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A closer look at the indications of q-generalized Central Limit Theorem behavior in quasi-stationary states of the HMF model

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Abstract

We give a closer look at the Central Limit Theorem (CLT) behavior in quasi-stationary states of the Hamiltonian Mean Field model, a paradigmatic one for long-range-interacting classical many-body systems. We present new calculations which show that, following their time evolution, we can observe and classify three kinds of long-standing quasi-stationary states (QSS) with different correlations. The frequency of occurrence of each class depends on the size of the system. The different microscopic nature of the QSS leads to different dynamical correlations and therefore to different results for the observed CLT behavior.

Keywords: Metastability in Hamiltonian dynamics; Long-range interactions; Central Limit Theorem behavior; Nonextensive statistical mechanics

1. Introduction

Very recently there has been a lot of interest in generalizations of the Central Limit Theorem (CLT) [1–3] and on their possible (strict or numerically approximate) application to systems with long-range correlations [4,5], at the edge-of-chaos [6], nonlinear dynamical systems the maximal Lyapunov exponent of which is either exactly zero or tends to vanish in the thermodynamic limit (increasingly large systems) [7], hindering in this way mixing and thus the application of standard statistical mechanics. A possible application of nonextensive statistical mechanics [8,9] has been advocated in these cases. Along this line we discuss in the present paper a detailed study of a paradigmatic *toy model* for long-range interacting Hamiltonian systems [10–16], i.e. the Hamiltonian Mean Field (HMF) model which has been intensively studied in the last years. In a recent article [17], we presented molecular dynamics numerical results for the HMF model showing three kinds of quasi-stationary states (QSS) starting from the same water-bag initial condition with unitary magnetization ($M_0 = 1$). In the following we present how the applicability of the standard or q-generalized CLT is influenced by the different microscopic dynamics observed in the three classes of QSS. In general, averaging over the three classes can be misleading. Indeed, the frequency of appearance of each of these classes depends on the size of the system under investigation, and there is no clear evidence that a predominant class exists.

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2. Quasi-stationary behavior in the HMF model

The HMF model consists of N fully-coupled classical inertial XY spins (rotors) $\vec{s}_i = (\cos\ \theta_i, \sin\ \theta_i), i = 1, \ldots, N$, with unitary module and mass [10]. One can also think of these spins as rotating particles on the unit circle. The Hamiltonian is given by

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

where θ_i ($0 < \theta_i \leq 2\pi$) is the angle and p_i the conjugate variable representing the rotational velocity of spin i.

At equilibrium the model can be solved exactly and the solution predicts a second-order phase transition from a high-temperature paramagnetic phase to a low-temperature ferromagnetic one [10]. The transition occurs at the critical temperature $T_c = 0.5$ which corresponds to a critical energy per particle $U_c = E_c/N = 0.75$. The order parameter is the modulus of the *average magnetization* per spin defined as $M = (1/N)|\sum_{i=1}^{N} \vec{s}_i|$. Above T_c, the spins are homogeneously distributed on the circle so that $M \sim 0$, while below T_c, most spins are aligned, i.e. rotors are trapped in a single cluster, and $M \neq 0$. The out-of-equilibrium dynamics of the model presents very interesting dynamical anomalies. For energy densities $U \in [0.5, 0.75]$, special classes of initial conditions such as those called *water-bag*, characterized by an initial magnetization $0 \leq M_0 \leq 1$ and uniform distribution of the momenta, drive the system, after a violent relaxation, towards metastable QSS. The latter slowly decay towards equilibrium with a lifetime which diverges like a power of the system size N [10]. Along the QSS regime, in the microcanonical ensemble, the dynamics exhibits a glassy behavior, hierarchical structures, velocity correlations, aging, vanishing Lyapunov exponents, etc., and the statistical description of the QSS is strongly dependent on the initial conditions [11–13]. However, even for the same type of initial conditions, we have observed different dynamical behaviors [17]. In particular we have found three typical classes of events, as illustrated in Fig. 1. Here we plot the temperature of the system (defined as twice the average kinetic energy per particle) versus time. We focused on a system with size $N = 20\,000$, the energy per particle being $U = 0.69$, for which anomalies are more evident. Initial conditions were chosen to be of the water-bag kind, with initial magnetization equal to unity ($M_0 = 1$). For details about the accuracy of the calculations and the integration algorithm adopted see Ref. [12]. Only single events are plotted in Fig. 1, each one representative of a given class. One immediately realizes that there are two extreme events (which we indicated with 1 and 3) and an intermediate one (indicated as 2) which stays close to event 1 at the beginning, but collapses towards the plateau of the event 3 after some time. The relative frequency of occurrence of these three classes of events is illustrated in Fig. 2 as a function of the size N of the system. A total of 20 realizations for each N was considered. It is important to note that the event of class 3 shown in Fig. 1, and all the events of class 3 in general, are very similar to the QSS obtained for initial conditions with zero initial magnetization ($M_0 = 0$), which are almost homogeneous and have very small correlations [12]. In this case a Lynden–Bell kind of approach, or one based on the Vlasov equation has been applied [15]. Therefore, due to the different nature of these QSS, which have in general different microscopic correlations, one could expect a different result for the central limit theorem behavior shown in Refs. [16,18,19].

3. Discussion of numerical results for the CLT

In this section, following the prescription of the CLT and the procedure adopted in Refs. [16,18,19], we construct probability density functions (pdf) of quantities expressed as a finite sum of stochastic variables and we select these variables along the deterministic time evolutions of the N rotors. More formally, we study the pdf of the quantity y defined as

$$y_i = \frac{1}{\sqrt{n}} \sum_{k=1}^{n} p_i(k) \quad \text{for } i = 1, 2, \ldots, N, \tag{2}$$

where $p_i(k)$, with $k = 1, 2, \ldots, n$, are the rotational velocities of the ith rotor taken at fixed intervals of time δ along the same trajectory obtained integrating the HMF equations of motions. The product $\delta \times n$ gives the total simulation time over which the sum of Eq. (2) is calculated. As stressed in Ref. [18], the variables y's are also proportional to the *time average* of the velocities along the single rotor trajectories (in fact the $1/\sqrt{n}$ scaling is not necessary, and has been adopted just to conform to usage).