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On the non-Boltzmannian nature of quasi-stationary states in long-range interacting systems

Constantino Tsallis[a], Andrea Rapisarda[b,*], Alessandro Pluchino[b], Ernesto P. Borges[c]

[a]*Centro Brasileiro de Pesquisas Fisicas, Rua Xavier Sigaud 150, 22290 180 Rio de Janeiro, RJ, Brazil*
[b]*Dipartimento di Fisica e Astronomia, Universitá di Catania and INFN sezione di Catania, Via S. Sofia 64, I 95123 Catania, Italy*
[c]*Escola Politecnica, Universidade Federal da Bahia, Rua Aristides Novis 2, 40210 630 Salvador, BA, Brazil*

Abstract

We discuss the non-Boltzmannian nature of quasi-stationary states in the Hamiltonian mean field (HMF) model, a paradigmatic model for long-range interacting classical many-body systems. We present a theorem excluding the Boltzmann–Gibbs exponential weight in Gibbs Γ-space of microscopic configurations, and comment a paper recently published by Baldovin and Orlandini [Phys. Rev. Lett. 96 (2006) 240602]. On the basis of the points here discussed, the ongoing debate on the possible application, within appropriate limits, of the generalized q-statistics to long-range Hamiltonian systems remains open.
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1. Introduction

The Hamiltonian mean field (HMF) model is a paradigmatic *toy model* for long-range interacting Hamiltonian systems [1]. In a recent paper [2], Baldovin and Orlandini presented new molecular dynamics numerical results for the HMF model in contact with a thermal bath. They conclude that the energy distribution in its *quasi-stationary state* (QSS) is of the Boltzmann–Gibbs (BG) form. In view of their own numerical results, we cannot agree with their conclusions. In this paper we present three points that are relevant for the interesting questions raised in Ref. [2].

*Corresponding author. Tel.: +39 095 3785408; fax: +39 095 3785231.
E-mail addresses: tsallis@cbpf.br (C. Tsallis), andrea.rapisarda@ct.infn.it (A. Rapisarda), alessandro.pluchino@ct.infn.it (A. Pluchino), ernesto@ufba.br (E.P. Borges).

2. Discussion

In what follows we present three important points regarding the non-Boltzmannian nature of the QSS in the HMF model.

2.1. The nature of the QSS in the canonical setup presents differences with that in the microcanonical setup

It has already been demonstrated that, in the microcanonical ensemble, the anomalous dynamics (concerning the presence of a glassy phase, hierarchical structures, velocity correlations, aging, vanishing Lyapunov exponents, etc.), and therefore the statistical description of the QSS, is strongly dependent on the initial conditions [3–5]. *A fortiori*, it is thus not at all justified to *extrapolate* the conclusions for the canonical QSS studied in Refs. [2,6] to the microcanonical ones. Although the authors themselves state in Ref. [6] that the canonical QSSs are only *reminiscent* of the microcanonical ones (in fact they differ in the lifetimes, the relaxation times, and, most probably, also in the correlations), they neglect it in Ref. [2]. In order to stress this point, in Fig. 1(a) we plot three numerical simulations in the microcanonical ensemble (averaged over 10 events) for energy density $U = E/N = 0.69$, size $N = 5000$ and for different initial magnetizations M_0. Water-bag initial conditions were used [3]. Following the Central Limit Theorem aspects recently revealed in Ref. [7], we illustrate in Fig. 1(b) the non-Boltzmannian nature of this QSS regime by studying the probability density functions (pdfs) of the stochastic values y defined as follows: $y_j = \sum_{i=1}^{n} l_j(i)$, for $j = 1, 2, \ldots, L$, where $l_j(i)$ are the momenta of the jth-rotator taken at fixed intervals of time i inside the QSS regime. We considered $L = 5000$ and $n = 500$ intervals, one every 10 units of time. The length of the time interval was varied as shown in Fig. 1(c) for the initial magnetization $M_0 = 0.8$ without any relevant change in the pdfs. An average over 10 events was also considered, in order to have 50 000 values for the y variables for each pdf. In case of no global correlations, as one would expect at equilibrium, the resulting pdf should be a Gaussian. As Fig. 1(b) shows, in our case, the Gaussian distribution does *not* occur. In fact we have pdfs whose shape depends on the initial magnetization M_0 and the central region (up to a few mean standard deviations) of most of them is well fitted by q-Gaussians. In particular for $M_0 = 0.8$ we get a q-Gaussian with $q = 1.75$ as in Ref. [7]. We do not think that this is a universal value in this case, since we do not have a strictly zero largest Lyapunov exponent as in Ref. [7]. For the HMF model, the latter goes to zero as $1/N^{1/9}$ in the QSS regime [4], while it remains finite at equilibrium at this energy value. We normalized the data to the corresponding standard deviations in order to compare them. This comparison clearly shows that strong correlations are present in our case indicating a deviation from the standard Central Limit Theorem, as in Ref. [7]. A more complete study on this point will be reported elsewhere. In any case the arguments discussed in Ref. [2], and in particular in Fig. 1(a) of Ref. [2], do not apply to the microcanonical QSS. The effects become increasingly stronger when the initial magnetization gets closer and closer to 1.

2.2. The energy distribution of the QSS cannot be of the BG exponential form

As clearly seen in Fig. 1(a) of Ref. [2], the one-body momentum distribution is *non*-Gaussian. This excludes the BG exponential form as the energy distribution in full phase space Γ, as proved (*by reduction to the absurd*) in what follows. This analytical fact can easily be enlarged to n-dimensional rotators, $n > 1$: $n = 1, 2, d$, and ∞ correspond respectively to the Ising, *XY*, Heisenberg, and spherical models. In what follows we illustrate it, however, for $n = 2$, the case addressed in Ref. [2].

Theorem. *Let $H = K + V$ be the Hamiltonian of a M-body classical system, where the kinetic energy is $K = \sum_{i=1}^{M}(l_i^2/2I), I > 0$, and the potential energy V contains arbitrary* integrable *one-body, two-body, three-body, ... terms, concerning (isotropic or anisotropic) rotators localized at a (irregular or regular d-dimensional) lattice (each term might be characterized by a distance-dependent coupling constant, which can be summable or not in the $M \to \infty$ limit). And let the one-momentum marginal probability distribution*

$$p(l_1) \equiv \int dl_2 \, dl_3 \ldots dl_M \, d\theta_1 \, d\theta_2 \ldots d\theta_M \, p(l_1, l_2, \ldots, l_M, \theta_1, \theta_2, \ldots, \theta_M)$$
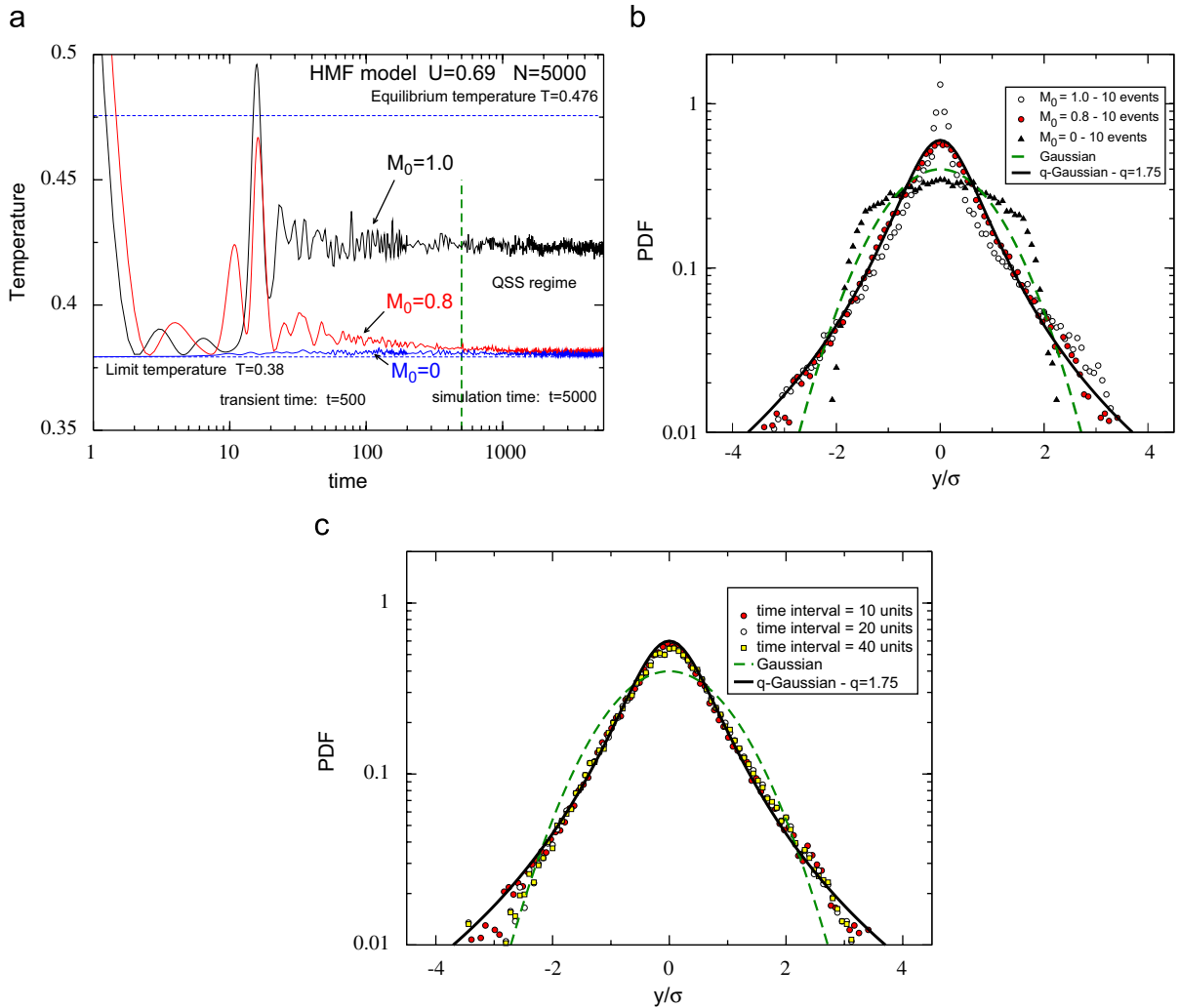
Fig. 1. (a) The temperature as a function of time for the HMF model at energy density $U = 0.69$ and size $N = 5000$ obtained for three initial magnetization values, respectively, $M_0 = 1, 0.8, 0$, and averaged over 10 events. The system remains trapped in a QSS at a temperature value lower than the equilibrium one. The latter is drawn together with the limit temperature at this energy [3]. (b) The pdf of stochastic values y obtained by summing rotators momenta in the QSS regime illustrated in panel (a), see text. Different initial magnetizations M_0 are reported. A Gaussian (dashed curve) and a q-Gaussian with $q = 1.75$ (full curve) are also reported for comparison. (c) For the initial magnetization $M_0 = 0.8$, we plot the pdfs obtained changing the time interval for recording the momenta of the rotators. No significant change is observed. See text for further details.

associated with the joint distribution

$$p(l_1, l_2, \ldots, l_M, \theta_1, \theta_2, \ldots, \theta_M)$$

be non-Gaussian. *Then*

$$p(l_1, l_2, \ldots, l_M, \theta_1, \theta_2, \ldots, \theta_M)$$

cannot *be proportional to*

$$e^{-\beta H(l_1, l_2, \ldots, l_M, \theta_1, \theta_2, \ldots, \theta_M)}, \quad \beta > 0.$$

Proof. Assume that

$$p(l_1, l_2, \ldots, l_M, \theta_1, \theta_2, \ldots, \theta_M) = \frac{e^{-\beta H}}{\int e^{-\beta H}},$$

then

$$
\begin{aligned}
p(l_1) &= \frac{\int dl_2\, dl_3 \ldots dl_M\, d\theta_1\, d\theta_2 \ldots d\theta_M\, e^{-\beta H}}{\int dl_1\, dl_2\, dl_3 \ldots dl_M\, d\theta_1\, d\theta_2 \ldots d\theta_M\, e^{-\beta H}} \\
&= \frac{\int dl_2\, dl_3 \ldots dl_M\, e^{-\beta K}}{\int dl_1\, dl_2\, dl_3 \ldots dl_M\, e^{-\beta K}} \frac{\int d\theta_1\, d\theta_2\, d\theta_3 \ldots d\theta_M\, e^{-\beta V}}{\int d\theta_1\, d\theta_2\, d\theta_3 \ldots d\theta_M\, e^{-\beta V}} = \frac{e^{-\beta l_1^2/2I} \prod_{i=2}^{M} \int dl_i\, e^{-\beta l_i^2/2I}}{\prod_{i=1}^{M} \int dl_i\, e^{-\beta l_i^2/2I}} \\
&= \frac{e^{-\beta l_1^2/2I}}{\int dl_1\, e^{-\beta l_1^2/2I}},
\end{aligned}
$$

which is a Gaussian, thus contradicting the hypothesis.　□

Hence, the Central Limit Theorem verification exhibited in Ref. [2] refers to a necessary but insufficient property.

2.3. The Baldovin–Orlandini results do not exclude the non-extensive statistical mechanics q-exponential form

Contrary to what is stated in Ref. [2], q-statistics [8] cannot be excluded on the basis of what they exhibit in their Fig. 3(d). Indeed, in Fig. 2 we plot the statistical weights corresponding to BG statistics (full circles), and to a typical illustration of non-extensive statistics ($q = 1.5$; solid line), for the size $M = 1000$ example exhibited in Fig. 3(d) of Ref. [2]. We used nearly the same number of points of Fig. 3(d) in the interval $E_{HMF} \in [664, 720]$, which covers 4% around its central value 692. The linear correlation is $r = -0.99996$ ($r = -0.99997$ in Ref. [2] for a similar analysis). The remarkable closeness of the $q = 1$ and 1.5 examples comes
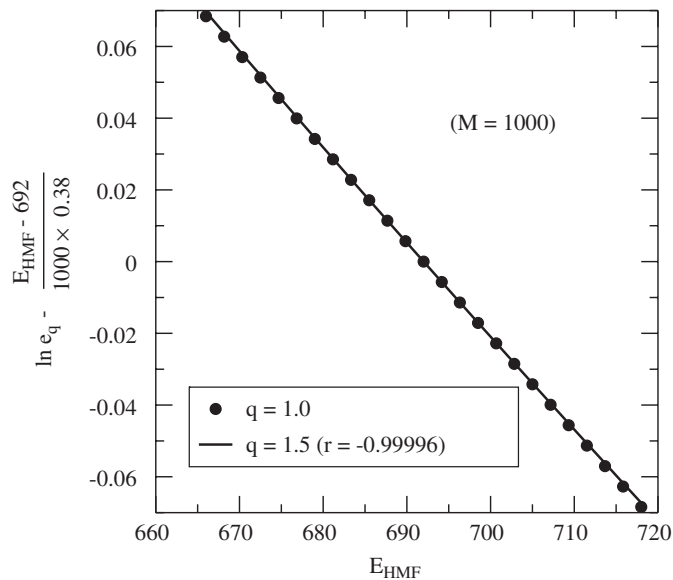

Fig. 2. The statistical weights corresponding to BG statistics (full circles), and to a typical illustration of non-extensive statistics ($q = 1.5$; solid line), for the size $M = 1000$ example exhibited in Fig. 3) of Ref. [2], see text for details.

from two facts. The first one is that

$$e_q^x \equiv [1 + (1-q)x]^{1/(1-q)} = e^x[1 + \tfrac{1}{2}(q-1)x^2 + \cdots] \quad \text{for } x \to 0.$$

Notice the absence of the term *linear* in x in the latter expression. While the second one is that the spreading around the central value 692 is very small. Notice also that we rescaled the temperature $T = 0.38$ by a factor M, which corresponds to multiplying Hamiltonian (1) of Ref. [2] by M and then rescaling time in the kinetic energy (see Ref. [9]). This makes the *microscopic* two-body interaction of the model *independent* from the *macroscopic* quantity M, as desirable. Consider also that, in the q-statistical weight of Fig. 2, we have subtracted from E_{HMF} a characteristic macroscopic energy, namely the central value 692. This procedure is long known to be mandatory (see Ref. [10]) for any $q \neq 1$ in order to preserve the invariance of probabilities with regard to an uniform shift of the energy scale, i.e., in order to preserve the freedom of the choice of the zero of energies. Such subtraction, although allowed for all values of q, is clearly *not* mandatory for the BG exponential weight ($q = 1$), since the desired invariance is anyhow guaranteed by the fact that the exponential of a sum factorizes into the product of exponentials (whereas the q-exponential of a sum does *not* factorize into the product of q-exponentials if $q \neq 1$).

3. Conclusions

On the basis of the points here discussed, the results presented in Ref. [2] should be considered with extreme care, and by no means they close the ongoing debate on the possible application, in appropriate limits, of generalized q-statistics to long-range Hamiltonian systems. Finally, let us mention for completeness that neither the arguments recently advanced in Ref. [11] exclude the possible application of q-statistics, especially for initial magnetization close to 1, but this point is beyond the scope of the present paper and it will be discussed elsewhere.

Acknowledgments

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