nx_1)! (Nx_2)! \dots (Nx_q)!}. \quad (37)$$

Thus, the x_σ are of the form N_σ/N with N_σ an integer $\in [0, N]$, and obey the constraint $x_1 + \dots + x_q = 1$.

32) From Stirling formula, we have

$$\lim_{N \rightarrow \infty} \frac{1}{N} \ln \mathcal{N}_{x_1, \dots, x_q}^N = - \sum_{\sigma=1}^q x_\sigma \ln x_\sigma. \quad (38)$$

This is the expression of Shannon entropy for a random variable having q possible values, with probabilities x_1, \dots, x_q . To leading exponential order, we can write

$$Z \sim \sum_{x_1, \dots, x_q} \exp \left[-N\beta \hat{f}(x_1, \dots, x_q, T) \right], \quad (39)$$

and evaluate this sum by Laplace method when $N \rightarrow \infty$. In the minimization, the variables x_σ are real numbers between 0 and 1, with the constraint $x_1 + \dots + x_q = 1$.

33) We could have written directly the expression of the free energy following the Bragg-Williams route.

34) At high T , the free energy is entropy dominated, and its minimum is reached at the symmetric point $(x_1^*, \dots, x_q^*) = (1/q, \dots, 1/q)$. This is the paramagnetic phase.

35) When $T = 0$, minimizing the free energy amounts to minimizing the energy. For a vanishing field, we thus have to maximize $x_1^2 + \dots + x_q^2$ under the constraint that $x_1 + \dots + x_q = 1$. There are q equivalent solutions $(x_1^*, \dots, x_q^*) = (1, 0, \dots, 0)$ or $(0, 1, \dots, 0), \dots$, or $(0, \dots, 0, 1)$, which correspond to ferromagnetic phases. This can be seen from the identity

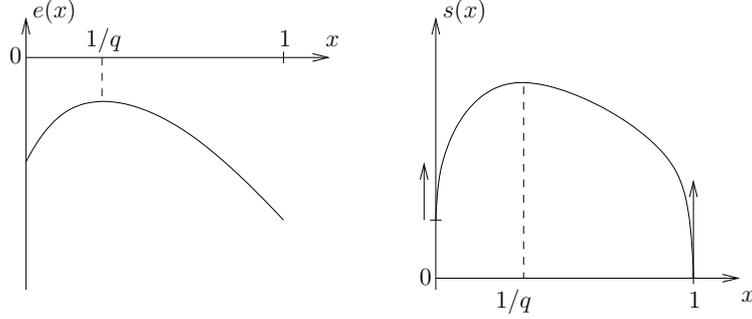
$$1 = \left(\sum_{\sigma=1}^q x_\sigma \right)^2 = \sum_{\sigma=1}^q x_\sigma^2 + \sum_{\sigma \neq \sigma'} x_\sigma x_{\sigma'}. \quad (40)$$

The ground state is q -fold degenerate; these states correspond to microscopic configurations with $\sigma_1 = \sigma_2 = \dots = \sigma_N$.

36) We have $x_2 = \dots = x_q = \frac{1-x}{q-1}$. We thus find

$$e(x) = -J \frac{q}{q-1} \left(x - \frac{1}{q} \right)^2 - \frac{J}{q}, \quad \frac{s(x)}{k_B} = -x \ln(x) - (1-x) \ln(1-x) + (1-x) \ln(q-1). \quad (41)$$

37) The function $e(x)$ has a maximum at $x = 1/q$, and finite slopes (derivatives) at 0 and 1; the function $s(x)$ has a maximum for $x = 1/q$, and vertical tangents in 0 and 1 :



38) The entropy $s(x)$ reaches its maximum for $x_0 = 1/q$. This point also is an extremum of $e(x)$, so that $\hat{f}'(x_0) = 0$ for all temperature. To determine the nature of this point, we compute the second derivative

$$\hat{f}''(x) = -2J \frac{q}{q-1} + k_B T \frac{1}{x(1-x)}, \quad \text{and} \quad \hat{f}''(x_0) = \frac{q}{q-1} (-2J + k_B T q). \quad (42)$$

Thuq x_0 is a local minimum (resp. maximum) of \hat{f} for $T > T_c^{(2)}$ (resp. $T < T_c^{(2)}$), with $k_B T_c^{(2)} = \frac{2J}{q}$.

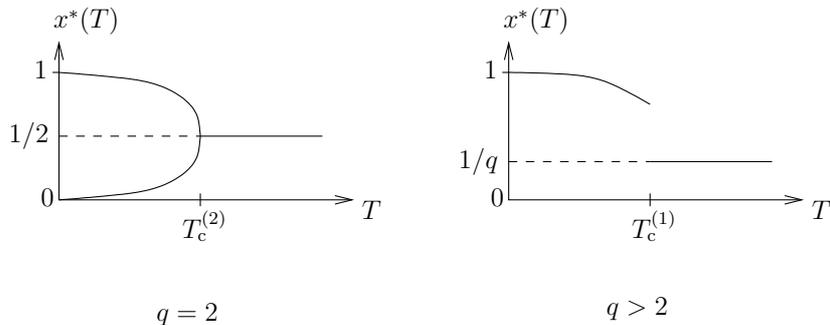
39) For $T = T_c^{(2)}$, we have $\hat{f}'''(x_0) = -2J \left(\frac{q}{q-1} \right)^2 (q-2) < 0$ since $q > 2$. Hence \hat{f} goes below its value at x_0 for $x > x_0$. Since \hat{f} features a slope $+\infty$ for $x = 1$, there is necessarily a local minimum for a value $x^* > x_0$, with $\hat{f}(x^*) < \hat{f}(x_0)$. Because $\hat{f}(x, T)$ is monotonous in T , there is a temperature $T_c^{(1)} > T_c^{(2)}$ below which x_0 is no longer the global minimum.

40) For $q > 2$, the profile of $\hat{f}(x, T)$ for different temperatures is sketched in Fig. 2.

41) The conditions determining $T_c^{(1)}$ et $x^{(1)}$ are
$$\begin{cases} \hat{f}(x^{(1)}, T_c^{(1)}) = \hat{f}(x_0, T_c^{(1)}) \\ \left. \frac{\partial \hat{f}}{\partial x} \right|_{(x^{(1)}, T_c^{(1)})} = 0 \end{cases}, \quad \text{as can be seen in the}$$

figure below at T_d . By inserting the proposed forms, we find $\alpha = 1$.

42) For $q = 2$ (resp. $q > 2$) the function $x^*(T)$ is continuous (resp. discontinuous) :



One can define $x^*(T) - 1/q$ as an order parameter (see above), since this quantity vanished in the paramagnetic phase at high temperature. For $q = 2$, the transition is second order, $\beta = 1/2$ since

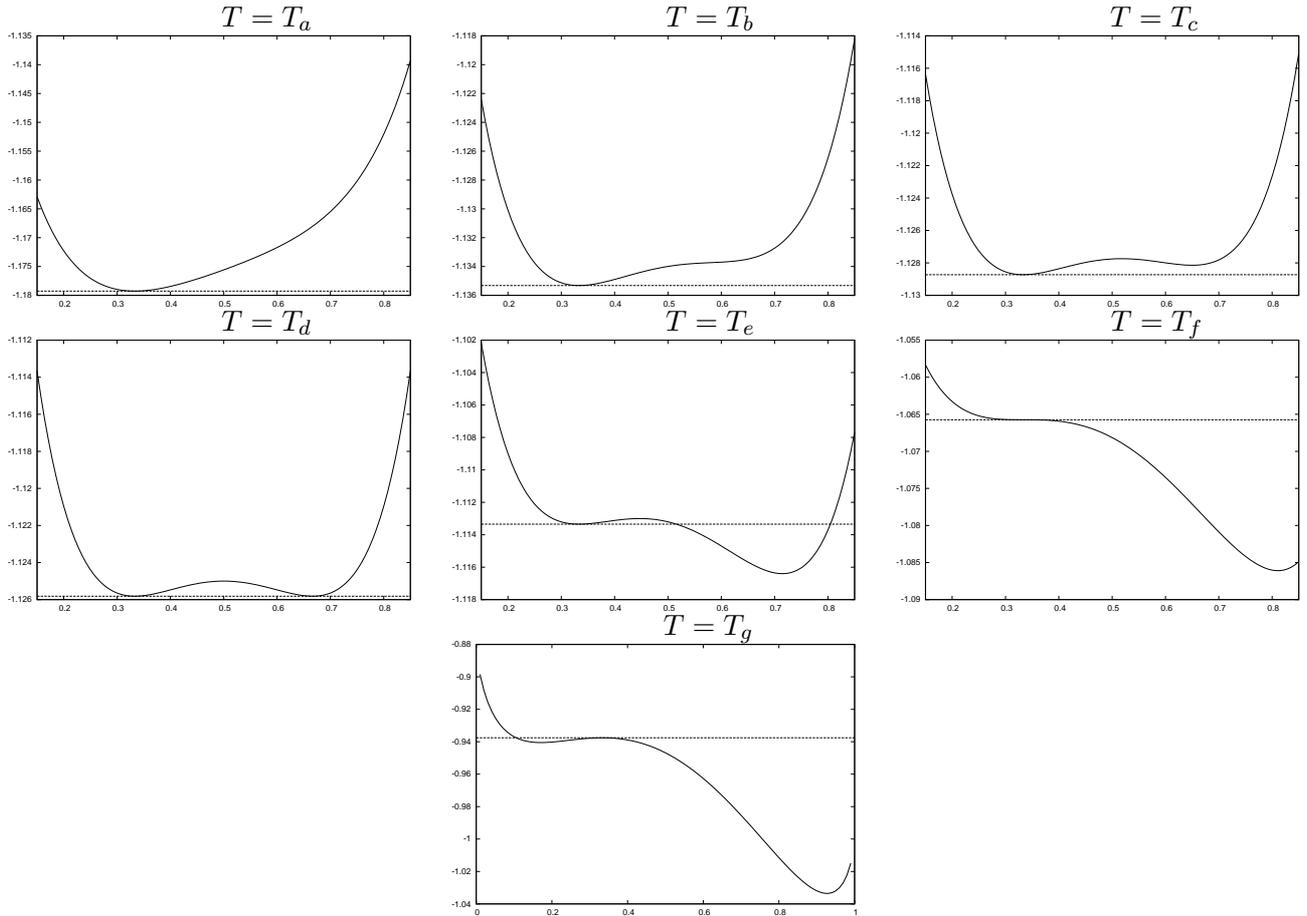


FIGURE 2 – Sequence of profiles $\hat{f}(x, T)$ as functions of x , for $T_a > T_b > \dots > T_g$, and $T_d = T_c^{(1)}$, $T_f = T_c^{(2)}$. The dashed horizontal line corresponds to the value of $\hat{f}(x_0, T)$. We have here $q = 3$, i.e. $x_0 = 1/3$.

$x^*(T = T_c^{(2)} - \varepsilon) - (1/2) \sim \varepsilon^{1/2}$. For $q > 2$ the transition is first order, the order parameter is discontinuous at the transition point, and one therefore cannot define critical exponents.

- 43) A phase separation would ensue, with domains where one of the q spin values is predominant, separated by domain walls, with a given surface tension (cost for creating an interface).

E. Exact results (miscellanea)

- 44) From

$$Z(K) = Z(\tilde{K}) \left(\frac{(e^K - 1)^2}{q} \right)^N \quad \text{and} \quad (e^{\tilde{K}} - 1)(e^K - 1) = q. \quad (43)$$

we know that if there would be a critical point K_c , then \tilde{K}_c would also be critical. If the (non-trivial) critical point is unique, it thus obeys

$$(e^{K_c} - 1)^2 = q. \quad (44)$$

As a consequence,

$$k_B T_c = \frac{J}{\log(1 + \sqrt{q})}. \quad (45)$$

- 45) We discuss here the two dimensional case. The renormalization flow tells us that

$$\boxed{\text{for } q < 4, \text{ the transition is second order while for } q > 4, \text{ it is first order}.} \quad (46)$$

In this respect the critical number of “colors” (spin values) is $q_c = 4$. Mean-field predicts a similar scenario, although it fails in getting the correct q_c , which we found to be 2 at mean-field level.

- 46) Those results are compatible with the figure. Indeed, for $q \leq 4$, we observe the same pattern at criticality, with domains of the q states that would presumably not allow to find order nor disorder upon coarse-graining. For $q > 4$, the pattern changes, and one state (the blue color), is largely predominant. It is then not necessary to coarse-grain to obtain strongly ordered states.
- 47) The comparison requires a bit of care, since mean-field does not predict the correct value of q_c . We have to consider q values for which the transition is second order, and that mean-field considers to be second order. This restricts the analysis to $q \leq 2$. Then, we expect mean-field to overestimate the correct critical temperature, due to discarded fluctuations. The mean-field prediction is (here $d = 2$)

$$T_c^{\text{mf}} = \frac{4J}{k_B q} \quad \text{and indeed} \quad \frac{4J}{q} > \frac{J}{\log(1 + \sqrt{q})}. \quad (47)$$

Note that in the Ising case, for $q = 2$, remembering the connection (5) between Potts and Ising spins (the factor 2), we recover Onsager’s exact result for the critical temperature :

$$k_B T_c = \frac{J}{\log(1 + \sqrt{2})}. \quad (48)$$

F. Open question

- 48) We first take for granted that $\nu = 1/2$, for it simplifies the analysis. It is rather straightforward to realize that our cubic Landau expansion yields a mean-field prediction $\beta = 1$. We can find look for the spatial dimension where the mean-field free energy per spin f_{mf} is dominated, close to T_c , by the typical free energy of a fluctuation, given by kT/ξ^d , where ξ is the correlation length. From the Landau expansion, we see that

$$f_{\text{mf}} \propto |t|m^2 \propto |t|^3, \quad (49)$$

where $t = (T - T_c)/T_c$, and here, $T^* = T_c$. The regime $d < d_u$, where d_u is the upper critical dimension, corresponds, scaling-wise, to

$$f_{\text{mf}} \ll \xi^{-d} \quad \text{meaning that} \quad |t|^3 \ll |t|^{\nu d} = |t|^{d/2}. \quad (50)$$

The corresponding d -range is $d \leq 6$, from which we conclude that $\boxed{d_u = 6}$.

What remains is to show $\nu = 1/2$, as for the Ising model. To this end, we may construct a Ginzburg-Landau free energy functional from the (by definition mean-field) Landau expression, adding a square gradient term and suitably coarse-graining our order parameter $\mathbf{m} = [q\mathbf{x} - (1, 1 \dots 1)]/(q - 1)$ so that it depends on position \mathbf{r} . Note that the composition vector $\mathbf{x} = (x_1, x_2 \dots, x_q)$ obeys the constraint $\sum_{\sigma=1}^q x_\sigma = 1$. We get

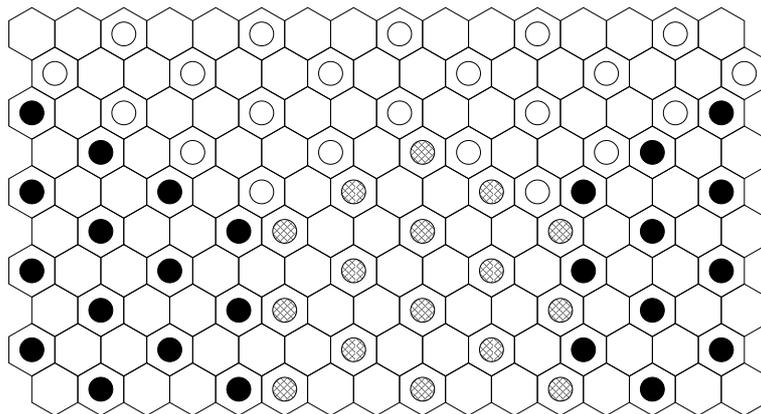
$$\mathcal{R}\{\mathbf{m}\} = \int d\mathbf{r} \left\{ \frac{a_2}{2} \mathbf{m}^2 + \frac{a_3}{3} \mathbf{m}^3 + \frac{a_4}{4} \mathbf{m}^4 + \frac{b}{2} \sum_{\sigma=1}^q (\nabla m_\sigma)^2 \right\}. \quad (51)$$

This functional was met in class. It leads to a correlation functions of the form $\int d\mathbf{q} e^{i\mathbf{q}\cdot\mathbf{r}} / (q^2 + \xi^{-2})$ with $\xi^{-2} \propto |a_2| \propto |t|$, hence $\nu = 1/2$ (and $\eta = 0$).

G. Application

- 49) We have here $q = 3$, and the spin value encodes the atom’s position adsorbed at one of the 3 possible sites. For the configuration proposed, the domains are represented below. The energetical cost is arguably most important for the junctions AB, AC et CB in the right half of the figure below, as well as at the corners where domains of the 3 types meet.

State A



State B

State C

State B