Chaotic Properties of Systems with Markov Dynamics

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(Received 30 March 2005; published 27 June 2005)

We present a general approach for computing the dynamic partition function of a continuous-time Markov process. The Ruelle topological pressure is identified with the large deviation function of a physical observable. We construct for the first time a corresponding finite Kolmogorov-Sinai entropy for these processes. Then, as an example, the latter is computed for a symmetric exclusion process. We further present the first exact calculation of the topological pressure for an N-body stochastic interacting system, namely, an infinite-range Ising model endowed with spin-flip dynamics. Expressions for the Kolmogorov-Sinai and the topological entropies follow.

DOI: 10.1103/PhysRevLett.95.010601 PACS numbers: 05.40.−a, 02.50.−r, 05.45.−a

In statistical mechanics, bridging the microscopics to the macroscopics remains the ultimate goal, be it in or out of equilibrium. The development of the theory of dynamical systems and of their chaotic properties has led to major advances in equilibrium and nonequilibrium statistical mechanics. All those approaches make extensive use of such concepts as Lyapunov exponents, Kolmogorov-Sinai (KS) or topological entropies, topological pressure, etc., all quite mathematical in nature, and for which very few results (even nonrigorous) are available, as far as systems with many degrees of freedom are concerned. One of the central ideas in constructing a statistical physics out of equilibrium is that of Gibbs ensembles [1] in which time is seen to play the role of the volume in traditional equilibrium statistical mechanics. A central quantity called the dynamical partition function is, in general, defined as

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

The so-called thermodynamic formalism allows us to derive from this quantity a number of chaotic properties such as the topological entropy which is defined through the number of possible trajectories a system can follow, or the KS entropy which is a measure of the complexity of a process and characterizes its dynamical randomness. Within that framework there exists a mathematical construction of smooth stationary measures for nonequilibrium steady states—the Sinai-Ruelle-Bowen (SRB) measures—the determination of which precisely rests on the dynamic partition function and the KS entropy [2].

It must, however, be acknowledged that the determination of any of these quantities has only been carried out for toy models of dynamical systems, such as the baker's map [3]. Most of the efforts for physically relevant systems have borne on the Lorentz gas [4–6], and more recently on hard-sphere systems in the dilute limit [7]. It is possible to relate discrete-time Markov processes to dynamical systems (see [4] for a pedagogical account), yet very few examples going beyond the simple random walk have been investigated. More importantly, when the discrete-time scale is sent to zero, infinities arise [8], so that no viable definition of the dynamical partition function in the physical limit of continuous time has hitherto been proposed. Continuous-time Markov processes are ubiquitous. Many systems governed by a Hamiltonian dynamics can be mapped, within some well-controlled approximation schemes, onto Markov processes. An extensive activity in the physical modeling of complex systems, from interacting spins to interacting gases, from avalanches in sandpiles to chemical reactions, relies on a continuous-time Markov description. In the present letter we construct, apparently for the first time in the literature, the dynamical partition function for such Markov processes. We do not rely on a discrete-to-continuum limit [8], and by working directly with continuous time, we obtain finite results. From this we show how to extract the KS entropy. We further connect it, in the spirit of Gaspard [9], to the Markov analog of a fluctuating entropy flow, as identified by Lebowitz and Spohn [10]. In order to exemplify our findings, we then perform an exact calculation on the infinite-range (i.e., mean-field) Ising model, endowed with spin-flip dynamics as introduced by Ruijgrok and Tjon [11]. To the best of our knowledge, this is the first available result for a many-body interacting stochastic system.

The outline of this Letter is as follows: First we construct the dynamical partition function and the related topological pressure, which is identified as the large deviation function of a physical observable. From this we deduce an expression for the KS entropy. Then we establish a connection to the time-integrated entropy current. Finally, we explore the consequences of our formulation on three examples, a random walk with absorbing boundaries, a symmetric exclusion process, and an infinite-range Ising model, for which explicit and exact calculations are performed.

We begin with a generic Markov process characterized by transition rates $W(C \to C')$ from configuration C to configuration C'. The mean residence time in configuration C is $1/r(C)$, with $r(C) = \Sigma_{C'} W(C \to C')$. This means, in particular, that the probability of hopping from configuration C after a time interval t to some other configuration between t and $t + dt$ is $r(C)\exp(-r(C)t)dt$. Among the allowed target configurations, the system hops to the particular configuration C' with probability $W(C \to C')/r(C)$. Various properties of the master equation evolution operator $\mathbf{W}$ for the probability $P(C, t)$ to be in state C at time t, such that, in matrix notation, $\partial_t P = \mathbf{W}P$, can be found in [12]. We define the dynamic partition function $Z(s, t)$ as the sum over all possible histories of the process over the interval $[0, t]$ of the probabilities of the histories raised to the power $(1 - s)$ [13]. It is a matter of carefully applying the definition to realize that

$$Z(s, t) = \sum_{\text{histories from } 0 \to t} (\text{Prob}\{\text{history}\})^{1-s} = \langle e^{-sQ_+(t)} \rangle, \tag{2}$$

where the observable $Q_+(t)$ depends on the sequence of states $C_0, \ldots, C_k$ occupied by the system over $[0, t]$ through the relationship

$$Q_+(t) = \sum_{n=0}^{k-1} \ln \frac{W(C_n \to C_{n+1})}{r(C_n)}. \tag{3}$$

It is necessary to describe the meaning of the brackets in (2): they stand for an average over the number k of successive states occupied over $[0, t]$, over the various configurations $C_0, \ldots, C_k$ visited by the system, and, finally, over the time lapses that the system has been staying in each of those k states. All these quantities define a *history*. Note that the topological or Ruelle pressure $\psi(s)$, canonically defined as $\psi(s) = \lim_{t\to\infty} \frac{1}{t} \ln Z$, is also the generating function of the cumulants of the physical observable Q_+. It is possible to write an evolution equation for $P(C, Q_+, t)$, the probability to be in state C at time t with $Q_+(t) = Q_+$, and a similar one for the related generating function $\int dQ_+ e^{-sQ_+} P(C, Q_+, t)$. The latter obeys a master-equation-like evolution with an operator $\mathbf{W}_+$ whose matrix elements are given by

$$\mathbf{W}_+(C, C') = W(C' \to C)^{1-s} r(C')^s - r(C)\delta_{C,C'}. \tag{4}$$

An important consequence is that $\psi(s)$ is simply the largest eigenvalue of the evolution operator $\mathbf{W}_+$. The analog was already known [8] for a discrete-time Markov process, but appears to be a new result for continuous-time processes. We stress that ψ is finite even though we are working in continuous time. Having reduced the computation of chaotic properties to a mere technical challenge, we later present concrete physical examples in which the entire spectrum of $\mathbf{W}_+$ can be determined. We temporarily continue with abstract considerations by defining a similar quantity Q_- for the time-reversed process,

$$Q_-(t) = \sum_{n=1}^{k} \ln \frac{W(C_n \to C_{n-1})}{r(C_{n-1})}, \tag{5}$$

which verifies that

$$Q_+(t) - Q_-(t) = \sum_{n=1}^{k} \ln \frac{W(C_{n-1} \to C_n)}{W(C_n \to C_{n-1})} = Q_S(t). \tag{6}$$

The quantity $Q_S(t)$ appearing in the right-hand side of (6) is precisely the time-integrated fluctuating entropy flow introduced by Lebowitz and Spohn [10], which verifies, as $t \to \infty$, the Gallavotti-Cohen symmetry $\langle e^{-sQ_S} \rangle \simeq \langle e^{-(1-s)Q_S} \rangle$. A similar property for discrete-time Markov processes, discussed at the level of the averages, was already noted by Gaspard [9]. In the same way as it can be seen that the entropy current

$$J_S(C) = \sum_{C'} W(C \to C') \ln \frac{W(C \to C')}{W(C' \to C)} \tag{7}$$

verifies $d\langle Q_S \rangle/dt = \langle J_S(C) \rangle$, one can verify that

$$J_\pm(C) = \sum_{C'} W(C \to C') \ln \frac{W(C \rightleftarrows C')}{r(C)} \tag{8}$$

govern the evolutions of $Q_\pm$ according to $d\langle Q_\pm \rangle/dt = \langle J_\pm(C) \rangle$, and they have the property that $J_+(C) - J_-(C) = J_S(C)$. The entropy current is usually proportional to a particle current [14–16] or to an energy current [17]; hence, its physical meaning is clear. However, neither of $J_\pm$ receives such a straightforward interpretation. In equilibrium, which is when the rates W satisfy the detailed balance condition, both Q_+ and Q_- have the same large deviation function. It requires one to relate Q_+ to quantities familiar in the dynamical systems theory to endow it with a more transparent physical meaning. The KS entropy, h_{KS}, which is defined [2] as

$$h_{\text{KS}} = -\frac{1}{t} \sum_{\text{hist.}} \text{Prob}\{\text{history}\} \ln \text{Prob}\{\text{history}\} \tag{9}$$

is also obtained, for a system without escape, from

$$h_{\text{KS}} = \psi'(0) = -\langle J_+ \rangle. \tag{10}$$

Therefore J_+ appears to convey the physical meaning of an information content flow. Another quantity of interest is the topological entropy $h_{\text{top}} = \psi(1)$, which counts the number of possible trajectories over $[0, t]$. We close our construction with a remark on SRB measures. Following the procedure outlined in Beck and Schlögl [2], the stationary SRB measure can be obtained from a variational principle: in our case, this is the invariant measure P that renders the combination $\psi_P(s) = h_{\text{KS}}[P] - (1 - s)\langle Q_+ \rangle_P / t$ maximum when $s = 0$. The master equation possesses a unique stationary solution. The SRB measure can only be this stationary solution, for which the above combination becomes $\psi(s) = s h_{\text{KS}}$ if $s \to 0$ and one recovers the fact that $h_{\text{KS}} = \psi'(0)$.

We now present three simple applications of increasing complexity. Consider first a particle diffusing with diffusion constant D on a one-dimensional infinite line. We can illustrate on this example how a deterministic map allows one to define for a stochastic system a Lyapunov exponent compatible with the thermodynamic formalism exposed above. Each jump of the particle can be described by a deterministic map as indicated in [3,4]. This allows one to define a corresponding Lyapunov exponent from the exponential divergence between initially close trajectories, averaging over the time lapses between jumps (which are randomly distributed as for the Markov process). Here we find $\lambda = 2D\ln 2$ which is related to the topological pressure $\psi(s) = 2D(2^s - 1)$ through $\psi'(0) = \lambda$.

The same example can be used to illustrate the case of systems with escape. The particle now jumps on an infinite two-dimensional lattice slab of width ℓ with absorbing boundaries. It is a trivial matter to diagonalize the corresponding $\mathbf{W}_+$ and to find its largest eigenvalue $\psi(s)$, which reads, for large ℓ

$$\psi(s) = 4D(4^s - 1) - 4^s D\pi^2/\ell^2. \tag{11}$$

Hence the topological pressure verifies $\psi(0) = -\gamma$, where $\gamma = D\pi^2/\ell^2$ is the escape rate of the particle. This result is, of course, consistent with that established for the Lorentz gas and stands as yet another manifestation of the link between transport coefficients and the topological pressure [18].

Our second example is the *symmetric exclusion process,* a gas of N mutually excluding particles diffusing on a one-dimensional lattice of L sites with periodic boundary conditions. Their hopping rate is denoted by D, and for simplicity we have confined our analysis to determining the KS entropy. Denoting by ρ the average density, and by $\sigma(\rho) = 2\rho(1-\rho)$ (twice) its compressibility, we find that

$$h_{\rm KS}/D = L\sigma\ln(L\sigma) + \sigma\ln(L\sigma) + \tfrac{3}{2}\sigma + \mathcal{O}(\ln L/L). \tag{12}$$

In order to establish this result we started from $h_{\rm KS} = -\langle J_+\rangle$ and we exploited that the equilibrium state is perfectly random [19]. Our first comment on (12) is that $h_{\rm KS}$ is not extensive in the system size. Second, the effect of the interaction is felt through a given combination of the system size and of its compressibility. At half-filling the system shows its largest KS entropy, and this is likely related to the fact that also the number of allowed distinct microscopic states is maximum at $\rho = 1/2$. The dependence of $h_{\rm KS}$ on ρ through σ arises only from the particle-hole symmetry.

As a third example, we consider an infinite-range Ising model with Hamiltonian $\mathcal{H} = -(\sum_{i=1}^N \sigma_i)^2/2N$, endowed with spin-flip dynamics. Each spin σ_i flips independently with a rate $\exp(-\beta\sigma_i M/N)$, where β is the inverse temperature and where $M = \sum_i \sigma_i$ is the total magnetization before the spin flip. These flipping rates satisfy the detailed balance property with respect to the canonical distribution $\exp(-\beta\mathcal{H})$. This system has the advantage of exhibiting a second-order phase transition, the generic effect of which on Lyapunov exponents has hitherto never been explicitly probed. Technically speaking, the master equation has an evolution operator that can be exactly diagonalized [11]. We now describe, skipping all technical details [20], our results for the topological pressure for this system. On the one hand, we may follow the procedure outlined in the first part of this Letter, and identify a state C with a configuration $\{\sigma_i\}$ of the N spins. There are 2^N such configurations, and restricting ourselves to the high temperature phase $\beta < 1$, the exact diagonalization of $\mathbf{W}_+$ as defined in (4) leads to the eigenvalues (or Ruelle-Pollicott resonances) $\psi(s) - n\phi(s)$ with $n \in \mathbb{N}$, where

$$\begin{aligned} \psi(s) &= (N^s - 1)N + N^s[1 - (1-s)\beta] - \phi(s), \\ \phi(s) &= N^{s/2}\sqrt{N^s[1 + s\beta(2-\beta)] - \beta(2-\beta)}. \end{aligned} \tag{13}$$

Again we note that the topological pressure (13) is not extensive in the number of spins, which also reflects on the KS entropy:

$$h_{\rm KS} = N\ln N - \frac{\beta(2-\beta)}{2(1-\beta)}\ln N - \frac{\beta^2}{2(1-\beta)}. \tag{14}$$

What can also be observed in (14) is that, because of the diverging susceptibility $\beta/(1-\beta)$ at the critical point $\beta = 1$ our calculational technique [11] ceases to be valid for systems with $N(1-\beta) \sim 1$.

Another viewpoint, on the other hand, would have consisted in adopting a coarse-grained description of the same spin system and choosing to characterize its states by their total magnetization M (there are $2N$ such magnetization states). Even though we are talking about the same system we are not talking about the same Markov process, hence the spectrum of $\mathbf{W}_+$ differs from its previous expression and the Ruelle pressure is now given by

$$\begin{aligned} \psi(s) = {} & N(2^s - 1) + 2^s(1-s)(1-\beta) \\ & - 2^{s/2}\{2^s[1 - s(1-\beta)^2] - \beta(2-\beta)\}^{1/2}. \end{aligned} \tag{15}$$

Now the corresponding KS entropy is extensive in the system size. The leading term in the system size expresses that, roughly speaking, the total magnetization undergoes a simple random walk. Interactions, and the effects of correlations, just as in (12) or (14), are felt to the next order in the system size. This is where interesting physical features are to be looked for.

We now summarize our findings. We have defined and constructed a dynamical partition function in the manner of Ruelle, along with the related topological pressure for continuous-time Markov processes. The topological pressure appears to be the largest eigenvalue of some operator, and is therefore a finite quantity, in spite of working within a continuous-time formulation. A key quantity for characterizing dynamical randomness, the KS entropy, follows, along with the topological entropy and the sum of positive

Lyapunov exponents. We have put our definitions to work on a few simple examples, thus illustrating how straightforward the connection between topological pressure and escape rate is, and making a significant step towards realistic systems (with a large number of degrees of freedom and interactions). Our formulation has the advantage of bringing concepts and quantities pertaining to other fields of studies—dynamical systems theory—back into the statistical mechanics community, and to which the available toolbox (simulations, mean-field approximations, low density expansions, field theory, exact results, etc.) will apply. We insist that the observable $Q_+(t)$ from which the main dynamical quantities arise can be easily monitored when performing numerical simulations.

We believe that our formulation opens a series of new research routes. To begin with, it would be interesting to see, e.g., for a lattice gas, how the precise form of the interactions and of the microscopic dynamics affects the KS entropy, and possibly to help clarify ongoing debates [21]. To what extent is the result obtained in (12) universal? Next, it would be instructive to see if ergodicity-breaking features, which are suspected to characterize systems with glassy dynamics, can be identified on h_{KS}. This could be first examined on simple systems like a particle diffusing in a random scenery, and then on a many-body glass forming lattice gas, such as the Kob-Andersen model. Even if no conceptual progress is to be expected from that, it would certainly be useful to specialize our approach to a widely used class of Markov processes, that which rests on Langevin equations (this could be achieved by resorting to the description used by Kurchan in [22]). This includes, in particular, fluctuating hydrodynamics, but also phenomenological models of chemical reactions, surface growth, turbulence, etc. It would also be interesting to see how the nonequilibrium nature can be traced back on the form and properties of the topological pressure. In that sense it would be useful to compare the dynamical entropies of a gas in equilibrium and for the same gas driven out of equilibrium by the system boundaries or by a bulk field. Such a system develops long range correlations and, in the case of a bulk drive, nonequilibrium phase transitions may be observed [23,24]; how these features affect the dynamical entropies deserves to be investigated. Finally, the link with dynamical system theory that we have presented in our first example still involves a stochastic part (the residence time in each visited state). It would be interesting to formalize a relationship between continuous-time Markov processes and fully deterministic flows. This identification, if possible, would perhaps allow for an interpretation of our KS entropy in terms of the sum of Lyapunov exponents for the corresponding flow. We hope that the present work will stand as a contribution towards welding communities somewhat impervious to each other.

The authors thank M. Courbage, H. J. Hilhorst, J. R. Dorfman, and H. van Beijeren for useful discussions and for critical comments.

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