Nonergodicity and central-limit behavior for long-range Hamiltonians

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received 27 June 2007; accepted in final form 1 September 2007
published online 21 September 2007

PACS 64.60.My – Metastable phases
PACS 89.75.-k – Complex systems

Abstract – We present a molecular dynamics test of the Central-Limit Theorem (CLT) in a paradigmatic long-range-interacting many-body classical Hamiltonian system, the HMF model. We calculate sums of velocities at equidistant times along deterministic trajectories for different sizes and energy densities. We show that, when the system is in a chaotic regime (specifically, at thermal equilibrium), ergodicity is essentially verified, and the PDFs of the sums appear to be Gaussians, consistently with the standard CLT. When the system is, instead, only weakly chaotic (specifically, along longstanding metastable Quasi-Stationary States), nonergodicity (i.e., discrepant ensemble and time averages) is observed, and robust \( q \)-Gaussian attractors emerge, consistently with recently proved generalizations of the CLT.

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Introduction. – During recent years there has been an increasing interest in generalizations of the Central-Limit Theorem (CLT). This theorem — so called because of its central position in theory of probabilities — has ubiquitous and important applications in several fields. It essentially states that a (conveniently scaled) sum of \( n \to \infty \) independent (or nearly independent) random variables with finite variance has a Gaussian distribution. Understandingly, this theorem is not applicable to those complex systems where long-range correlations are the rule, such as those addressed by nonextensive statistical mechanics [1,2]. Therefore, several papers [3–10] have recently discussed extensions of the CLT and their corresponding attractors. In this paper, following [5,6], we present several numerical simulations for a long-range Hamiltonian system, namely the Hamiltonian Mean-Field (HMF) model. This model is a paradigmatic one for classical Hamiltonian systems with long-range interactions which has been intensively studied in the last decade (see, for example, [6,11–21], and references therein). In [5] it was shown that the probability density of rescaled sums of iterates of deterministic dynamical systems (e.g., the logistic map) at the edge of chaos (where the Lyapunov exponent vanishes) violates the CLT. Here we study rescaled sums of velocities considered along deterministic trajectories in the HMF model. It is well known that, in this model, a wide class of out-of-equilibrium initial conditions induce a violent relaxation followed by a metastable regime characterized by nearly vanishing (strictly vanishing in the thermodynamic limit) Lyapunov exponents, and glassy dynamics [14–16]. We exhibit that correlations and nonergodicity created along these Quasi-Stationary States (QSS) can be so strong that, when summing the velocities calculated during the deterministic trajectories of single rotors at fixed intervals of time, the standard CLT is no longer applicable. In fact, along the QSS, \( q \)-Gaussian PDFs emerge as attractors instead of simple Gaussian PDFs, consistently with the recently advanced \( q \)-generalized CLT [4,5,9], and ensemble averages are different from time averages.

Numerical simulations. – The HMF model describes a system of \( N \) fully-coupled classical inertial \( XY \) spins (rotors) \( \vec{\mathbf{r}}_i = (\cos \theta_i, \sin \theta_i) \), \( i = 1, \ldots, N \), with unitary module and mass [11,12]. These spins can also be thought of as particles rotating on the unit circle. The Hamiltonian is given by

\[
H = \sum_{i=1}^{N} \frac{p_i^2}{2} + \frac{1}{2N} \sum_{i,j=1}^{N} \left[ 1 - \cos (\theta_i - \theta_j) \right],
\]
where $\theta_i$ ($0 < \theta_i \leq 2\pi$) is the angle and $p_i$ the conjugate variable representing the rotational velocity of spin $i$.

The equilibrium solution of the model in the canonical ensemble predicts a second-order phase transition from a high-temperature paramagnetic phase to a low-temperature ferromagnetic one [11]. The critical temperature is $T_c = 0.5$ and corresponds to a critical energy per particle $U_c = E_c/N = 0.75$. The order parameter of this phase transition is the modulus of the magnetization per spin defined as: $M = (1/N) \sum_{i=1}^{N} |\vec{S}_i|$. Above $T_c$, the spins point to different directions and $M \sim 0$. Below $T_c$, most spins are aligned (the rotators are trapped in a single cluster) and $M \neq 0$. The out-of-equilibrium dynamics of the model is also very interesting. In a range of energy densities between $U \in [0.5, 0.75]$, special initial conditions called water-bag (characterized by initial magnetization $M_0 = 1$ 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 $N$ [13–15].

In this section we simulate the dynamical evolution of several HMF systems with different sizes and at different energy densities, in order to explore their behavior either inside or outside the QSS regime. For each of them, following the prescription of the CLT, we construct probability density functions of quantities expressed as a finite sum of stochastic variables. But in this case, following the procedure adopted in ref. [5] for the logistic map, we will select these variables along the deterministic time evolutions of the $N$ rotors. More formally, we study the PdF of the quantity $y$ defined as

$$y_j = \frac{1}{\sqrt{n}} \sum_{i=1}^{n} (p_j(i) - \langle p_j \rangle) \quad \text{for} \quad j = 1, 2, \ldots, N,$$  

(2)

where $p_j(i)$, with $i = 1, 2, \ldots, n$, are the velocities of the $j$-th rotor taken at fixed intervals of time $\delta$ along the same trajectory. The latter are obtained integrating the HMF equations of motions (see [14] for details about these equations and the integration algorithm adopted). The quantity $\langle p_j \rangle = (1/n) \sum_{i=1}^{n} p_j(i)$ is the average of the $p_j(i)$’s over the single trajectory. The product $\delta \times n$ gives the total simulation time. Note that the variables $y$’s are proportional to the time average of the velocities along the single rotor trajectories. In the following we will distinguish this kind of average, i.e. time average, from the standard ensemble average, where the average of the velocities of the $N$ rotators is calculated at a given fixed time and over many different realizations of the dynamics. The latter can also be obtained from eq. (2) considering the $y$’s variables with $n = 1$ and $\langle p_j \rangle = 0$. In general, although the standard CLT predicts a Gaussian shape for sum of $n$ independent stochastic values strictly when $n \to \infty$, in practice a finite sum converges quite soon to the Gaussian shape and this, in the absence of correlations, is certainly true at least for the central part of the distribution [22]. Typically we will use in this section a sum of $n = 50$ values of velocities along the deterministic trajectories for each of the $N$ rotors of the HMF system, though larger values of $n$ were also considered.

In the following we will show that, if correlations among velocities are strong enough and the system is weakly chaotic, CLT predictions are not verified and, consistently with recent generalizations of the CLT, $q$-Gaussians appear [3–5]. The latter are a generalization of Gaussians which emerge in the context of nonextensive statistical mechanics [1,2] and are defined as

$$G_q(x) = A(1 - (1 - q)x^2)^{1/1-q},$$  

(3)

being $q$ the so-called entropic index (for $q = 1$ one recovers the usual Gaussian), $\beta$ another suitable parameter (characterizing the width of the distribution) and $A$ a normalization constant (see also ref. [10] for a simple and general way to generate them). In particular we will show in this section that:

i) \textit{at equilibrium}, when correlations are weak and the system is strongly chaotic (hence ergodic) standard CLT is verified, and time average coincides with ensemble average (both corresponding PdFs are Gaussians, either in the limit $n \to \infty$ or $\delta \to \infty$);

ii) \textit{in the QSS regime}, where velocities are strongly correlated and the system is weakly chaotic and nonergodic, the standard CLT is no longer applicable, and $q$-Gaussian attractors replace the Gaussian ones; in this regime ensemble averages do not agree with time averages.

For all the present simulations, water-bag initial conditions with initial magnetization $M_0 = 1$, usually referred as M1, will be used. In general, several different realizations of the initial conditions will be performed also for the time average PdFs case, but only in order to have a good statistics for small values of $N$ (for $N = 50000$, on the contrary, only one realization has been used: see fig. 7(b)). Finally, to allow a correct comparison with standard Gaussians (represented as dashed lines in all the figures) and $q$-Gaussians (represented as full lines), the PdF curves were always normalized to unit area and unit variance, by subtracting from the $y$’s their average $\langle y \rangle$ and dividing by the correspondent standard deviation $\sigma$ (hence, the traditional $\sqrt{n}$ scaling adopted in eq. (2) is in fact irrelevant).

The case $N = 100$. We start the discussion of the numerical simulations for the HMF model considering a size $N = 100$ and two different energy densities, $U = 0.4$ and $U = 0.69$. In the first case no QSS exist, while in the second case QSS characterize the out-of-equilibrium dynamics and correlations formed during the first part of the dynamics decay slowly while the system relaxes towards equilibrium [14,15]. With $N = 100$ this relaxation takes however a reasonable amount of time steps, thus one can easily study also the equilibrium regime. The situation is illustrated in fig. 1, where we show the time evolution of the temperature —calculated as twice the average
kinetic energy per particle— for the two energy densities considered, starting from $M_0 = 1$ initial conditions. As expected, QSS are clearly visible only in the case $U = 0.69$, although a small transient regime exists also for $U = 0.4$.

$N = 100$ and $U = 0.4$. Here we discuss numerical simulations for the HMF model with size $N = 100$ and $U = 0.4$. In this case it has been shown in the past that the equilibrium regime is reached quite fast and is characterized by a very chaotic dynamics [11,12].

In fig. 2 a transient time of 40000 units has been performed before the calculations, so that the equilibrium is fully reached (see fig. 1). In (a) we consider the ensemble average of the velocities, i.e. the $y$ variables defined as in (2) with $n = 1$, at $t = 40000$ and taking 1000 different realizations of the initial conditions (events). The Pdf compares very well with the Gaussian curve (dashed line), as expected at equilibrium. On the other hand, we consider in (b), (c) and (d) the Pdfs for the variable $y$ with $n = 50$ and with different time intervals $\delta$ over an increasing simulation time at equilibrium. As previously explained, this procedure corresponds to performing a time average along the trajectory for all the rotors of the system. In this case only the central part of the curve exhibits a Gaussian shape. On the other hand, Pdfs have long fat tails which can be very well reproduced with $q$-Gaussians (full lines). If one increases the time interval $\delta$ going from $\delta = 100$ (b), to $\delta = 200$ (c) and finally to $\delta = 1000$ (d), the tails tend to disappear, the entropic index $q$ of the $q$-Gaussians decreases from $q = 1.45 \pm 0.05$ towards $q = 1$ and the Pdf tends to the standard Gaussian. This means that, as expected, summed velocities are less and less correlated as $\delta$ increases [see also ref. [5]] and therefore the assumptions of the CLT are satisfied as well as its prediction. Notice that $n = 50$ terms and a time interval $\delta = 1000$ are sufficiently large to reach a Gaussian-shaped Pdf. This situation reminds similar observations in the analysis of returns in financial markets [22], or in turbulence [23].

$N = 100$ and $U = 0.69$. Let us to consider now numerical simulations for the HMF model with size...
plateaux, for \( N = 100 \) it is not possible to use greater values of \( \delta \) or \( n \) in the numerical calculations of the \( y \)'s.

In fig. 4 we repeat the previous simulations for \( N = 100 \) and \( U = 0.69 \), but adopting a transient time of 40000 steps, in order to study the behavior of the system after the QSS regime. The ensemble average Pdf (over 1000 realizations) of the single rotor velocities at the time \( t = 40000 \) is shown in (a) and indicates that equilibrium seems to have been reached. In fact the agreement with the standard Gaussian is almost perfect up to \( 10^{-4} \). In the other figures we plot the time average Pdfs for the variable \( y \) with \( n = 50 \) and for different time intervals \( \delta \), and for different realizations of the initial conditions. We are here always starting with \( U = 0.69 \), always starting with \( M1 \) initial conditions. We are here always starting with \( U = 0.69 \), always starting with \( M1 \) initial conditions. We are here always starting with \( U = 0.69 \), always starting with \( M1 \) initial conditions. We are here always starting with \( U = 0.69 \), always starting with \( M1 \) initial conditions.

The last statements are confirmed by panels (e) and (f) of fig. 4, where the effect of increasing the number \( n \) of summed velocities, keeping fixed the value of \( \delta \), has been investigated. More precisely \( \delta = 100 \) and \( n = 5000 \) in (e) and \( n = 50000 \) in (f). As expected, the increment of \( n \) makes the Pdf closer to the Gaussian, essentially because the total time over which the sum is considered increases (for \( n = 50000 \) we cover a simulation time of \( 5 \times 10^5 \)) and therefore correlations become asymptotically weaker and weaker, thus finally satisfying the prediction of the standard CLT.

In order to study in more details the ensemble-time inequivalence along the QSS regime in the next subsection we will increase the system size and discuss numerical results for \( N = 5000 \) and \( N = 50000 \).

For \( N = 5000 \) and \( N = 50000 \) at \( U = 0.69 \). In fig. 5 we show the time evolution of the temperature for the cases \( N = 5000 \) and \( N = 50000 \) at \( U = 0.69 \), always starting (as usual) from the M1 initial conditions. It is evident that, for both systems, the length of the QSS plateaux is very much greater than for \( N = 100 \).

We discuss first numerical simulations done inside the QSS for \( N = 5000 \) and \( U = 0.69 \).

In fig. 6 we show in (a) the ensemble average Pdf of velocities calculated over 1000 realizations at \( t = 100 \), i.e. at the beginning of the QSS regime. Its shape, constant...
along the entire QSS regime, is clearly not Gaussian and looks similar to that of fig. 3(a). In panels (b)-(d) we show the effect of increasing the number of velocity terms in the $y$ sum on the time average PDFs, calculated using a fixed value of $\delta = 100$. An average over 200 different realizations of the initial conditions was also considered in order to have good statistics. In this case only for $n = 1000$ a $q$-Gaussian, with $q = 1.45 \pm 0.05$, emerges. This is most likely due to the effective number of $n$ used but, consistently with fig. 6, to the fact that when choosing a large $n$ one is averaging over a larger interval of time and thus considers in a more appropriate way the average over the entire QSS regime. In any case the observed behavior goes in the opposite direction to the prescriptions of the standard CLT and to the trend shown in panels (e)-(f) of fig. 4. Indeed, increasing $n$, the PDF tails do not vanish but become more and more evident, thus supporting even further the claim about the existence of a non-Gaussian attractor for the nonergodic QSS regime of the HMF model. Moreover, the results of fig. 6 confirm the robustness of the $q$-Gaussian shape along the entire QSS regime and the inequivalence between ensemble and time averages in the metastable regime.

Let us now definitively demonstrate this inequivalence considering the case $N = 50000$ at $U = 0.69$. In fig. 7(a) we plot the ensemble average PDF of the velocities calculated (over 100 different realizations) at $t = 200$, i.e. at the beginning of the QSS regime, and after a very long transient, at $t = 250000$ (full circles). In panel (b) we plot the time average PDF for the normalized variable $y$ with $n = 5000$ and $\delta = 100$, after a transient of 200 time units and over a simulation time of 500000 units along the QSS. It is important to stress that in this case only one single realization of the initial conditions has been performed, realizing this way a pure time average. The shape of the time average PDF (b) results to be again a robust $q$-Gaussian, with $q = 1.4 \pm 0.05$, not only in the tails, but also in the center (see inset). The time average PDF is completely different from the ensemble average PDF of fig. 7(a) (that is also very robust over all the plateaus), thus confirming definitively the inequivalence between the two kinds of averages and the existence of a $q$-Gaussian attractor in the QSS regime of the HMF model. These results indicate that standard statistical mechanics based on the ergodic hypothesis cannot be applied in this case, while a generalized version, like the $q$-statistics [1,2] is likely more suitable [15].

**Conclusions.** The numerical simulations presented in this paper strongly indicate that dynamical correlations...
and ergodicity breaking, induced in the HMF model by the initial out-of-equilibrium violent relaxation, are present along the entire QSS metastable regime and decay very slowly even after it. In particular, considering finite sums of \( n \) correlated variables (velocities in this case) selected with a constant time interval \( \delta \) along single rotor trajectories, allowed us to study this phenomenon in detail. Indeed, we numerically showed that, in the weakly chaotic QSS regime, i) ensemble average and time average of velocities are inequivalent, hence the ergodic hypothesis is violated, ii) the standard CLT is violated, and iii) robust \( q \)-Gaussian attractors emerge. On the contrary, when no QSS exist, or at a very large time after equilibration, i.e., when the system is fully chaotic and ergodicity has been restored, the ensemble average of velocities results to be equivalent to the time average and one observes a convergence toward the standard Gaussian attractor. In this case, the predictions of CLT are satisfied, even if we have only considered a finite sum of stochastic variables. How fast this happens depends on the size \( N \), on the number \( n \) of terms summed in the \( y \)-variables and on the time interval \( \delta \) considered.

These results are consistent with the recent \( q \)-generalized forms of the CLT discussed in the literature [3–6, 9], and pose severe questions to the often adopted procedure of using ensemble averages instead of time averages. Nonergodicity in coupled many particle systems goes back to the famous FPU experiment [24], but in our case is due to the long-range nature of the interaction. More recently, nonergodicity was found in deterministic iterative systems exhibiting subdiffusion [25], but also in real experiments of shear flows, with results that were fitted with Lorentzians, i.e., \( q \)-Gaussians with \( q = 2 \) [26]. The whole scenario reminds that found for the leptokurtic returns Pdf in financial markets [22], or in turbulence [23], among many other systems, and could probably explain why \( q \)-Gaussians appear to be ubiquitous in complex systems. Finally, we would like to add that, although it is certainly nontrivial to prove analytically whether the attractor in the nonergodic QSS regime of the HMF model precisely is a \( q \)-Gaussian or not (analytical results, as well as numerical dangers, have been recently illustrated in ref. [8] for various models), our numerical simulations unambiguously provide a very strong indication towards the existence of a robust \( q \)-Gaussian attractor in the case considered. This opens new ways to the possible application of the \( q \)-generalized statistics in long-range Hamiltonian systems which will be explored in future papers.

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We thank M. IACONO MANNO for many technical discussions and help in the preparation of the scripts to run our codes on the GRID platform. The numerical calculations here presented were done within the TRIGRID project. AP and AR acknowledge financial support from the PRIN05-MIUR project “Dynamics and Thermodynamics of Systems with Long-Range Interactions”. CT acknowledges financial support from the Brazilian Agencies Pronex/MCT, CNPq and Faperj.

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