Zeroth principle of thermodynamics in aging quasistationary states

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We show that the zeroth principle of thermodynamics applies to aging quasistationary states of long-range interacting \(N\)-body Hamiltonian systems. We also discuss the measurability of the temperature in these out-of-equilibrium states using a short-range interacting thermometer. As many connections are already established between such quasistationary states and nonextensive statistical mechanics, our findings constitute a strong suggestion that these basic concepts apply to systems that the nonextensive formalism aims to describe.

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The zeroth principle — if systems \(A\) and \(B\) are in thermal equilibrium with \(C\), they are in thermal equilibrium among them —, is one of the basic principles in physics. It establishes the transitivity of the temperature, and its importance can hardly be overestimated, being essential to the logical formulation of thermodynamics. In particular, it is fundamental in thermometry, which resides at the very grounds of experimental physics. Recently, considerable attention has been driven to \(N\)-body Hamiltonian systems that constitute paradigmatic models for long-range interactions [1–4]. These systems present several anomalies in their behavior. Among them, negative microcanonical specific heat, inequivalence between canonical and microcanonical ensembles, vanishing Lévy walks and anomalous diffusion. Quite remarkably, aging has also been exhibited [5]. In this Letter we focus on the appearance of long-lasting (possibly infinite-lasting in the thermodynamical limit) metastable or quasistationary states (QSS), characterized by a non-Gaussian velocity distribution and by a temperature that does not coincide with the one predicted by the Boltzmann-Gibbs (BG) theory [6,7]. The BG thermal equilibrium is attained at much later times, after a crossover time which diverges with \(N\). Using a standard dynamical definition of the temperature, we show that the zeroth principle of thermodynamics applies to these QSS in a manner which is essentially the same as for conventional thermal equilibria. Moreover, we exhibit that thermalization occurs even if measured with a thermometer that, in contrast with the ‘thermal bath’ that is probed, is short-range interacting. As these systems present a considerable number of connections [2,3,5–8] with nonextensive statistical mechanics [9], our findings constitute a strong suggestion that these basic concepts apply to situations that the nonextensive formalism aims to describe.

Long-range interacting systems constitute nowadays an exciting frontier topic in many areas of physics (astrophysics, nuclear physics, plasma physics, Bose-Einstein condensates, atomic clusters, hydrodynamics, among others) [10]. They also provide an interesting arena in a trans-disciplinary perspective as prototypical systems that enable the study of analogies or differences between alternative approaches. In particular, interesting results are now available which exhibit [4,6,7] inequivalences between standard BG approaches and methods of dynamical systems. If we consider, as Einstein pointed out in 1910 [11], that the foundations of statistical mechanics lies on dynamics, this is a major point worthwhile to be deeply analyzed.

As a representative example of such a richness of behavior, the Hamiltonian Mean Field model, which describes a system of \(N\) planar classical spins interacting through an infinite-range potential, has been largely considered in the literature [1–6]. This Hamiltonian can be written as

\[
H = K + V = \sum_{i=1}^{N} \frac{p_i^2}{2} + \frac{1}{2N} \sum_{i,j=1}^{N} \left[1 - \cos(\theta_i - \theta_j)\right],
\]

where \(\theta_i\) is the \(i\)th angle and \(p_i\) is the conjugate variable representing the angular momentum (unit inertial moment is assumed). It is the inertial version of the XY ferromagnetic spin model, with the interaction terms connecting not only first neighbors but all couples. Note that it is common use, although not necessary [2], to divide the potential term by \(N\) in order to make the Hamiltonian formally extensive. Defining the mean field vector \(\mathbf{M} \equiv \sum_{i=1}^{N} \mathbf{m}_i / N\) (with \(\mathbf{m}_i = (\cos \theta_i, \sin \theta_i)\)), an analytical BG canonical solution of this system predicts a second-order phase transition from a low-energy ferromagnetic phase with magnetization \(M \equiv |\mathbf{M}| \neq 0\), to a high-energy one with the spins homogeneously ori-
ent on the unit circle and $M = 0$. The critical point is at energy density $u_c = 0.75$, and a caloric curve can be exactly obtained [4]. On the other hand, it is quite simple to integrate numerically the equations of motion and to study the dynamical behavior of the system by means of molecular dynamics simulations for a relatively large number of spins $N$. When this is done for energy densities (slightly) below the critical point, with some non-zero-measure class of out-of-equilibrium initial conditions [6], one finds that the system is dynamically stuck in quasistationary nonequilibrium states whose duration diverges with $N$. Consistently with standard equilibrium statistical mechanics, a ‘dynamical temperature’ $T$ can be defined as

$$T(t) \equiv 2K(t)/N,$$

where $K$ is the kinetic energy and $t$ is time. In the present approach, we use the qualification dynamical in the sense that this definition purely descends from dynamics and not from a thermal contact with a thermostat. For system (1), during the QSS, the temperature $T_{QSS}$ evolves into a first plateau below the BG equilibrium temperature $T_{BG}$, before relaxing to a second plateau that coincides with $T_{BG}$. The difference between $T_{QSS}$ and $T_{BG}$ is maximal for energy density around $u = 0.69$. $T_{QSS}$ depends on the size $N$ of the system, but tends to a well defined value $T_\infty \simeq 0.38$ as $N \to \infty$. Notice that other long-range interacting models display QSS with temperature above $T_{BG}$ [7]. Moreover, aging [5] and non-Gaussian one-body marginal velocity distributions characterize the QSS. As strong numerical evidences indicate [6,7], in the thermodynamic limit $N \to \infty$, the QSS lasts forever. If we are attempting a thermodynamical description of such a system, it is fundamental to discuss the zeroth principle under these conditions. Furthermore, we would like to know what would be the response of a thermometer testing the quasistationary temperature.

In order to provide an answer to these questions we numerically integrate the Hamilton equations using the 4th order symplectic Neri-Yoshida integrator [12] with energy conservation $\Delta E/E \simeq 10^{-4}$, under different setups. In our first simulation we examine precisely the textbook construction for deriving the canonical ensemble as a subsystem of the microcanonical ensemble. First, we consider the isolated Hamiltonian system (1), composed by $N$ spins. Our out-of-equilibrium initial conditions consist in setting every angle parallel, e.g., $\theta_i = 0$, $\forall i$, and the angular momenta distributed inside an interval around the origin with a fixed separation between them, but each with a random shift that could be up to $a$. We renormalize the distribution in order to have total energy density $u = 0.69$ and zero total angular momentum. These initial conditions are very similar to the ones normally used in the literature, the so-called ‘waterbag’ initial conditions, but the present setup yields a lower initial temperature, just above $T_\infty$, which results in both smaller fluctuations and a longer duration of the anomalous plateau. Then, we take into account two distinct subsystems of the isolated system, each of them consisting of $M$ spins, with $M \ll N$. The first (second) subsystem is composed by the most (least) energetic initial data, so that its initial temperature $T_M(0) = 2K_M(0)/M$ is larger (smaller) than the one, $T_N(0) = 2K_N(0)/N$, of the isolated system as a whole. Fig. 1 shows the result of a single typical simulation, with $N = 10^4$ and $M = 5 \times 10^2$. In both cases we see that $T_M$ relaxes after some time to $T_N$, while the isolated system is still in the QSS. This situation lasts until all systems undergo together the expected relaxation to $T_{BG}$, due to finite-size effects. It is important to stress that the subsystem starting with the higher temperature, in its relaxation to the temperature of the isolated system, crosses $T_{BG}$ with no signs of attempts to relax to $T_{BG}$ itself. This result, for the QSS, precisely complies with the zeroth principle of equilibrium thermodynamics. Indeed, two systems are in thermal (meta)equilibrium with a third system, and in thermal (meta)equilibrium with each other. Also, this verification clearly opens the possibility for a generalized canonical treatment of the QSS, as all subsystems with $M \ll N$ share the same dynamical temperature after an initial transient. Such a detailed study is presently under course [13].

Our second simulation addresses the question of the measurability of the QSS dynamical temperature. We do this by considering the system (1) as a thermostat and by constructing a thermometer very different from the system (1), in the sense that it complies with the usual BG laws. The difference lies, more precisely, in the fact that we choose short-range interactions for the thermometer, both for its own dynamics and for its coupling with the thermostat. The thermometer is then composed by $M$ classical spins whose Hamiltonian is

$$H_{thermometer} = \sum_{j=1}^M p_j^2/2 + \sum_{j=1}^M [1 - \cos(\theta_j - \theta_{j+1})].$$

It has the same potential as the thermostat, but it only connects first neighbors. This short-range interaction results in a standard BG system as we will see below. The thermometer is prepared as follows: before entering into contact with the thermostat, we set the thermometer coordinates to $\theta_j = 0$, $\forall j$, and $p_j$ taken from a Gaussian distribution whose standard deviation is chosen in order to start with a particular temperature of our choice. We then let the system evolve freely for enough time until complete BG equilibrium is achieved with a Maxwellian one-body marginal velocity distribution. The $2M$ resulting coordinates are then used as initial conditions for the contact with the thermostat. In this way we are confident that we are starting with a thermometer in a usual BG equilibrium. On the other side, the thermostat is
prepared in the ‘water bag’ initial conditions previously described and we let evolve the two systems separately, until any quick transient states have disappeared. At a convenient time $t_{\text{contact}}$ they are “connected” through an interaction term

$$H_{\text{int}} = \epsilon \sum_{j=1}^{M} \left[ 1 - \cos(\theta_j - \theta_{\xi(j)}) \right],$$

(4)

where $\xi(i)$ is a random natural number between 1 and $N$ (fixed once for ever) that describes the connection between thermometer and thermostat spins. We include also a coupling constant $c$ to regulate the intensity of the interaction term (the coupling constant between spins of the same system is equal to unity). If we call $H_{\text{thermostat}}$ the Hamiltonian (1), the total system after $t_{\text{contact}}$ is then described by the Hamiltonian

$$H = H_{\text{thermostat}} + H_{\text{thermometer}} + H_{\text{int}}.$$  

(5)

Results of a single typical simulation with $N = 10^5$, $M = 50$ and $c = 5 \times 10^{-2}$ are shown in Fig. 2. It is important to appropriately choose the range of the numerical value of the coupling constant $c$. Indeed, we want on one hand to establish a significative coupling between the systems, but on the other hand to produce a not too large perturbation of the thermostat. We expect this care to become less and less restrictive as we numerically approach the theoretical limit $(N, M, N/M) \rightarrow (\infty, \infty, \infty)$. We see that the thermometer temperature $T_M = 2K_{\text{thermometer}}/M$, chosen in order to start below the thermostat temperature, stays few time steps in its initial equilibrium state and afterwards starts to grow rapidly to reach the thermostat temperature $T_N = 2K_{\text{thermostat}}/N$, and relaxation occurs completely within the QSS, for $\Delta t \approx 10^5$ time steps (fluctuations are of course present because of finite-size effects). Differently with the previous case, the thermometer eventually begins to relax to its equilibrium temperature, before the thermostat starts its final thermalization. As explained below, we consider this as one more finite-size effect. Note in the inset of Fig. 2 that the time at which the thermometer leaves the thermostat temperature approximately coincides with its minimum, that is known to be present just after the thermostat finally relaxes to $T_{BG}$.

When the thermometer is prepared in order to have, before contact, a temperature which is higher than that of the thermostat, our results show no clear signs of thermalization. $T_M$ increases steadily until it attains its definite equilibrium. This behavior will hopefully disappear when computers will allow simulations with even larger systems. It is also interesting to notice that, even preparing the thermometer with a temperature below $T_\infty = 0.38$, thermalization occurs only for $N$ and $N/M$ sufficiently large. For example, simulations with $N = 5 \times 10^5$ and $M = 5 \times 10^2$ do not show any thermalization.

Taking all these facts in consideration, namely, thermometer temperature reaching BG equilibrium before the thermostat, no relaxation for $T_M(t_{\text{contact}}) > T_N(t_{\text{contact}})$, no relaxation for too small $N$ and $N/M$, and also taking into account the fact that the system is aging, one may suspect what follows. The model (1) behaves like having some internal mechanism that, after a certain amount of time, for finite $N$, pulls the system out of the QSS to a BG equilibrium. This mechanism works like an internal clock that regulates this thermalization time, and may function like a potential well whose deepness decreases with time. A system with large enough fluctuations, compared to the well depth, will never be confined by the potential well. A system with small enough fluctuations is constrained to the well, but just for a limited amount of time, until the well becomes shallow and its depth becomes comparable to the fluctuations. In our case, the effect of the well would be to restrict the system to visit just a part of the phase space, while not being in any way during a long time would be associated to an homogeneous visit, the system thus becoming ergodic and relaxing to the expected BG temperature (see [14] for a low-dimensional analogy). Consequently, within this picture, fluctuations would greatly influence the system permanence in the QSS. Note that this scenario is also consistent with the relaxation of subsystems of an isolated system as observed in Fig. 1.

In order to state our conclusions, let us recall that in the last years considerable interest has been raised in the study of long-range interacting systems [10]. Significant progress has been made in the description and comprehension of out-of-equilibrium QSS that by no means accommodate within the BG scenario. These QSS display an anomalous temperature plateau [6] and various other anomalies that are consistent with the nonextensive statistical mechanics [9] picture. Among them, vanishing Lyapunov exponents [2] (see [15] for illustrative connections between nonextensive statistical mechanics and vanishing Lyapunov exponents), Lévy walks and anomalous diffusion [3], aging involving $q$-exponential (i.e., asymptotically power-law) time correlation functions [5], $q$-exponential one-body marginal velocity distributions [6], and $q$-exponential relaxation to the BG equilibrium [8]. Summarizing, if one wants to design a generalized statistical mechanical approach for the description of these QSS, a fundamental step concerns the validity of the zeroth principle. Our present results exhibit that this basic law of thermodynamics also applies to the QSS, and has therefore a domain of validity which is wider that the one normally associated with it within BG statistical mechanics. Furthermore, we have provided evidence that the QSS dynamical temperature is actually detectable by a normal short-range thermometer. We believe that the present findings establish fundamental grounds for forth-
coming research in the area.

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