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Thermodynamic formalism and large deviation functions in continuous time Markov dynamics

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Abstract

The thermodynamic formalism, which was first developed for dynamical systems and then applied to discrete Markov processes, turns out to be well suited for continuous time Markov processes as well, provided the definitions are interpreted in an appropriate way. Besides, it can be reformulated in terms of the generating function of an observable, and then extended to other observables. In particular, the simple observable K giving the number of events occurring over a given time interval turns out to contain already the signature of dynamical phase transitions.

For mean-field models in equilibrium, and in the limit of large systems, the formalism is rather simple to apply and shows how thermodynamic phase transitions may modify the dynamical properties of the systems. This is exemplified with the q -state mean-field Potts model, for which the Ising limit $q = 2$ is found to be qualitatively different from the other cases.

Résumé

Formalisme thermodynamique et grandes déviations dans les systèmes à dynamique markovienne.

Le formalisme thermodynamique, qui a d'abord été développé dans le cadre des systèmes dynamiques puis appliqué aux processus de Markov, s'avère également pertinent pour les dynamiques de Markov en temps continu, à condition toutefois d'interpréter les définitions en jeu de façon appropriée. Ce formalisme peut être reformulé en termes de fonction génératrice d'une observable, puis étendu à d'autres observables. En particulier, l'observable K donnant le nombre d'événements ayant lieu dans un intervalle de temps donné, bien que très simple, contient déjà la signature de transitions de phases dynamiques.

Pour les modèles de champ moyen à l'équilibre, et dans la limite des grands systèmes, le formalisme peut s'appliquer simplement et montre comment les transitions de phase thermodynamiques peuvent affecter les propriétés dynamiques de ces systèmes. Cela est illustré sur le cas du modèle de Potts en champ moyen, et il s'avère que le cas d'Ising diffère qualitativement des autres cas.

Key words: thermodynamic formalism ; large deviations ; chaos

Mots-clés : formalisme thermodynamique ; grandes déviations ; chaos

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1. Introduction

The theory of chaos has first been developed in the frame of dynamical systems. In particular the well-known Lyapunov exponents were then defined, which characterize the exponential divergence between initially closely trajectories in phase space. Lyapunov exponents characterize individual directions, and if at least one of these exponents is positive, the system is said to be chaotic. The Kolmogorov-Sinai entropy provides a more global measurement of chaos. This can directly be seen from Pesin's theorem, which relates the KS entropy to the sum of positive Lyapunov exponents: $h_{KS} = \sum_{\lambda_i > 0} \lambda_i$ for a closed system. In practice, in order to obtain the h_{KS} entropy, one has to partition phase space. A trajectory in phase space becomes, in this coarse grained description, a sequence of cells which are visited by the actual trajectory. By doing so, the deterministic dynamics can be turned into a stochastic one. The KS entropy is then defined as $h_{KS} = -\lim_{t \rightarrow \infty} \frac{1}{t} \sum_{\text{histories}} \text{Prob}\{\text{history}\} \ln \text{Prob}\{\text{history}\}$. Then, in order to mimic the formalism that is used for equilibrium systems, a so-called thermodynamic formalism was introduced [1], in which various quantities – and in particular the KS entropy – are derived from a partition function

$$Z(s, t) = \sum_{\text{histories from } 0 \rightarrow t} (\text{Prob}\{\text{history}\})^{1-s} \quad (1)$$

This function is called *dynamical partition function*, as the sum is not taken over configurations but over histories. We have replaced the usual exponent β by $1-s$ for reasons that will become obvious later. Anyhow, this exponent has nothing to do with a temperature. It is just a parameter that allows to scan the distribution $\text{Prob}\{\text{history}\}$. In the same way as a free energy is defined for equilibrium systems, one introduces the so-called topological pressure, or Ruelle pressure, defined by

$$\psi(s) = \lim_{t \rightarrow \infty} \frac{1}{t} \ln Z(s, t) \quad (2)$$

where the thermodynamic limit is replaced by a long time limit. The KS entropy is immediately obtained from $\psi(s)$ via the relation $h_{KS} = \psi'(0)$. Other quantities that can be obtained from ψ are for example the topological entropy, $h_{\text{top}} = \psi(1)$, which counts the number of trajectories within a certain time interval, or the escape rate (for open systems) which is equal to $\gamma = -\psi(0)$.

As the deterministic dynamics had to be turned into a stochastic dynamics in order to apply this formalism, the latter is of course particularly well-suited for systems which are stochastic from the beginning, as Markov processes are. The formalism was successfully applied to a number of Markov processes in discrete time, and in this frame, it was shown that h_{KS} could be efficiently calculated via the formulation $h_{KS} = -\frac{1}{\tau} \langle \sum_{\mathcal{C}'} w(\mathcal{C} \rightarrow \mathcal{C}') \ln w(\mathcal{C} \rightarrow \mathcal{C}') \rangle_{\text{st}}$ where $w(\mathcal{C} \rightarrow \mathcal{C}')$ is the probability to jump from a configuration \mathcal{C} to a configuration \mathcal{C}' , and τ is the time step of the process [2].

If one tries to extend the calculations of h_{KS} to continuous time by letting the time step τ tend to zero, the probability $w(\mathcal{C} \rightarrow \mathcal{C}')$ (which is proportional to τ) also tends to zero and h_{KS} diverges. In the same way, a finite continuous time limit for the thermodynamic formalism cannot be obtained by taking $\tau \rightarrow 0$.

A first remark is that this divergence of h_{KS} does reflect the fact that the dynamical complexity of the trajectories is infinite when continuous time dynamics is considered, since one needs an infinite amount of information to describe the continuum of time intervals between configuration changes (see Sec.2). In that sense, the divergence is meaningful. On the other hand, this divergence indicates that the glasses one is wearing to look at Markov processes (discrete time) may not be the most appropriate ones if one is interested in Markov dynamics (i.e. with continuous time).

In this paper, we shall summarize which glasses should be used, i.e. how the thermodynamic formalism should be applied in the case of Markov dynamics in order to get finite quantities [5,6]. The formalism will be rephrased in terms of large deviations of observables - or more precisely in terms of cumulant generating functions, which are the Legendre transforms of large deviation functions. This allows to cast the thermodynamic formalism into a more general frame including the much-discussed fluctuation theorem.

The computation of the topological pressure $\psi(s)$ for physically relevant models is in general a difficult task. Here, we shall show that in the special case of mean-field models at equilibrium, the dominant term of $\psi(s)$ in the limit of large systems can be obtained quite simply from the minimization of a given functional. As a result, one obtains a description of the dynamical properties of the aforementioned equilibrium systems. This will be illustrated on the example of the Potts model.

2. The thermodynamic formalism for continuous time Markov dynamics

We shall start with some obvious remarks on the origin of stochasticity of the trajectories. In order to define a trajectory, one has to determine:

- which configurations will be visited: this is the configurational part of the trajectory, and it is just a sequence of configurations $\mathcal{C}_0 \rightarrow \dots \rightarrow \mathcal{C}_K$ where successive configurations are different. Once we know that the system will jump from configuration \mathcal{C} to another one, the probability to chose a specific configuration \mathcal{C}' is $\frac{W(\mathcal{C} \rightarrow \mathcal{C}')}{r(\mathcal{C})}$ where $r(\mathcal{C})$ is the rate of escape from configuration \mathcal{C} :

$$r(\mathcal{C}) = \sum_{\mathcal{C}' \neq \mathcal{C}} W(\mathcal{C} \rightarrow \mathcal{C}'). \quad (3)$$

The probability of the configurational part of the trajectory thus reads:

$$\text{Prob}\{\text{history}\} = \prod_{n=0}^{K-1} \frac{W(\mathcal{C}_n \rightarrow \mathcal{C}_{n+1})}{r(\mathcal{C}_n)} \quad (4)$$

- when shall the system jump from one configuration to the next one:

$$\begin{array}{cccccc} 0 & t_1 & t_2 & \cdots & t_K & t \\ \mathcal{C}_0 & \implies & \mathcal{C}_1 & \implies & \mathcal{C}_2 & \cdots \implies & \mathcal{C}_K \end{array} \quad (5)$$

The probability density for not leaving the configuration \mathcal{C}_{n-1} during the time interval $t_n - t_{n-1}$ and for changing configuration at time t_n is $r(\mathcal{C}_{n-1})e^{-(t_n - t_{n-1})r(\mathcal{C}_{n-1})}$. For the last time interval, one must only ensure that the system does not leave configuration \mathcal{C}_K during the time interval $t - t_K$, and the associated probability density is $e^{-(t - t_K)r(\mathcal{C}_K)}$.

The key point when applying the definition for the dynamical partition function is that only the probability of the configurational part of the trajectory should be raised to the power $1 - s$, i.e.

$$\begin{aligned} Z(s, t | \mathcal{C}_0, t_0) &= \sum_{k=0}^{+\infty} \sum_{\mathcal{C}_1, \dots, \mathcal{C}_k} \int_{t_0}^t dt_1 r(\mathcal{C}_0) e^{-(t_1 - t_0)r(\mathcal{C}_0)} \dots \\ &\int_{t_{k-1}}^t dt_k r(\mathcal{C}_{k-1}) e^{(t_k - t_{k-1})r(\mathcal{C}_{k-1})} e^{-(t - t_k)r(\mathcal{C}_k)} \left[\prod_{n=1}^k \frac{W(\mathcal{C}_{n-1} \rightarrow \mathcal{C}_n)}{r(\mathcal{C}_{n-1})} \right]^{1-s} \end{aligned} \quad (6)$$

At this stage, it may seem quite arbitrary. The justification for this point of view is mainly that it gives a coherent picture, and that the value of $Z(s, t)$ and derived quantities can effectively be computed in several models. Actually, the idea was already implicitly present in a work by van Beijeren, Dorfman and Latz [3,4], in the case of a Lorentz gas with discs scatterers, and a hard sphere gas.

In order to give a unified picture, it is useful to notice that $Z(s, t)$ can be expressed in terms of an observable

$$Q_+ = \sum_{n=0}^{K-1} \ln \frac{W(\mathcal{C}_n \rightarrow \mathcal{C}_{n+1})}{r(\mathcal{C}_n)} \quad (7)$$

Indeed one has $Z(s, t) = \langle e^{-sQ_+} \rangle$ and the dynamical partition function appears as the moment generating function of Q_+ . Then $\psi(s)$ is the corresponding cumulant generating function. The average sign $\langle \dots \rangle$ includes the average both on configurations and times. From now on, ψ will be denoted by $\psi_+(s)$ to recall that it is associated to the observable Q_+ .

In practice, $Z(s, t)$ is rarely evaluated directly from its definition (6). One rather evaluates directly $\psi(s)$, which turns out to be the largest eigenvalue of an operator $\mathbb{W}_+(\mathcal{C}, \mathcal{C}') = W(\mathcal{C}' \rightarrow \mathcal{C})^{1-s} r(\mathcal{C}')^s - r(\mathcal{C}) \delta_{\mathcal{C}, \mathcal{C}'}$ which is a kind of evolution operator weighted according to the parameter s . In [6], we found that not only the eigenvalue but also the eigenvector associated with this operator can yield useful information on the dynamical structure of the system dynamics, in particular when dynamical transitions occur.

The KS entropy can then be obtained from several definitions which can be shown to be equivalent:

$$h_{\text{KS}} = - \lim_{t \rightarrow \infty} \frac{1}{t} \left\langle \sum P(\mathcal{C}_0, \mathcal{C}_1, \dots, \mathcal{C}_K) \ln P(\mathcal{C}_0, \mathcal{C}_1, \dots, \mathcal{C}_K) \right\rangle \quad (8)$$

$$= \psi'_+(0) \quad (9)$$

$$= - \lim_{t \rightarrow \infty} \frac{\langle Q_+ \rangle}{t} \quad (10)$$

$$= - \left\langle \sum_{\mathcal{C}'} W(\mathcal{C} \rightarrow \mathcal{C}') \ln \frac{W(\mathcal{C} \rightarrow \mathcal{C}')}{r(\mathcal{C})} \right\rangle_{st} \quad (11)$$

The last relation was obtained by a similar derivation as the one performed for discrete time Markov processes by Gaspard [2].

In the spirit of Gaspard [7], once the thermodynamic formalism is expressed in terms of an observable, one can generalize it to a whole family of observables

$$A(t) = \sum_{n=0}^{K-1} \alpha(\mathcal{C}_n, \mathcal{C}_{n+1}) \quad (12)$$

which depends only on the configurational part of the trajectory. Then $\psi_A(s) = \lim_{t \rightarrow \infty} \frac{1}{t} \ln \langle e^{-sA} \rangle$ is the moment generating function of A and can be obtained as the largest eigenvalue of an operator \mathbb{W}_A defined in a way similar to \mathbb{W}_+ .

Among all these observables, at least two other ones than Q_+ seem interesting. The first one is K , i.e. the number of configuration changes within the time interval $[0, t]$. It is the simplest one one could think of, and still already contains some relevant information on dynamical phase transitions.

The second one was introduced by Lebowitz and Spohn [8]

$$Q_S = \sum_{n=0}^{K-1} \ln \frac{W(\mathcal{C}_n \rightarrow \mathcal{C}_{n+1})}{W(\mathcal{C}_{n+1} \rightarrow \mathcal{C}_n)} \quad (13)$$

It is this observable that verifies the fluctuation relation which, in terms of the moment generating function ψ_S , reads $\psi_S(s) = \psi_S(1-s)$ (we assume through the whole paper that the systems under consideration can take only a finite number of states). Moreover, in the steady state, Q_S was identified as the integrated entropy flux [8] (we are now referring to the Boltzmann entropy $S(t) = - \sum_{\mathcal{C}} P(\mathcal{C}, t) \ln P(\mathcal{C}, t)$).

We have shown that, if one defines a twin observable Q_- for the reversed trajectories, namely $Q_- = \sum_{n=0}^{K-1} \ln \frac{W(\mathcal{C}_{n+1} \rightarrow \mathcal{C}_n)}{r(\mathcal{C}_{n+1})}$, then the observable Q_+ that we have introduced in the frame of the thermodynamic formalism can be related to Q_S via the relation

$$Q_S = Q_+ - Q_- \quad (14)$$

and, similarly to what Gaspard did for discrete time systems [2], one can define a reversed KS entropy $h_{\text{KS}}^R = - \lim_{t \rightarrow \infty} \frac{\langle Q_- \rangle}{t}$ which relates, in the stationary state, to the entropy flux:

$$\sigma_{\text{f}} = -\sigma_{\text{irr}} = h_{\text{KS}} - h_{\text{KS}}^R \quad (15)$$

where h_{KS} is defined by (8-11).

3. Mean-Field models

In general, calculating the cumulant generating function ψ_A associated with the observable A is a difficult task (see [6,9] for examples). However, for mean-field models which can be described by a macroscopic order parameter (such as a magnetization), and for which a detailed balance relation is available, one can quite easily get the leading order of ψ_A in the limit of large systems, at least for $A = K$ and $A = Q_+$.

The derivation is based on the fact that for a *symmetric* operator, the largest eigenvalue can be expressed as

$$\lambda_{\text{max}} = \max_V \left\{ \frac{\langle V | \mathbb{W}^{\text{sym}} | V \rangle}{\langle V | V \rangle} \right\} \quad (16)$$

3.1. Symmetrization of the operators \mathbb{W}_K and \mathbb{W}_+

One can check, using the detailed balance relation

$$\frac{P_{\text{eq}}(\mathcal{C}')}{P_{\text{eq}}(\mathcal{C})} = \frac{W(\mathcal{C} \rightarrow \mathcal{C}')}{W(\mathcal{C}' \rightarrow \mathcal{C})}, \quad (17)$$

that the following operators obtained by a similarity transformation from \mathbb{W}_K and \mathbb{W}_+ are symmetric

$$\mathbb{W}_K^{\text{sym}} = \mathcal{T}^{-1} \mathbb{W}_K \mathcal{T} \ ; \ \mathcal{T}(\mathcal{C}, \mathcal{C}') = P_{\text{eq}}^{1/2}(\mathcal{C}) \delta_{\mathcal{C}, \mathcal{C}'} \quad (18)$$

$$\mathbb{W}_+^{\text{sym}} = \mathcal{T}^{-1} \mathbb{W}_+ \mathcal{T} \ ; \ \mathcal{T}(\mathcal{C}, \mathcal{C}') = P_{\text{eq}}(\mathcal{C})^{\frac{1-s}{2}} r(\mathcal{C})^{-\frac{s}{2}} \delta_{\mathcal{C}, \mathcal{C}'} \quad (19)$$

As a property of similarity transformations, these symmetric operators have the same spectrum - and thus the same largest eigenvalue - as the original ones.

To make the presentation easier to follow, we shall exemplify the remaining of the approach in the case of the Potts model.

3.2. Definition of the mean-field Potts model

In each site of a lattice of size N , a spin variable σ_i can be in q different states. The mean-field Potts model is defined by the Hamiltonian

$$\mathcal{H} = -\frac{J}{2N} \sum_{i,j} [q \delta_{\sigma_i, \sigma_j} - 1] = -\frac{J}{2N} \sum_{k=1}^q [N_k^2 - N^2] = -\frac{J}{2} N \left[q \sum_{k=1}^q \theta_k^2 - 1 \right]$$

where N_k is the number of spins in state k and $\theta_k = \frac{N_k}{N}$ the corresponding fraction. When a site switches from state n to state m , the corresponding energy variation writes

$$\Delta \mathcal{H} = -\frac{Jq}{N} [N_m - N_n + 1] = -Jq [\theta_m - \theta_n + 1/N] \quad (20)$$

The model is endowed with a continuous time Glauber like dynamics with transition rates

$$W(\sigma_i = n \rightarrow \sigma_j = m) = e^{-\beta \frac{\Delta \mathcal{H}}{2}} \quad (21)$$

The equilibrium probability distribution

$$P_{\text{eq}}(\{\sigma_i\}) = \frac{1}{Z} e^{-\beta \mathcal{H}} \quad (22)$$

verifies detailed balance. However, in what follows, we shall rather describe the system at the level of the occupation numbers $\mathbf{N} = \{N_k\}_{k=1..q}$. Then the equilibrium distribution that obeys detailed balance reads

$$P_{\text{eq}}(\mathbf{N}) = \frac{1}{Z} \frac{N!}{\prod_{k=1}^q N_k!} e^{-\beta \mathcal{H}} \quad (23)$$

with the transition rates

$$W(\mathbf{N}', \mathbf{N}) = W(\mathbf{N} \rightarrow \mathbf{N}') = N_n e^{\beta \frac{Jq}{2N} [N_m - N_n + 1]} \quad (24)$$

where $\mathbf{N}' = \{N_1, \dots, N'_n = N_n - 1, \dots, N'_m = N_m + 1, \dots, N_q\}$.

In the following, we shall consider the operator associated with the observable K :

$$\mathbb{W}_K(\mathbf{N}', \mathbf{N}) = z \sum_n \sum_{m \neq n} \delta_{N'_n, N_n - 1} \delta_{N'_m, N_m + 1} \prod_{k \neq n, k \neq m} \delta_{N'_k, N_k} W(\mathbf{N} \rightarrow \mathbf{N}') - \prod_{k=1}^q \delta_{N'_k, N_k} r(\mathbf{N}) \quad (25)$$

where $z = e^{-s}$. Using the same transformation as in (18), one obtains the symmetric operator

$$\begin{aligned} \mathbb{W}_K^{\text{sym}}(\mathbf{N}', \mathbf{N}) &= z \sum_n \sum_{m \neq n} \delta_{N'_n + 1, N_n} \delta_{N'_m - 1, N_m} \prod_{k \neq n, k \neq m} \delta_{N'_k, N_k} [(N'_n + 1) N'_m]^{1/2} \\ &\quad - \prod_{k=1}^q \delta_{N'_k, N_k} \sum_n \sum_{m \neq n} N'_n e^{\beta \frac{Jq}{2N} [N'_m - N'_n + 1]} \end{aligned}$$

For large N , and outside of the thermodynamic transition, one expects that the eigenvector associated with the largest eigenvalue will take the form

$$V(\mathbf{N}) \sim e^{Nf(\{\theta_k\}_{k=1..q})}$$

Indeed, this is the case in particular for $z = 1$ ($s = 0$), i.e. for the equilibrium distribution with

$$f(\{\theta_k\}_{k=1..q}) = \beta \frac{Jq}{2} \sum_{k=1}^q \theta_k^2 \quad (26)$$

An expansion in the large N limit yields

$$\begin{aligned} & \sum_{\mathbf{N}'} \mathbb{W}^{\text{sym}}(\mathbf{N}, \mathbf{N}') Q(\mathbf{N}') \\ &= z \sum_n \sum_{m \neq n} \sqrt{(N_n + 1)N_m} e^{Nf(\theta_1, \dots, \theta_n + \frac{1}{N}, \dots, \theta_m - \frac{1}{N}, \dots, \theta_q)} - \sum_n \sum_{m \neq n} N_n e^{\beta \frac{Jq}{2N} [N_m - N_n + 1]} e^{Nf(\theta_1, \dots, \theta_q)} \\ &= N e^{Nf(\theta_1, \dots, \theta_q)} \sum_n \sum_{m \neq n} \left\{ z \sqrt{\theta_n \theta_m} e^{\frac{\partial f}{\partial \theta_n} - \frac{\partial f}{\partial \theta_m}} - \theta_n e^{\beta \frac{Jq}{2} [\theta_m - \theta_n]} \right\} \end{aligned} \quad (27)$$

The quantity to maximize is

$$\frac{\sum_{\mathbf{N}} \sum_{\mathbf{N}'} V(\mathbf{N}) \mathbb{W}^{\text{sym}}(\mathbf{N}, \mathbf{N}') V(\mathbf{N}')}{\sum_{\mathbf{N}} [V(\mathbf{N})]^2} = \frac{\sum_{\mathbf{N}} N e^{2Nf(\theta_1, \dots, \theta_q)} \sum_n \sum_{m \neq n} \left\{ z \sqrt{\theta_n \theta_m} e^{\frac{\partial f}{\partial \theta_n} - \frac{\partial f}{\partial \theta_m}} - \theta_n e^{\beta \frac{Jq}{2} [\theta_m - \theta_n]} \right\}}{\sum_{\mathbf{N}} e^{2Nf(\theta_1, \dots, \theta_q)}} \quad (28)$$

For each function f , in the large N limit, the sum is dominated by the maximum of f , for which $\frac{\partial f}{\partial \theta_n} = 0 \forall n = 1..q$, i.e.

$$\frac{\psi_K(s)}{N} = \max_{\mathbf{N}} \left\{ \sum_n \sum_{m \neq n} \left[z \sqrt{\theta_n \theta_m} - \theta_n e^{\beta \frac{Jq}{2} [\theta_m - \theta_n]} \right] \right\} \quad (29)$$

We shall now apply this result to various values of q .

3.3. Arbitrary value of q

As in [10], we assume a symmetry breaking along one particular direction $k = 1$ (assume for example that a very small field along this direction breaks the symmetry of the system). Then the system can be described by one order parameter $m \in [-1/(q-1), 1]$ with $\theta_k = \frac{1-m}{q} \forall k > 1$ and $\theta_1 = \frac{1+(q-1)m}{q}$.

The cumulant generating function for K is then obtained from

$$\begin{aligned} \frac{\psi_K(s)}{N} &= \max_m \left\{ 2 \frac{q-1}{q} z \sqrt{(1-m)[1+(q-1)m]} + \frac{(q-1)(q-2)}{q} (z-1)(1-m) \right. \\ &\quad \left. - \frac{q-1}{q} [1+(q-1)m] e^{-\frac{\beta Jq}{2} m} - \frac{q-1}{q} (1-m) e^{\frac{\beta Jq}{2} m} \right\} \end{aligned} \quad (30)$$

We shall now take special values of q to explore the consequences of this maximization condition.

3.4. $q = 2$: the mean-field Ising model

For $q = 2$, spins can take only two values $S_i = \pm 1$. The corresponding fractions can be expressed in terms of a unique order parameter, the magnetization m :

$$\theta_1 = \frac{1+m}{2} \quad \text{and} \quad \theta_2 = \frac{1-m}{2}$$

with $\theta_1 - \theta_2 = m$, and the Hamiltonian reads with these notations

$$\mathcal{H} = -\frac{J}{2N} \sum_{i,j} S_i S_j. \quad (31)$$

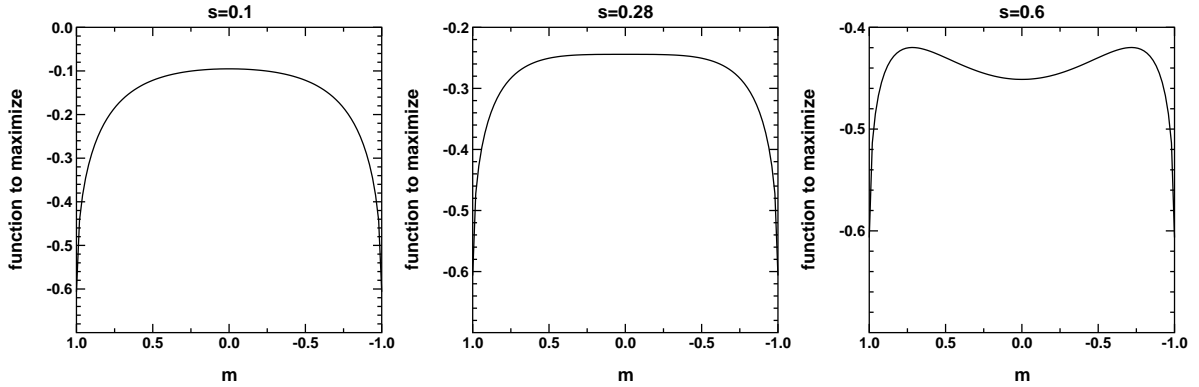


Figure 1. The function that must be maximized in order to find the value of $m_K(s)$ and $\frac{\psi_K(s)}{N}$, in the case of the Ising model ($q=2$), for a temperature $\beta = 0.5$ above the critical temperature (disordered phase), $J = 1$, and for the s values 0.1, $s_c = 0.28$, and 0.6.

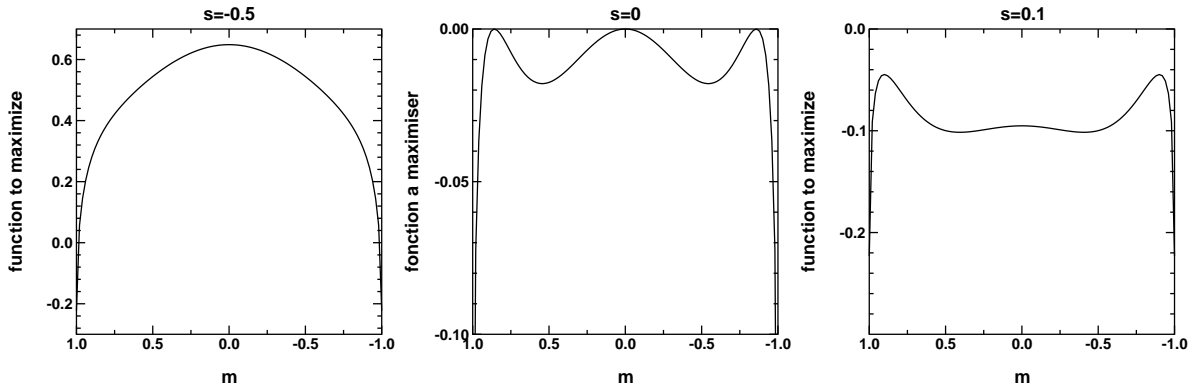


Figure 2. The function that must be maximized in order to find the value of $m_K(s)$ and $\frac{\psi_K(s)}{N}$, in the case of the Ising model ($q=2$), for a temperature $\beta = 1.5$ under the critical temperature (ordered phase), $J = 1$, and for the s values -0.5 , 0, and 0.1.

Then the maximization condition (30) becomes

$$\frac{\psi_K(s)}{N} = \max_m \left\{ z\sqrt{1-m^2} - \cosh \beta J m + m \sinh \beta J m \right\} \quad (32)$$

The behavior of this function is illustrated in figures 1 and 2. The magnetization for which the maximum is obtained is called $m_K(s)$. In the high temperature phase, it is vanishing for a whole range of s values. This was of course expected for $s = 0$, where m_K coincides with the physical magnetization of the system. But above a certain threshold s_c , the maximum splits into two symmetrical ones. The transition is continuous (see figure 3, left), and corresponds to a discontinuity in the second derivative of $\psi_K(s)$ (figure 4). A clear difference appears between the disordered and ordered phases. In the latter case ($\beta > 1$), the transition value s_c is exactly at zero (figure 3, right). Besides, the transition in m_K is now discontinuous, and the first derivative of $\psi_K(s)$ already shows a discontinuity.

Once we know that the transition above T_c is continuous, and thus that $m_K(s)$ is close to zero at the transition, it is possible to determine the value for s_c by expanding the expression for $\psi_K(s)$ for small m_K values. Then the condition $\frac{d\psi_K}{dm_K} = 0$ yields a non-zero m_K solution for

$$z_c = \beta J (2 - \beta J) \quad (33)$$

It is of course much harder to perform these calculations in finite dimension. It may nevertheless be argued that the dynamical phase transition occurring in the paramagnetic phase for $s > s_c > 0$ has an upper critical dimension $d_c = 6$ characterized by critical exponents that are apparently unrelated to those of the static phase transition at $\beta = 1$ and $s = 0$.

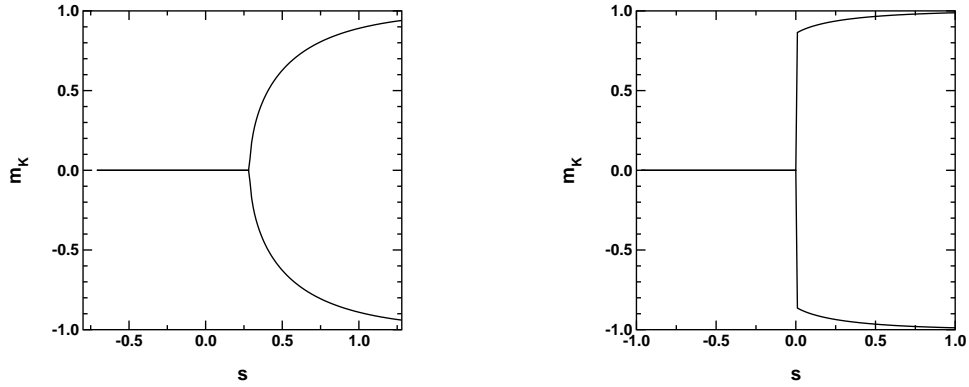


Figure 3. The value of the magnetization for which the function of (32) is maximal, as a function of s , in the case of the Ising model ($q=2$), for $\beta = 0.5$ (left) and $\beta = 1.5$ (right). We took $J = 1$.

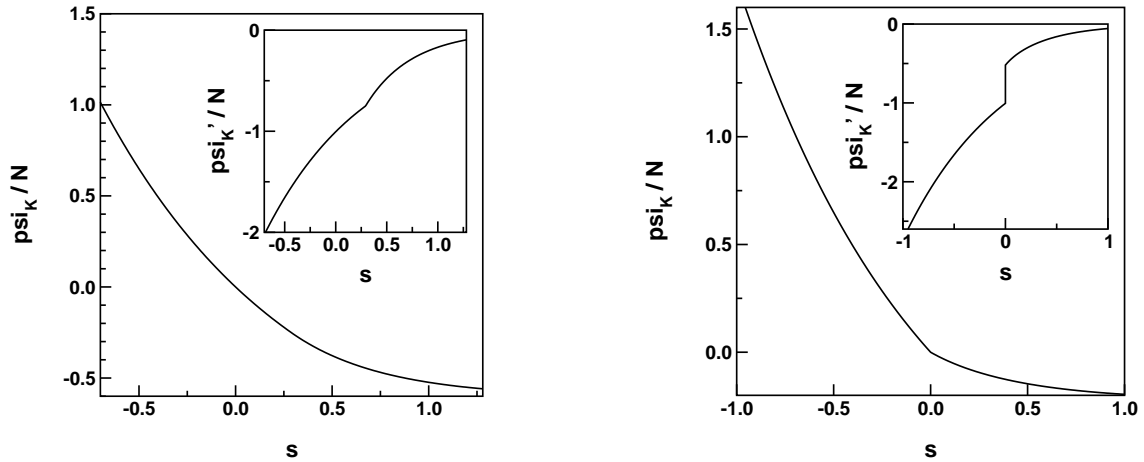


Figure 4. $\psi_K(s)$ in the case of the Ising model ($q=2$), for $\beta = 0.5$ (left) and $\beta = 1.5$ (right). We took $J = 1$. The derivative $\psi'_K(s)$ is plotted in the inset. It is continuous (resp. discontinuous) in the disordered (ordered) phase.

3.5. $q = 3$: the three states Potts model

For $q = 3$, the critical temperature of the thermodynamic phase transition corresponds to $\beta_c = 2.7725$ [10]. As we shall show graphically, the dynamical phase transition is now discontinuous both above and under the critical temperature

For $\beta = 0.5$, figure 5 shows the behavior of the function to maximize. By contrast with the Ising case, now the transition in the m_K parameter is discontinuous even in the high temperature phase (figure 6). Both for high and low temperatures, the discontinuity occurs in the first derivative of $\psi_K(s)$, as seen in figure 7. However, while the transition at high temperature occurs at $s = s_c \neq 0$, it occurs at $s = 0$ under the critical temperature.

3.6. The $q = 1$ limit

The limit $q = 1$ is interesting because it can be related to percolation (see [11] for example). In order to have a well defined limit, one considers

$$\tilde{\psi}_K(s) = \lim_{q \rightarrow 1} \frac{\psi_K(s)}{q-1} = N \max_{m \leq 1} \left\{ z (2\sqrt{1-m} + m - 1) + (1-m) \left(1 - e^{\frac{\beta J}{2} m} \right) - e^{-\frac{\beta J}{2} m} \right\}$$

In the case $z = 1$, this expression can be factorized

$$\frac{\tilde{\psi}_K(s)}{N} = \max_{m \leq 1} \left\{ \sqrt{1-me}^{\frac{\beta J}{4} m} - e^{-\frac{\beta J}{4} m} \right\}^2 \quad (34)$$

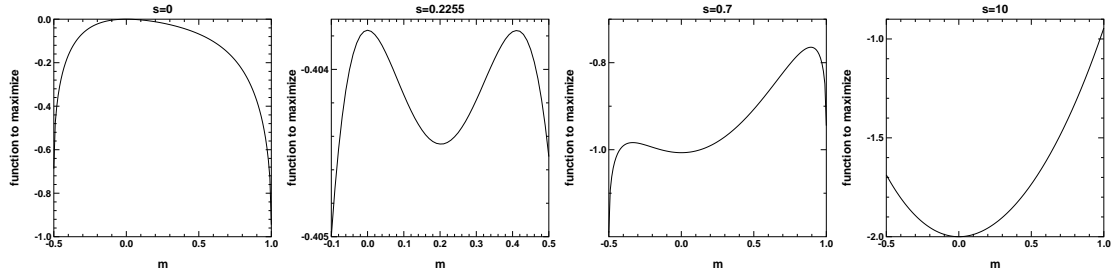


Figure 5. The function that must be maximized in order to find the value of $m_K(s)$ and $\frac{\psi_K(s)}{N}$, in the case of the Potts model for $q = 3$, for a temperature $\beta = 0.5$ above the critical temperature, for $J = 1$, and for the s values $0, s_c = 0.2255, 0.7$ and 10 .

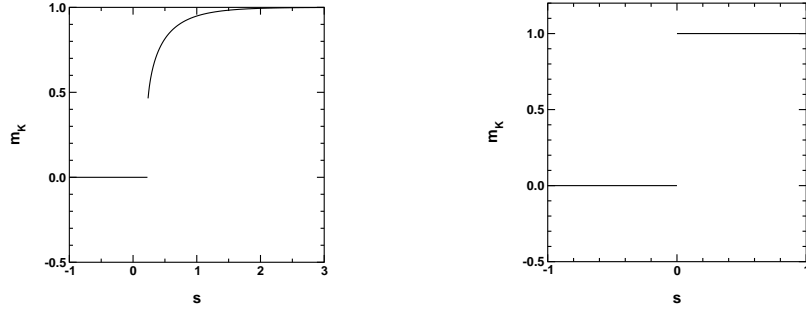


Figure 6. The value of the magnetization for which the function of (32) is maximal as a function of s , in the case of the Potts model for $q = 3$, for $\beta = 0.5$ (left) and $\beta = 5$ (right). We took $J = 1$.

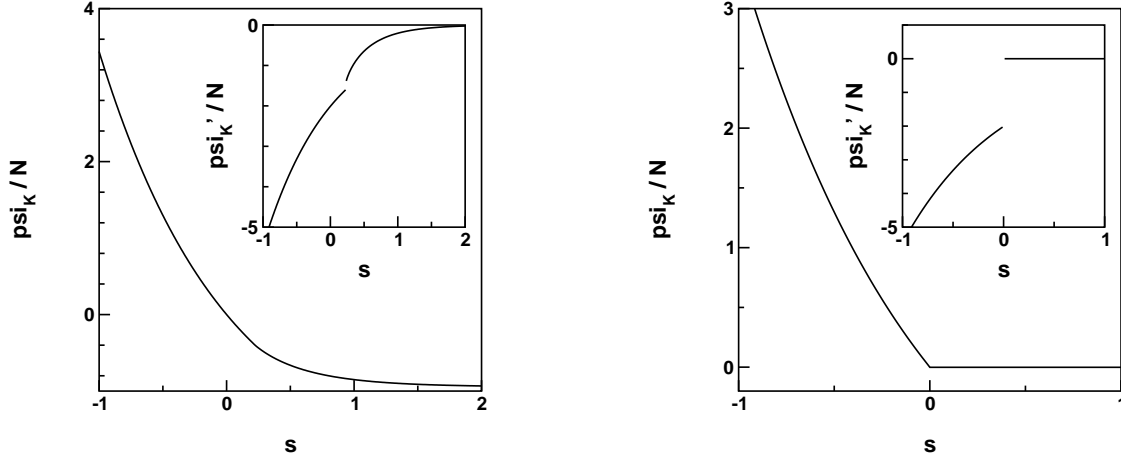


Figure 7. $\psi_K(s)$, in the case of the Potts model for $q = 3$, for $\beta = 0.5$ (left) and $\beta = 5$ (right). We took $J = 1$. The derivative $\psi'_K(s)$ is plotted in the inset. It is discontinuous in both cases.

As in the case $q = 3$, one finds that the dynamical phase transition that occurs at $s = 0$ for $\beta > 1$ or < 1 is characterized by a discontinuous $m_K(s)$, and a continuous cumulant generating function (the discontinuity occurs in the first derivative of $\psi_K(s)$).

4. Conclusion

Though the thermodynamic formalism was designed in order to study out-of-equilibrium systems, it is also a useful tool to shed a new light on equilibrium systems. Their dynamical properties turn out to be richer than could be expected. Actually, some dynamical phase transitions do occur even in apparently dull phases as the disordered

phase in the Ising model. Dynamical phase transitions and thermodynamic ones are connected : in all examples that we studied, the features of the dynamical phase transition are different on each side of the thermodynamic phase transition. The understanding of the interplay between dynamical and thermodynamic phase transitions could lead to a renewed vision of equilibrium systems.

Here the case of the Potts model was studied for a various number of states q . Interestingly, the case $q = 2$ turns out to be quite special in the sense that the paramagnetic phase of the Ising model is the only one where a continuous phase transition occurs in the order parameter $m_K(s)$, corresponding to a discontinuity which appears only in the second derivative of $\psi_K(s)$. By contrast, both for $q = 1$ or $q = 3$, all dynamical transitions were found to be discontinuous in the order parameter $m_K(s)$, and it is the first derivative of $\psi_K(s)$ that shows a discontinuity.

In a research field which often requires very technical and heavy calculations, the method that we present here is interestingly simple. We applied it in this paper to the calculation of the cumulant generating function of K for the mean-field Potts model in the large N limit, but more generally it can be applied to any mean-field model which can be described by a macroscopic order parameter, and for which a detailed balance relation at the macroscopic scale is available (in particular, the transition rates of the dynamics must be functions only of the aforementioned order parameter). Though all the results we presented were dealing with the observable K , the same kind of calculations - with the same kind of conclusions in the case of the Potts model - can be performed for the observable Q_+ (the corresponding cumulant generating function is then the so-called topological pressure). It should be noticed however that in the case of Q_+ , the large N expansion of equation (27) is only valid for $s < 1$, as a consequence of $1 - s$ powers. A generalization to other observables of the form (12) with $\alpha(\mathcal{C}, \mathcal{C}') = \alpha(\mathbf{N}, \mathbf{N}')$ is often possible.

References

- [1] David Ruelle. *Thermodynamic Formalism*. Addison Wesley Publ. Co. (Reading, Mass, 1978)., 1978.
- [2] P. Gaspard. Time-reversed dynamical entropy and irreversibility in markovian random processes. *J. Stat. Phys.*, 117:599–615, 2004.
- [3] H. van Beijeren and J.R. Dorfman. A note on the Ruelle pressure for a dilute disordered Sinai billiard. *J. Stat. Phys.*, 108:516, 2002.
- [4] A. Latz, H. van Beijeren, and J.R. Dorfman. Lyapunov spectrum and the conjugate pairing rule for a thermostated random Lorentz gas: kinetic theory. *Phys. Rev. Lett.*, 78:207–210, 1997.
- [5] V. Lecomte, C. Appert-Rolland, and F. van Wijland. Chaotic Properties of Systems with Markov Dynamics *Phys. Rev. Lett*, 95:010601, 2006.
- [6] V. Lecomte, C. Appert-Rolland, and F. van Wijland. Thermodynamic formalism for systems with Markov dynamics. *To appear in J. Stat. Phys*, 2007.
- [7] P. Gaspard. *Chaos, scattering and statistical mechanics*. Cambridge Nonlinear Science Series vol. 9 (Cambridge UP, 1998), 1998.
- [8] J.L. Lebowitz and H. Spohn. A Gallavotti-Cohen type symmetry in the large deviation functional for stochastic dynamics. *J. Stat. Phys.*, 95:333–365, 1999.
- [9] B. Derrida and C. Appert. Universal large deviation function of the Kardar-Parisi-Zhang equation in one dimension. *J. Stat. Phys.*, 94:1–30, 1999.
- [10] J.F.F. Mendes and E.J.S. Lage. Dynamics of the infinite ranged Potts model. *J. Stat. Phys.*, 64:653, 1991.
- [11] T.C. Lubensky. In Maynard Balian and Toulouse, editors, *Ill Condensed Matter, Les Houches XXXI*. North-Holland, Amsterdam, 1979.