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Boltzmann-Gibbs thermal equilibrium distribution for classical systems and Newton law: a computational discussion

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Abstract. We implement a general numerical calculation that allows for a direct comparison between nonlinear Hamiltonian dynamics and the Boltzmann-Gibbs canonical distribution in Gibbs Γ-space. Using paradigmatic first-neighbor models, namely, the inertial XY ferromagnet and the Fermi-Pasta-Ulam β-model, we show that at intermediate energies the Boltzmann-Gibbs equilibrium distribution is a consequence of Newton second law ($\mathbf{F} = m\mathbf{a}$). At higher energies we discuss partial agreement between time and ensemble averages.

PACS. 05.10.-a Statistical physics, thermodynamics, and nonlinear dynamical systems – 05.20.-y Classical statistical mechanics – 05.45.-a Nonlinear dynamics and chaos – 05.20.Gg Classical ensemble theory

The problem of the dynamical foundation of Boltzmann-Gibbs (BG) statistical mechanics dates back to the original proposal of this powerful formalism (see, e.g., [1]) and despite many important results this fundamental question [2] still presents open basic aspects (see, e.g., [3–7] and references therein). Thanks to the current computational capability we can numerically integrate the Hamilton equations of large enough systems and compare the results with the predictions of the BG formalism. Although this technique has been largely and successfully implemented in a microcanonical perspective (fixed-energy molecular dynamics), the methods used when addressing systems in contact with a thermostat (such as Monte Carlo and Nosé-Hoover [8]) usually impose an *ad hoc* dynamics. In this paper we introduce a scheme which enables the discussion of the canonical distribution in Gibbs Γ-space on the basis of the equations of motions. Within the present approach both time and ensemble averages are performed dynamically, so that we are able to discuss ergodicity. Using two paradigmatic first-neighbor nonlinear Hamiltonian systems — the one-dimensional inertial XY ferromagnet and the Fermi-Pasta-Ulam (FPU) β-model — we find a remarkable agreement between BG equilibrium calculations and dynamical ensemble averages. We also compare partial ergodicity failure with the maximum Lyapunov coefficient. Our numerical calculation can be implemented in systems that allow for a textbook definition of the canonical ensemble (i.e., part of a large isolated system). It would also be interesting to check the same procedure in situations where, due for example to the presence of long-range terms, important deviations from the BG predictions have been found [9,10]. We are presently making progress on this task.

Given some macroscopic conditions in the phase space of the system under consideration (Γ-space), the average value of a dynamical function can be defined using time or ensemble averages; ergodicity means that these two methods are equivalent. We remark that both approaches are dynamically realizable. In the first case one focuses on a single dynamical realization. The probability p_R of finding the system inside a coarse-grained region R of Γ-space is defined by the fraction of time t_R spent by the system inside that region during the (eventually infinite) total amount of time τ of its phase space trajectory: $p_R^t \equiv t_R/\tau$, where the superscript t stands for *time* definition. The second is achieved for instance by fixing a certain instant of time t^* and repeating the dynamical evolution up to t^*, under the same macroscopic (but different microscopic) initial conditions. Counting the number of times n_R the system is found in region R at time t^*, with respect to the (eventually infinite) total number of times n the calculation is performed, one defines $p_R^e \equiv n_R/n$, where the superscript e indicates *ensemble*.

For a typical N-body conservative Hamiltonian system (typical in the sense that it complies with the BG

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prescriptions) at fixed energy E_N (microcanonical setup), a standard introduction of the canonical ensemble is obtained defining the canonical system as composed by a subset of M interacting elements, with $1 \ll M \ll N$. The energy of the M elements satisfies $E_M \ll E_N$, and the interaction energy between the canonical system and the rest of the isolated system (thermal bath) is assumed to be much smaller than E_M. Under these circumstances, the probability p_j of finding the system in a M-microstate j is given by the BG equilibrium calculation $p_j \propto e^{-\beta E_j}$, where $\beta \equiv 1/T$ is the inverse temperature (without loss of generality, we set the Boltzmann constant $k_B \equiv 1$), and E_j is the energy of the microstate. A dynamical approach for the confirmation of this result must face the following numerical difficulty. The Γ-space is Md dimensional, d being the dimension of the single-particle phase space. If we implement a coarse-graining for example by making a partition of k intervals in each coordinate, the total number of (hyper)cells Ω_M is of order k^{Md}. Just to put some indicative numbers, with $k = 4$, $M = 100$ and $d = 2$ we get $\Omega_M \sim 4^{200} \sim 10^{120}$. We should hence implement a numerical integration of $2N(\gg 200)$ Hamilton equations with a total amount of time τ (or a total number of realizations n) much larger than 10^{120}, which is beyond what we can presently do numerically.

Nevertheless, we can proceed through an alternative path and, instead of focusing on the probability associated to a microstate, we could consider the probability of finding the canonical system with a given energy E_M. In this case the BG answer is

$$p(E_M) = \frac{\omega(E_M) e^{-\beta E_M}}{Z}, \tag{1}$$

where Z is the partition function and

$$\omega(E_M) = \int \prod_{i=1}^{M} (dp_i dq_i) \delta[E_M - H_M(p_i, q_i)] \tag{2}$$

is the phase-space density of states at energy E_M. As well known for a classical system, $\omega(E_M)$ does not depend on any particular thermal statistics, it only depends on the Hamiltonian of the system. In other words, we can calculate $\omega(E_M)$ by using *any* statistics, for example the BG one [11]. The density of states $\omega(E_M)$ can be analytically estimated through the thermodynamic relation linking the statistical entropy to the temperature: $\partial \ln \omega(E)/\partial E = \beta$. Integrating this relation we have that $\omega(E_M)$ is given through the caloric curve $T(E)$:

$$\frac{\omega(E_M)}{\omega(E_0)} = \exp\left[\int_{E_0}^{E_M} dE' \, \beta(E')\right], \tag{3}$$

where E_0 is the energy of the fundamental state. In brief, the Hamiltonian structure of the system defines the density of states as a function of the energy; once this relation is known it is sufficient to multiply $\omega(E_M)$ by the Boltzmann factor $e^{-\beta E_M}$ and to normalize, in order to obtain $p(E_M)$ for the whole spectrum of temperatures. Now, the dynamical computation of $p(E_M)$ is much easier than the one for p_j. All we have to do is to numerically integrate Hamilton equations and to calculate the value of the energy E_M for the canonical subset at each integration step. We can then coarse-grain the energy spectrum into bins of width ΔE_M and build up a normalized histogram of the occurrence of each of these bins. In analogy with the previous discussion,

$$p^{\,t}(E_M) \equiv \frac{t(E_M)}{\tau \, \Delta E_M} \;\text{ and }\; p^{\,e}(E_M) \equiv \frac{n(E_M)}{n \, \Delta E_M} \tag{4}$$

represent then the probability distribution of finding the canonical system with energy E_M, respectively using time and ensemble averages.

To illustrate this calculation, we consider next a specific class of analytically solvable nonlinear first-neighbor Hamiltonians,

$$H_N = K_N + V_N = \sum_{i=1}^{N} \left[\frac{p_i^2}{2} + V(q_{i+1} - q_i)\right], \tag{5}$$

with periodic boundary conditions ($q_{N+1} \equiv q_1$). As a first case we analyze a one-dimensional chain of rotors with $V(q_{i+1} - q_i) \equiv 1 - \cos(q_{i+1} - q_i)$, so that the canonical coordinates $q_i \in [0, 2\pi)$ and $p_i \in \mathbb{R}$ are respectively the angular coordinates and the angular momenta of the (unit inertial momenta) rotors. This Hamiltonian is an inertial version of the classical XY ferromagnetic spin model and constitutes a dynamical prototype for spin systems in statistical mechanics [5,7]. The model is nearly integrable for both low and high energies. The former regime is defined for $T < 0.05$ (specific energy $e < 0.05$) [5] and it is called strong coupling regime, for which the rotors constitute a set of oscillators almost linearly coupled. The latter is obtained say for $T > 10$ ($e > 6$) [5], where the rotors are almost free (weak coupling regime). For this model, dynamical deviation from BG statistics where detected both in the strong and in the weak coupling regimes. Since our main scope is to check our calculation scheme in standard situations, we will mainly concentrate in the intermediate energy range, and discuss partial disagreement that occurs at higher energies. The canonical partition function

$$Z_M = \int \prod_{i=1}^{M} (dp_i dq_i) \exp\left[-\beta H_M(p_i, q_i)\right], \tag{6}$$

gives, for this model, the specific free energy $f \equiv -\lim_{M\to\infty}[\ln Z_M/(M\beta)]$ (see. e.g., [5]):

$$f = -T\left[\frac{1}{2}\ln T + \ln I_0\left(\frac{1}{T}\right) + \ln 2\pi^{\frac{3}{2}}\right] + 1, \tag{7}$$

where $I_0(x)$ is the modified Bessel function of the first kind of order zero. Inversion of the relation $E(T) = F - T\partial F/\partial T$ furnishes the BG caloric curve $T(e)$, where $e \equiv \lim_{M\to\infty} E_M/M$. We then rescale the e-axis by a factor M and use the fact that the temperature is an intensive parameter to get $T(E_M)$. The integration in equation (3) finally gives $\omega(E_M)$ for any large-but-finite value

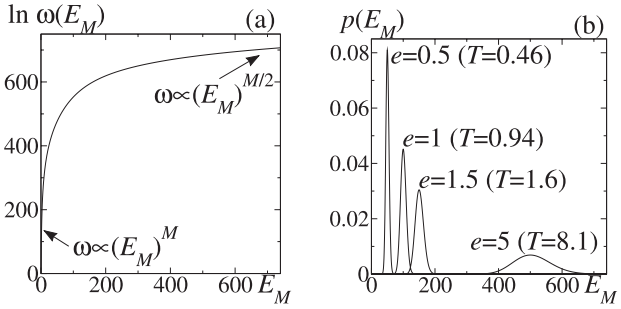

Fig. 1. BG analytical canonical prediction for the inertial XY-ferromagnetic rotors with $M = 100$. (a) Logarithm of the density of states $\omega_M(E_M)$. (b) $p(E_M) \equiv \omega_M(E_M)\exp(-E_M/T)/Z$, for different temperatures.

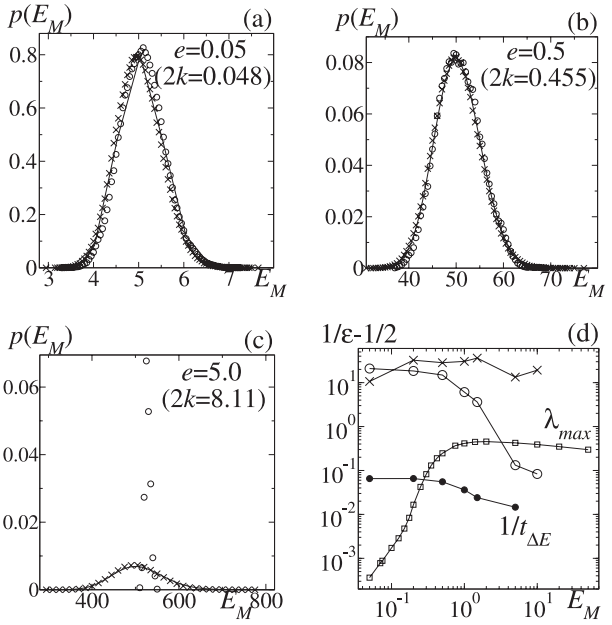

Fig. 2. (a–c) Comparison between the BG prediction $p(E_M)$ (full line), the ensemble dynamical average $p^e(E_M)$ (crosses), and the time dynamical average $p^t(E_M)$ (circles). $k \equiv K_M/M$ is the value of the specific kinetic energy. (d) Analysis of discrepancy between $p^e(E_M)$ and $p(E_M)$ (crosses), and $p^t(E_M)$ and $p(E_M)$ (empty circles). We also plot the largest Lyapunov coefficient λ_{max} (squares) and the inverse of the time-scale for a normal fluctuation $1/t_{\Delta E_M}$ (full circles). The lines are guides to the eye. See text for details.

of M. In Figure 1a we plot the logarithm of $\omega(E_M)$ for the first-neighbor rotors with $M = 100$ and Figure 1b displays BG $p(E_M)$ for different values of the temperature T (or of the specific energy e). We remark that, thanks to the elementary properties of the logarithmic function, it is possible to implement this calculation for quite large values of M, since one essentially deals with the exponents.

Because we are interested in very large values of τ and n, the dynamical integration of Hamilton equations has been performed using the 4th order symplectic Neri-Yoshida integrator [12] with an iteration parameter that assures an energy conservation $\Delta E_N/E_N \simeq 10^{-3}$ (a few runs with 10^{-5} showed that 10^{-3} is enough for our scopes). In particular, we checked that the energy fluctuations of the total system introduced by the finite precision of the integrator algorithm is order of magnitudes smaller than those that one would have in presence of a thermal coupling. An important point to perform an efficient calculation concerns the initial conditions, that must be close enough to equilibrium to avoid long transients. In this way we focus only on the equilibrium properties of the model, ruling out the possible presence of metastable or quasi-stationary states appearing with far-from-equilibrium initial conditions. Since the system does not display any phase transition for $T > 0$ but presents a tendency to clusterization at low temperatures, we have used a Maxwellian distribution for the angular momenta (with the appropriate temperature) and a set of l equidistant Gaussian distributions for the angles, each with the same variance appropriately calculated in order to yield the desired total energy E_N. In our calculation it was sufficient to use $l = 6$ for a fast enough relaxation to equilibrium in all our (microcanonical) setups. We have checked that this particular choice has no influence on the functional form of the equilibrium probability density functions: it is done to save computational time. Different close-to-equilibrium initial conditions eventually yield the same results. For all our results we have waited for 10^3 iteration steps before starting the measurements for a canonical system which is composed by a randomly chosen subset of M adjacent rotors.

In Figures 2a–2c we present a striking agreement between the BG analytical prediction for $p(E_M)$ (full line) and the dynamical estimation of $p^e(E_M)$ (crosses) for various order of magnitudes of the specific energy e with a setup $(M, N) = (10^2, 10^3)$ and a total number of realizations $n = 5 \times 10^6$. On the other hand, $p^t(E_M)$ (circles), calculated with a total number of iteration steps $\tau = 5 \times 10^7$, displays a good agreement with respect to the BG analytical distribution for intermediate energies, but starts to show large discrepancies when entering in the weak-coupling regime. In order to quantify this difference, we have defined the discrepancy $0 \leq \epsilon \leq 2$ between two distributions as the integral of the absolute value of the difference of the distributions. To allow for a comparison with the largest Lyapunov coefficient, in Figure 2d we plot the quantity $0 \leq 1/\epsilon - 1/2 \leq \infty$ which is zero for maximum discrepancy and infinite for perfect overlap of the distributions. While for ensemble averages $1/\epsilon - 1/2$ is large and almost constant with the energy, in the case of time averages such a quantity presents a dramatic decrease for large energies. In fact, we verified that the time necessary to have a typical energy fluctuation of the canonical subset ($\Delta E_M \sim E_M/\sqrt{M}$) grows with the energy (see full circles in Figure 2d, where we plot the inverse of this time), as a consequence of the fact that rotors are increasingly free (the potential is upper bounded). We point out that the

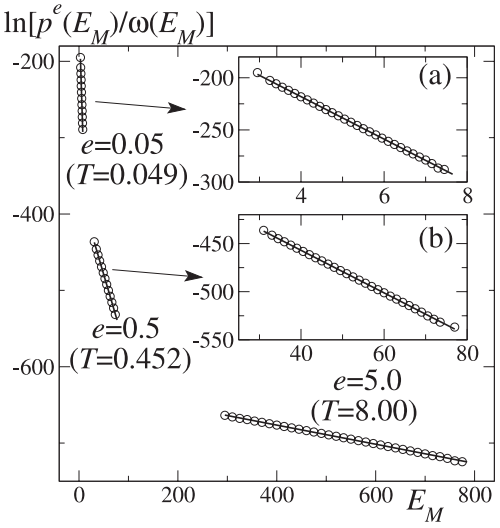

Fig. 3. Dynamical evidence of the Boltzmann factor. We plot $\ln[p^e(E_M)/\omega(E_M)]$ for the ensemble averages of Figure 2 (circles). T is the reciprocal of the slope of linear regressions (full lines) on the data. Insets (a) and (b) show a magnification of the results for $e = 0.05$ and $e = 0.5$ respectively.

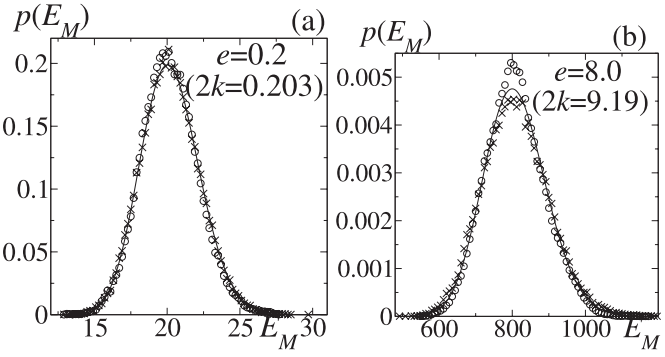

Fig. 4. Same as Figures 2a–2c for the FPU β-model. See text for details.

largest Lyapunov coefficient (squares in Fig. 2d) does not display a significant correlation with the time characterizing relaxation of $p^t(E_M)$ (circles in Figs. 2a–2c) towards the BG distribution $p(E_M)$ (see also [5] for a discussion of this point). This means that for the present system the positivity of the largest Lyapunov coefficient is a measure of local chaos that does not imply relaxation to global chaos.

An important result is the coincidence between the value of the BG temperature T and twice the specific kinetic energy $k \equiv K_M/M$ within an error of at most 2%. We stress that the probability density functions shown in Figure 2 are obtained by means of first principles only and with complete independence from the BG theory, which we are checking. The concurrence between dynamics and the Boltzmann factor appears satisfactorily in the linear regressions of Figure 3, where we plot $\ln[p^{\,e}(E_M)/\omega(E_M)]$ for the ensemble averages of Figures 2a–2c. With other values of (M, N), namely (50, 500) and $(10^3, 10^4)$, the results were qualitatively the same.

We also obtained a confirmation of our results by implementing the same calculation scheme for the FPU β-model, defined by the potential $V(q_{i+1} - q_i) \equiv (q_{i+1} - q_i)^2/2 + 0.1(q_{i+1} - q_i)^4/4$ with $q_i \in \mathbb{R}$, again considering close-to-equilibrium initial conditions (see, e.g., [5] for the analytical canonical solution and for a discussion of initial conditions). Although it is known that the FPU model presents, in common with the rotors model, a very rich anomalous behavior at low energies [4,5], for our initial conditions and for the energy-range we tested we found that $p^t(E_M)$ is in good agreement with the BG prediction (Fig. 4).

In summary, we recall that using the standard BG formalism and common numerical techniques, we have introduced a new calculation that allows for a comparison between nonlinear Newtonian dynamics and canonical statistical mechanics. Implementing a standard setup we have in fact shown that the BG energy distribution in Γ-space coincides with the one that is obtained dynamically (integrating Hamilton equations for close-to-equilibrium initial conditions) when an ensemble average is executed. We have checked this conclusion for two paradigmatic first-neighbor nonlinear Hamiltonians. As a side result, this calculation provides a dynamical confirmation of the very well known relation between temperature and specific kinetic energy $k = T/2$ (for one-dimensional systems). With respect to finite-time dynamical averages, at moderate low energies we have found a confirmation of the BG predictions. For the XY-model at high energies, if the time-scale is not very large, finite-time averages disagree with ensemble averages as a consequence of an increase of the time-scale of typical energy fluctuations. The energy dependence of this discrepancy does not display correlation with that of the largest Lyapunov coefficient (see also [5]).

Finally, let us emphasize that what we have shown here is that equilibrium thermal statistics descends from (finite-precision) mechanics, even for a system in contact with a thermostat (usually discussed through Monte Carlo or Nosé-Hoover techniques, which do not deduce the equilibrium distribution but impose it [8]). Indeed, this is the significance of Figures 2a–2c and 4, where circles and crosses have been obtained from Newton law, whereas full lines come from the BG theory. Equivalently, if we recall that the density of states is a purely mechanical concept, the same conclusion is shown in Figure 3. The present calculation scheme provides an insight onto the basic question of the dynamical foundation of statistical mechanics [1,2,5–7], and may serve as a useful tool in the discussion of complex situations (see e.g., [9]) where dynamical discrepancies with the BG theory have been found.

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