

exam 2019-2020

The Potts model

Pocket calculators and cell phones not allowed.

This part should be written on a separate paper.

La rédaction pourra se faire en français pour ceux qui le souhaitent.

The multinomial expansion formula, that can prove useful here, is reminded in the annex below. Besides, the different parts are essentially independent. In particular, the last question may be decoupled almost entirely from the others.

We consider a variant of Ising model, the so-called Potts model, where the N degrees of freedom (spins) $\sigma_1, \dots, \sigma_N$ may each take q different values, $\sigma_i \in \{1, \dots, q\}$, where q is, for the time being, an arbitrary integer ≥ 2 . The spins interact with the following Hamiltonian

$$H(\sigma_1, \dots, \sigma_N) = - \sum_{i,j=1}^N J_{i,j} \delta_{\sigma_i, \sigma_j} - \sum_{i=1}^N h_{\sigma_i}, \quad (1)$$

where $J_{i,j} \geq 0$ is the coupling constant between spins i and j , δ denotes the Kronecker symbol (giving one if the two arguments are equal, 0 otherwise) and h_1, \dots, h_q can be seen as magnetic fields acting on the q possible values of the spins. Such an approach is useful to study theoretically a variety of “hard” or “soft” condensed matter problems in a unified framework, and is also relevant to model some experimental systems (such as atomic adsorption, magnetic coarsening, foams, bubbles etc.). Interestingly, while q is taken here as an integer, it is possible to “continualize” the model for real q , and the $q \rightarrow 1$ limit connects Potts model with percolation. Other limits for q lead to problems in combinatorics or probability. Indeed, the Potts model enjoys fruitful connections with *a priori* remote domains, such as graph theory or computer science.

In the remainder, we shall work in the canonical ensemble, the system being in equilibrium at temperature T . We denote the Boltzmann constant by k_B and averages over the Boltzmann-Gibbs distribution by $\langle \cdot \rangle$; $\beta = 1/(k_B T)$.

A. Warming up : limiting cases, order parameter and connection to Ising model

- 1) What do you expect for the large T behaviour ?
- 2) When all fields $h_\mu = 0$ ($\mu = 1, \dots, q$), how many ground states are there ?
- 3) What if all fields $h_\mu \neq 0$ (all being different) ?
- 4) We assume $h_1 > 0$ while all other fields vanish. We denote by $\langle x \rangle$ the mean fraction of spins in state 1 (*i.e.* such that $\sigma_i = 1$). What order parameter m can you construct from $\langle x \rangle$, that would go from 0 in a disordered situation to 1 under perfect order ?
- 5) We consider here the $q = 2$ case. Establish that Potts model is then equivalent, up to a constant energy, to Ising model with variables $\sigma_i^{(1)} = \pm 1$ and a Hamiltonian

$$H(\sigma_1^{(1)}, \dots, \sigma_N^{(1)}) = - \sum_{i,j=1}^N J_{i,j}^{(1)} \sigma_i^{(1)} \sigma_j^{(1)} - h^{(1)} \sum_{i=1}^N \sigma_i^{(1)}. \quad (2)$$

Express $J_{i,j}^{(1)}$ and $h^{(1)}$ as functions of parameters pertaining to Potts model.

- 6) Do you expect a phase transition for $q = 2$ and if so, of what type ?

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

To investigate possible phase transitions, we resort to what is arguably the simplest treatment, inspired by the Curie-Weis method worked out for Ising model. It amounts to a single spin approximation, in a self-consistent effective field. The underlying lattice is hyper-cubic, of dimension d . The (ferromagnetic) couplings J_{ij} are all taken equal to J , restricted to nearest neighbors on the lattice.

- 7) How many nearest neighbors does a given spin have?
- 8) If $J = 0$ and the fields are such that $h_2 = h_3 = \dots = h_q$ while h_1 may differ from the others, show that $\langle x \rangle$, the mean fraction of spins in state 1 (which is also the probability that a given spin is in state 1), reads

$$\langle x \rangle = \frac{e^{\beta h_1}}{e^{\beta h_1} + \chi e^{\beta h_2}}. \quad (3)$$

What is χ ?

- 9) We address from now on the situation $J \neq 0$. In the Curie-Weis spirit, what is the origin of the so-called “molecular field”?
- 10) Express the molecular field acting on spins of type 1, and of type $\mu \neq 1$, with all fields h_μ vanishing.
- 11) Compute the mean fraction $\langle x \rangle$.
- 12) From $\langle x \rangle$, show that an eligible order parameter m obeys

$$m = \frac{e^{2d\beta J m} - 1}{e^{2d\beta J m} + q - 1}. \quad (4)$$

Before you are there, you can start by subtracting to $\langle x \rangle$ its value in the disordered phase, and then rescale this difference so that it tend to unity under perfect order. This will give you the relation between m and $\langle x \rangle$.

- 13) Sketch the behaviour of the right-hand-side in Eq. (4) as a function of m , for both low and high temperatures. How can one proceed to find the self-consistent order parameter? Discuss briefly the physics at play.
- 14) With a Taylor expansion of the right-hand-side in Eq. (4) for small m , one obtains :

$$m = \frac{T^*}{T} m + \mathcal{C}_2 (q - 2) m^2 + \mathcal{C}_3 m^3 + \mathcal{O}(m^4), \quad (5)$$

where $\mathcal{C}_2 > 0$. What is the value of T^* ?

- 15) Eq. (5) hides an interesting piece of information concerning the order of the phase transition, as a function of q . To bring this information to the fore, one needs to think in terms of a Landau-like free energy $\mathcal{R}(m)$, and we therefore write

$$\mathcal{R}(m) = \frac{a_2}{2} m^2 + \frac{a_3}{3} m^3 + \frac{a_4}{4} m^4 + \mathcal{O}(m^5) \quad (6)$$

Using the fact that for T close to T^* , $a_2 = \tilde{a}_2(T - T^*)$ where $\tilde{a}_2 > 0$ is some constant, relate the coefficients in (6) to those in (5). You have here to linearize a term in Eq. (5).

- 16) The above analysis teaches us the sign of a_3 , that is the key to our discussion. It is understood that ***the admissible values of m can only be positive (including 0)***. By sketching the profiles of $\mathcal{R}(m)$ for different T , conclude on the order of the phase transition under study. This order is affected by the q -value.
- 17) Are your results consistent with those from the Ising model? Are they compatible with what you see on Fig. 1?
- 18) Accepting that Potts model for $q \rightarrow 1$ describes percolation, what type of transition do you then expect there?

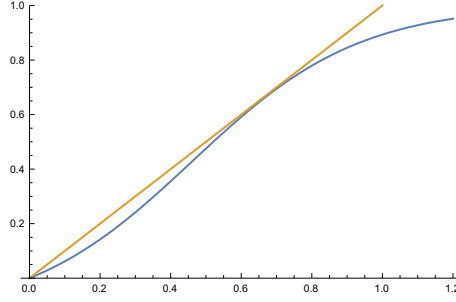


FIGURE 1 – Plot of the right hand side of Eq. (4) as a function of m , together with the first bissectrix, for $q = 8$, and some value of $2d\beta J$ (here close to 4.22).

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

The N spins live here on a chain, with periodic boundary conditions ($\sigma_1 = \sigma_{N+1}$). There is no external field and the Hamiltonian reads

$$H(\sigma_1, \dots, \sigma_N) = -J \sum_{i=1}^N \delta_{\sigma_i, \sigma_{i+1}} \quad (7)$$

- 19) Write the definition of the partition function Z , without attempting to compute it.
- 20) Rewrite Z introducing a $q \times q$ transfer matrix \mathbb{T} . Define \mathbb{T} explicitly for the case $q = 3$.
- 21) Here $q = 3$ unless otherwise stated. Show that \mathbb{T} admits a simple symmetric eigenvector. What is the corresponding eigenvalue? The other eigenvalue is degenerate. What is its expression? Write the corresponding eigenvectors (you can use the fact that they have to be perpendicular to the previous one).
- 22) Compute the partition function. What do you conclude?
- 23) Write the free energy per spin in the thermodynamic limit.
- 24) How do results generalize to arbitrary q ?

The transfer matrix technique allows to obtain the correlation length, but we switch here to a renormalization treatment. We note by a the original lattice spacing between two successive sites. One can prove that

$$\sum_{\sigma'=1, \dots, q} \exp(K\delta_{\sigma, \sigma'} + K\delta_{\sigma', \sigma''}) = A \exp(K'\delta_{\sigma, \sigma''}) \quad (8)$$

where A and K' depend on $K \equiv \beta J$.

- 25) Use this result to establish that

$$Z(K, N, a) = A^{N'} Z(K', N', b). \quad (9)$$

What are N' and b ?

- 26) The expression of K' as a function of K reads

$$e^{K'} = \frac{e^{2K} + q - 1}{p e^K + q - 2}. \quad (10)$$

What is p ? There are two fixed points only to the map $K \rightarrow K'$. What are they? Discuss their stability.

- 27) Sketch the “renormalization flow” diagram, obtained by iterating the above renormalization procedure. Discuss its physical meaning.
- 28) Is there a finite temperature critical point? Is that a surprise?

29) We denote by $\xi(K)$ the correlation length in the problem, and by $\tilde{\xi}$ its dimensionless counterpart, measured in units of the lattice spacing. How are $\xi(K')$ and $\tilde{\xi}(K)$ related?

30) Compute

$$\frac{e^{K'} + q - 1}{e^{K'} - 1} \quad \text{as a function of} \quad \frac{e^K + q - 1}{e^K - 1}. \quad (11)$$

Making use of the result in question 29, show that up to a constant

$$\tilde{\xi} \propto \frac{1}{\log[1 + q/(e^K - 1)]} \quad (12)$$

If you can remember the result for the 1D Ising chain, does it feature the same structure?

D. Mean-field analysis - take 2

In this section, we take $J_{i,j} = J/N$ for all values (i, j) , with $J > 0$.

31) Why can such an approach be coined “mean-field”? Making use of the fact that $\delta_{\sigma,\sigma'} = \sum_{\mu=1}^q \delta_{\sigma,\mu} \delta_{\sigma',\mu}$, show then that the partition function associated to the Hamiltonian (1) can be written in the form

$$Z = \sum_{x_1, \dots, x_q} \mathcal{N}_{x_1, \dots, x_q}^N e^{-N\beta e(x_1, \dots, x_q)}, \quad \text{with} \quad e(x_1, \dots, x_q) = -J \sum_{\sigma=1}^q x_\sigma^2 - \sum_{\sigma=1}^q h_\sigma x_\sigma. \quad (13)$$

What are the possible values for x_1, \dots, x_q ? What is their meaning? What is the constraint that links them? Write explicitly the expression of $\mathcal{N}_{x_1, \dots, x_q}^N$.

32) Stirling’s formula $\ln(X!) \sim X \ln X - X$ for $X \rightarrow \infty$ is reminded. Show that the free energy per spin reads, in the thermodynamic limit :

$$f(T) = -\frac{1}{\beta} \lim_{N \rightarrow \infty} \frac{1}{N} \ln Z = \inf_{x_1, \dots, x_q} \hat{f}(x_1, \dots, x_q, T), \quad \text{with} \quad (14)$$

$$\hat{f}(x_1, \dots, x_q, T) = e(x_1, \dots, x_q) - Ts(x_1, \dots, x_q) \quad \text{and} \quad s(x_1, \dots, x_q) = -k_B \sum_{\sigma=1}^q x_\sigma \ln x_\sigma. \quad (15)$$

What is the domain where the minimization should be performed? Comment on the expression of $s(x_1, \dots, x_q)$.

33) How could we have found directly the free energy \hat{f} above, and what name(s) does this approach bear?

We denote by (x_1^*, \dots, x_q^*) the point where the minimum of \hat{f} is reached. In the thermodynamic limit, one has $\langle \delta_{\sigma_i, \sigma} \rangle = x_\sigma^*$ for all i and all σ .

34) What is the value of (x_1^*, \dots, x_q^*) for high temperatures? How can we call the corresponding phase of the system?

35) We assume in what follows that $h_1 = \dots = h_q = 0$, and it is reminded that $J > 0$. What are the possible values of (x_1^*, \dots, x_q^*) at vanishing temperature? How can we call the corresponding phases? What is the degeneracy of the ground state?

We now wish to study the transition between the low T and high T regimes. We assume that the spontaneous symmetry breaking that occurs at low T , takes place along the $\sigma = 1$ direction, and does not distinguish among the other $q - 1$ possible values. We thus write $x_1 = x$, together with $x_2 = \dots = x_q$.

36) Express the common value $x_2 = \dots = x_q$ as a function of x . Show then that with the above parametrisation, we have $f(T) = \inf_x \hat{f}(x, T)$, with $\hat{f}(x, T) = e(x) - Ts(x)$. Provide the expressions of the functions $e(x)$ and $s(x)$.

From now on, q is taken as an arbitrary real number ≥ 2 , not necessarily an integer (there indeed exists an alternative definition to the partition function, that is meaningful for all possible real q).

- 37)** Plot schematically and separately the functions $e(x)$ and $s(x)$ for an arbitrary $q > 2$, emphasizing the behaviour close to the boundaries of their support (lower and upper bound), as well as the behaviour in the vicinity of their extrema (the position of which will be indicated).
- 38)** What is the value of x that minimizes $\hat{f}(x, T)$ at high temperature? This value will be denoted x_0 in the remainder. Below which temperature, denoted $T_c^{(2)}$, is x_0 no longer a local minimum of $\hat{f}(x, T)$? It may prove useful to show

$$\left. \frac{\partial^2 \hat{f}}{\partial x^2} \right|_T = -\gamma J \frac{q}{q-1} + k_B T \frac{1}{x(1-x)}, \quad \text{where } \gamma \text{ is a constant that will be given.} \quad (16)$$

- 39)** Expand $\hat{f}(x, T_c^{(2)})$ to third order around $x = x_0$. Show then that if $q > 2$, there exists a temperature $T_c^{(1)} > T_c^{(2)}$ such that x_0 no longer is the global minimum of \hat{f} for all temperatures $T < T_c^{(1)}$.
- 40)** Plot schematically the graphs of $\hat{f}(x, T)$ as a function of x for different temperatures.
- 41)** In the case $q > 2$, write the conditions that determine the value of $T_c^{(1)}$, and the position of the global minimum $x^{(1)}$ of \hat{f} at temperature $T_c^{(1)-}$, i.e. infinitesimally below $T_c^{(1)}$. Show that the conditions are met by

$$x^{(1)} = 1 - \frac{\alpha}{q}, \quad k_B T_c^{(1)} = J \frac{q-2}{(q-1) \ln(q-1)}. \quad (17)$$

What is the value of α ?

- 42)** Sketch the graph of the position of $x^*(T)$, the global minimum of \hat{f} , as a function of T . The cases $q = 2$ and $q > 2$ should be distinguished. Write down an admissible order parameter. In each case, what is the order of the transition and, if applicable, what is the value of the critical exponent β associated to the critical behaviour of $x^*(T)$?
- 43)** Explain qualitatively what would happen if one would consider the exact solution of the Potts model on a given lattice at $T = T_c^{(1)}$, imposing a fraction of spins $\sigma_i = 1$ between x_0 and $x^{(1)}$. It will be assumed that the mean-field scenario for $q > 2$ holds.

E. Exact results (miscellanea)

So-called duality transformations allow on some lattices to map Potts model onto itself, yet at a different coupling parameter $K = \beta J$. In doing so, one proves that the partition function on the square lattice (dimension $d = 2$) obeys the relation

$$Z(K) = Z(\tilde{K}) \left(\frac{(e^K - 1)^2}{q} \right)^N \quad \text{with} \quad (e^{\tilde{K}} - 1)(e^K - 1) = q. \quad (18)$$

- 44)** What is the explicit expression of the critical temperature?

In the 1970s, renormalization group treatments stumbled upon the Potts model for quite a while (in particular the change from first order for some q to second order for others), until it was realized that phase space should be enlarged to include “vacancies”. Indeed, mapping a region where the spins take many of the q possible values onto any one of those values leads to an overestimation of order. It is wiser to represent such areas by a vacancy on the renormalized lattice. Rather than the original Hamiltonian, we then consider

$$H_{\text{enlarged}} = - \sum_{\langle i,j \rangle} (L + J \delta_{\sigma_i, \sigma_j}) t_i t_j + \Delta \sum_i t_i, \quad (19)$$

where again $\sigma_i = 1, 2 \dots q$ while $t_i = 0$ or 1 . When the chemical potential $\Delta = -\infty$, all the $t_i = 1$ and we are back to Potts model. On the other hand, a finite value of Δ allows to have some $t_i = 0$, corresponding to vacant sites. Figure 2 shows the flow of the Hamiltonian (19) under a real-space renormalization transformation. The value of q is unchanged by the transformation, so all flows are along cross-sections of

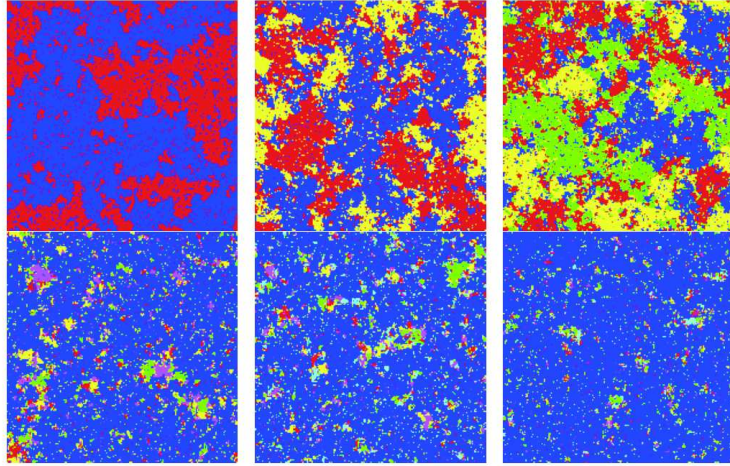


FIGURE 3 – Computer simulations of the Potts model at the critical temperature, for $q = 2, 3, 4$ (top row) and $q = 5, 6, 9$ (bottom row), from left to right. The different colors are for domains of like-spins; there are thus q colors in each Potts's plot. From H. Duminil-Copin, [arXiv:1707.00520](https://arxiv.org/abs/1707.00520).

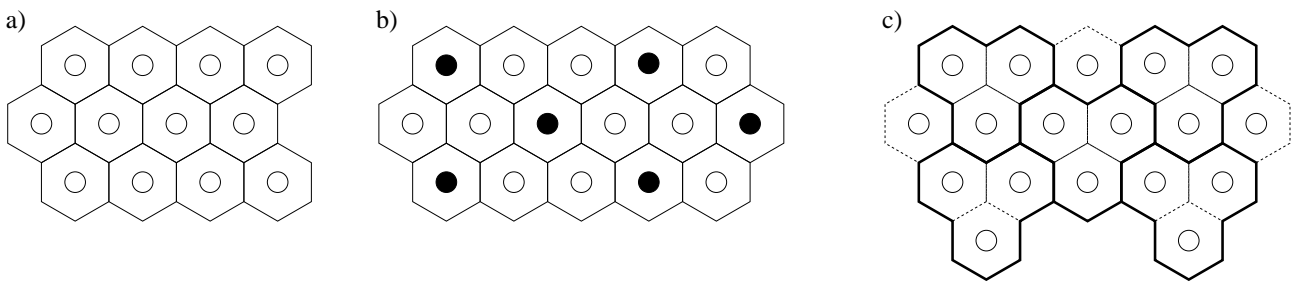


FIGURE 4 – a) Sketch of a graphite surface, where possible adsorption sites for Krypton atoms are represented by the circles. b) A possible ground state at filling fraction $1/3$. The sites occupied by Krypton correspond to the black disks. c) Groups of triplets of adsorption sites, to define the sites considered in the Potts model (where a q -states spin lives). Five such groups are shown in panel c).

- 49) What is then the value of q ? Figure 5 shows a configuration of Kr on the graphite plane, in which the possible ground states coexist, and occupy well defined domains. Show on the figure the domain walls (and do not forget to give this sheet back!). Which type of wall is the most energy consuming?

H. Annex

The multinomial expansion reads

$$\sum_{k_1+k_2+\dots+k_m=n} \frac{n!}{k_1! k_2! \dots k_m!} x_1^{k_1} x_2^{k_2} \dots x_m^{k_m} = (x_1 + x_2 + \dots + x_m)^n$$

References :

For question 49, see the cover of *Statistical Mechanics of Phase Transitions* by J. Yeomans (Oxford University Press), inspired from *Commensurate-incommensurate phase diagrams for overlayers from a helical Potts model*, M. Kardar and A. Berker, Phys. Rev. Lett. **48**, 1552 (1982). An authoritative review on the Potts model is that by F. Wu, Rev. Mod. Phys. **54**, 1 (1982) though not covering interdisciplinary applications (math, computer science, soft matter).

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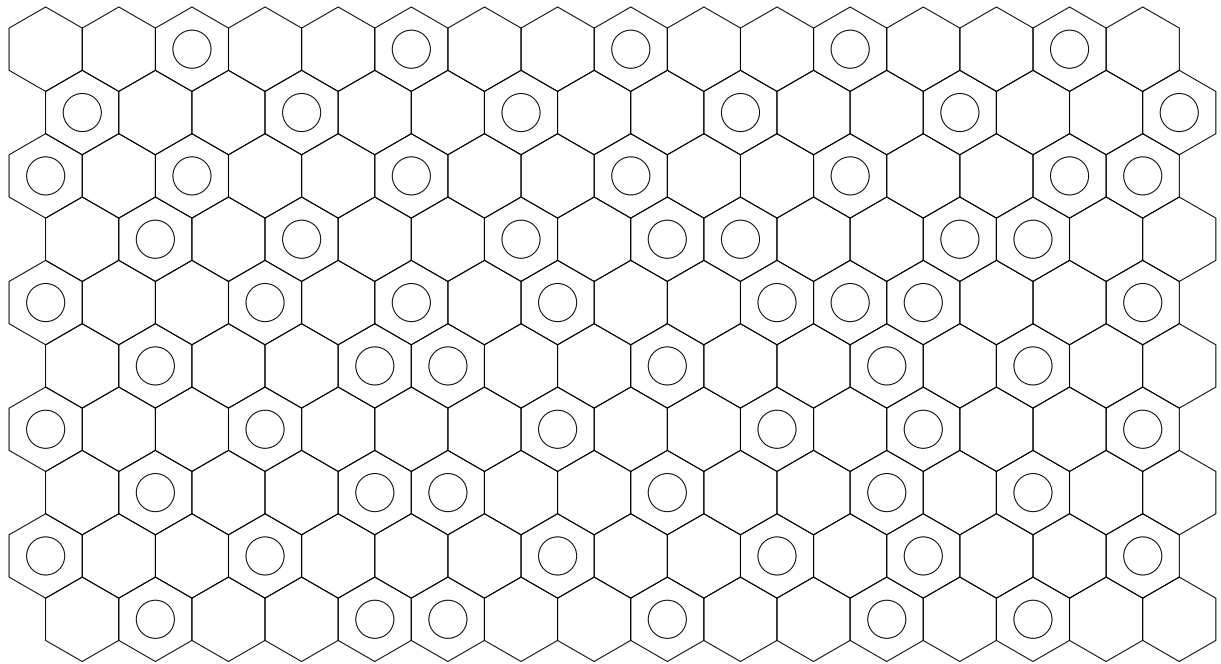


FIGURE 5 – An instantaneous configuration of adsorbed Kr atoms on graphite, at filling fraction $1/3$; the question is to identify the different ground states coexisting, and the domain walls between them. . .

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