ICFP M2 - Statistical Physics: Advanced and New Applications – Exam

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The exam is made of two parts. The first one is a series of short independent questions to check your knowledge and understanding of the contents of some of the lectures. You are expected to provide concise answers, without long computations. The second one consists in two longer independent problems.

Please write your answers to the two parts on separate pages.

No document nor calculator is allowed.

1 Questions on the lectures ($\approx 3/17$)

1. Give the definition of the Shannon entropy and recall its meaning in terms of information theory.
2. What is a topological defect ? Draw two examples of topological defect for the X-Y model.
3. What is the lower critical dimension for long-range order in case of continuous symmetries ? Give two examples of systems with quasi-long range order, i.e. characterized by power law correlations, in two dimensions.

2 Entropy production out of equilibrium ($\approx$ 7/17)

2.1 Introduction and notations

As explained during the lectures, even out of equilibrium is possible to obtain general thermodynamics identities. These are consequences of the breaking of time-reversal symmetry. The example explained in the lecture is the Jarzynski relation. In the following we are going to derive general relations for entropy and entropy production.
We consider a system, for simplicity in one-dimension, coupled to an environment and describe its dynamics by the Langevin equation :

$$\frac{dx}{dt} = F(x(t), \lambda(t)) + \xi(t) \qquad \langle \xi(t)\xi(t') \rangle = 2T\delta(t - t')$$

where $F(x(t), \lambda(t)) = -\frac{\partial V(x(t),\lambda(t))}{\partial x} + f(x)$ is an external force that depends on the external control parameter $\lambda(t)$ and the position $x(t)$.
We recall that the probability density $p(x, t)$ of x at time t verifies the Fokker-Planck equation :

$$\frac{\partial p}{\partial t} = \frac{\partial}{\partial x}\left(T\frac{\partial}{\partial x} - F\right)p = -\frac{\partial J}{\partial x}$$

where $J = -\left(T\frac{\partial}{\partial x} - F\right)p$ is the probability current.
The probability density of observing a trajectory $x[\tau]$ that starts in x_i at $t = t_i$ and ends in x_f at time t_f, conditioned on the starting point x_i, reads

$$p[x[\tau]] = \mathcal{N} \exp\left(-\int_{t_i}^{t_f} dt \left[\frac{1}{4T}\left(\frac{dx}{dt} - F\right)^2 + \frac{1}{2}\frac{\partial F}{\partial x}\right]\right)$$

where $\mathcal{N}$ is a normalization factor. Here and in the following we use the Stratonovich convention, which means that normal rules of calculus hold.

1. The work done in a small amount of time verifies the general thermodynamics relation $dw = dV + dq$, where dq is the amount of heat dissipated into the environment. Justify the "mechanical" definition of work
$$dw = \frac{\partial V}{d\lambda}\frac{d\lambda(t)}{dt}\,dt + f dx$$
and obtain that the dissipated heat $dq = F dx$.
2. Obtain the expression of the work done and the heat dissipated for a given trajectory $x[\tau]$. In particular justify why the entropy dissipated into the environment, i.e. the entropy created in the environment, reads
$$\Delta s_e = \frac{1}{T}\int_{t_i}^{t_f} F\frac{dx}{dt}dt$$
3. The instantaneous entropy of the system at time t and for a given path $x[\tau]$ has been defined by Seifert as $s_s = -\ln p(x(t), t)$, where $p(x, t)$ is the solution of the Fokker-Planck equation with initial condition x_i at time t_i and $x(t)$ is the position along the path at time t. Compute the average value of s_s and express it in terms of $p(x, t)$ only.
4. Show that at equilibrium $\langle s_s \rangle$ leads to the expected expression of the entropy of the system.
5. Show that there is a general relationship between the probability density of $x[\tau]$ and its time-reversed counterpart $p_R[x_R[\tau]]$ ($x_R[\tau]$ denotes the time reversed trajectory) :
$$p[x[\tau]] = p_R[x_R[\tau]]e^{\Delta s_e}$$
6. The variation of the total entropy Δs (of system plus environment) reads :
$$\Delta s = \Delta s_e + \Delta s_s = \Delta s_e - \ln p(x_f, t_f) + \ln p(x_i, t_i)$$

Using the two previous identities obtain :

$$\langle e^{-\Delta s} \rangle = 1$$

where the average is on the stochastic process.

7. Using the previous result show that the average variation of the *total* entropy s during an out of equilibrium process never decreases.
8. We are now going to obtain an expression for the average entropy production. Compute $\frac{ds_s}{dt}$.
9. Using the previous result, the definition of J and the expression of s_e obtain that the *total* entropy production reads
$$\frac{ds}{dt} = -\frac{1}{p}\frac{\partial p}{\partial t} + \frac{1}{T}\frac{J}{p}\frac{dx}{dt}$$
10. When using the Stratonovich convention averages such as $\langle h(x(t))\xi(t)\rangle$ are equal to $T\langle h'(x(t))\rangle$ (the proof of this statement is facultative). Using this identity show that the average entropy production reads
$$\langle \frac{ds}{dt} \rangle = \frac{1}{T}\int dx \frac{J(x,t)^2}{p(x,t)}$$
11. Show that the average entropy production is always non-negative and zero when the system is at equilibrium.

The relations we obtained are at the basis of what is called ”Stochastic Thermodynamics” which is an extension of thermodynamics used to study non-equilibrium systems, in particular small microscopic systems.

3 Percolation : Mean-Field Theory and Approximate Renormalization Group ($\approx 7/17$)

Percolation is a geometrical phase transition with several applications from physics to social sciences and computer science. In the following we are going to study its mean field theory and develop an approximate renormalization group treatment.
Consider an euclidean lattice, e.g. a square lattice in two dimensions. Each site in the lattice be occupied at random and independently with probability ρ. We call ρ the occupation probability or the concentration.
A *cluster* is a group of nearest neighbouring occupied sites.
In Fig. 1 we show what happens for the case of a square lattice in two dimensions. The occupied sites are shown in red while the sites belonging to the largest cluster are shown in black. Unoccupied sites are white. For $\rho \simeq 0.59$ a percolating cluster connecting two opposite boundaries appear for the first time. In the thermodynamic limit, this transition is sharp and can be understood using the framework of critical phenomena.

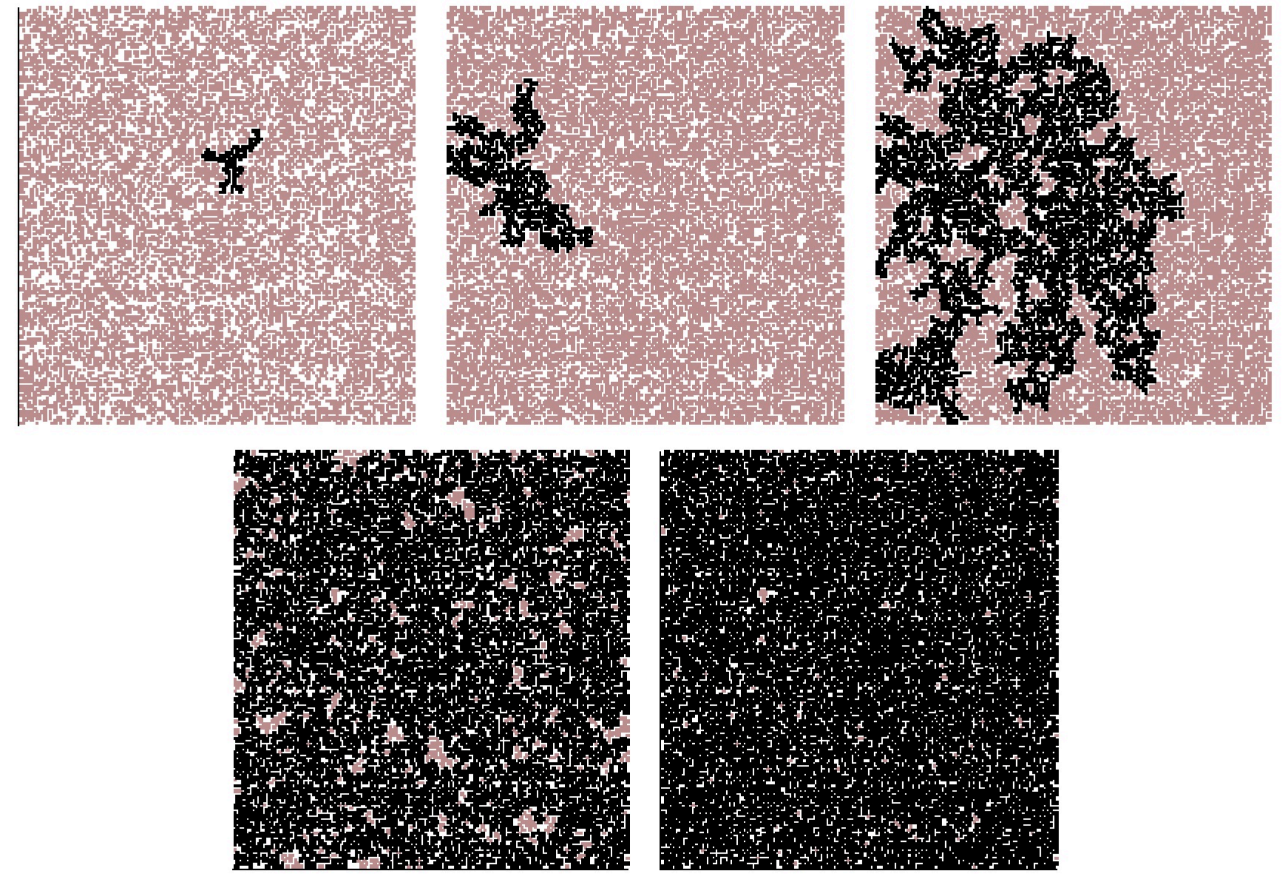

FIGURE 1 – Percolation in two dimensional square lattices with system size $L \times L = 150 \times 150$. Occupation probability $\rho = 0.45; 0.55; 0.59; 0.65$ and 0.75 respectively. Notice, that the largest cluster percolates through the lattice from top to bottom in this example when $p \simeq 0.59$.

3.1 Mean Field Theory

We are going to study percolation on a Bethe lattice, which provides a mean-field approximation to the problem. The particular feature of these lattices is that, as shown in Fig. 2, they are tree-like on any finite length-scale in the thermodynamic limit. We consider for simplicity the case with connectivity $z = 3$ which is an approximation of the hexagonal two dimensional lattice. The square lattice case would correspond to $z = 4$ (it's slightly more complicated).

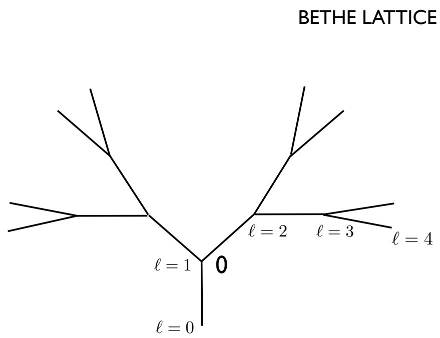

FIGURE 2 – Tree-like structure with connectivity $z = 3$. Neighbors of the site 0 are associated to a generation $\ell = 0, 1, 2, 3, 4$.

We choose to orient the lattice starting from an arbitrary site, called 0, as shown in Fig.2. We consider a recursive process explained below to determine when the percolation transition takes place. Let's call P the probability that a site at a given generation ℓ belongs to the infinite cluster (that we supposed unique) given that its neighbor at the previous generation $\ell - 1$ is occupied. This means that at least one of its neighbors at the next generation $\ell + 1$ belongs to the infinite cluster.

1. Justify that all the sites of the Bethe lattice are statistically identical.
2. Show that P verifies the self-consistent equation
$$P = \rho \left(2P - P^2\right)$$
3. Find the solutions of this equation for $\rho < \rho_c = 1/2$ and for $\rho > \rho_c = 1/2$. One can show that when there is more than one solution it is the largest solution that has to preferred.
4. Show that the probability $\overline{P}$ that a given site belongs to the infinite cluster reads :
$$\overline{P} = \rho \left(1 - (1 - P)^3\right)$$
Explain why this coincides with the fraction of sites belonging to the infinite cluster.
5. Plot $\overline{P}$ as a function of ρ and determine the critical exponent β defined by $\overline{P} \sim (\rho - \rho_c)^\beta$ for $(\rho - \rho_c) \ll 1$.
6. Start from a given site x at generation ℓ and focus on the sub-branch departing from that site, i.e. all sites belonging to the tree that starts from x and go up to higher generations. Call T the mean cluster size in a sub-branch. Show that T verifies the recurrence equation :
$$T = \rho \left(1 + 2T\right)$$
7. Compute the mean cluster size S to which a given site belongs to.
8. Plot S as a function of ρ and determine the critical exponent γ defined by $S \sim (\rho_c - \rho)^{-\gamma}$ for $(\rho_c - \rho) \ll 1$.

3.2 Approximate Renormalization Group Treatment

We are now going to develop an approximate RG theory of percolation. We will use a real space approach.
Within RG there are two fundamental steps : (1) replacing the original system defined on length-scale a by a new system defined on length-scale ℓa. (2) Rescaling the unit of length to complete the RG transformation.
We are interested in the percolation transition, i.e. whether a cluster connecting two opposite sides of the lattice appears for a certain value of ρ.

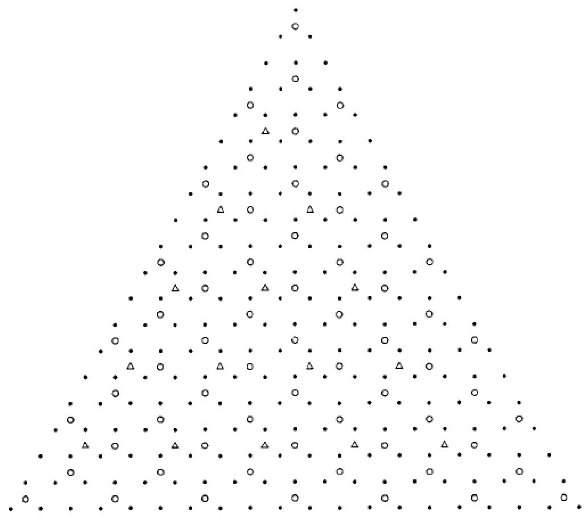

FIGURE 3 – Real space renormalization on a triangular lattice. At each iteration, three sites are combined into one supersite, denoted here by a different symbol. Circles, triangles and stars form triangular lattices and correspond to different steps in the RG flow.

1. We start by considering the one dimensional case. We divide the 1d lattice in blocks of consecutive three sites. The RG transformation consists in replacing the original lattice of L sites by a new system of $L/3$ sites. We focus on the probability p' of having a spanning cluster within the block. This verifies the equation $p' = R(p) = p^3$. This procedure can be then iterated leading to an RG flow. Study graphically the corresponding RG flow and identify the fixed points. Is there a transition in one dimension ?
2. We now consider the two dimensional case. For simplicity, we consider the triangular two-dimensional lattice. We divide it in triangular cells containing three sites each, see Fig.3. A renormalization step corresponds to a change of unit of length $\ell = \sqrt{3}$. Let's call p' the probability of having a spanning cluster in a triangular cell. Justify why the RG transformation reads :
$$p' = R(p) = p^3 + 3p^2(1-p) \ .$$
3. Study graphically the corresponding RG flow and identify the fixed points. What is the value of ρ_c found studying the RG flow. What is the value of p_c at the critical fixed point ?
4. From the analysis of the RG flow obtain the value of the critical exponent ν corresponding to the divergence of the correlation length, $\xi \sim (p_c - p)^{-\nu}$, which in the case of percolation corresponds to the linear size of the typical clusters.

The exact values for the percolation transition on the triangular two-dimensional lattice are $\rho_c = 1/2$ and $\nu = 4/3$. Our approximate RG treatment therefore provides a quite good approximation.