Lyapunov Instability and Finite Size Effects in a System with Long-Range Forces

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We study the largest Lyapunov exponent λ and the finite size effects of a system of N fully coupled classical particles, which shows a second order phase transition. Slightly below the critical energy density U_c, λ shows a peak which persists for very large N values ($N = 20\,000$). We show, both numerically and analytically, that chaoticity is strongly related to kinetic energy fluctuations. In the limit of small energy, λ goes to zero with an N-independent power law: $\lambda \sim \sqrt{U}$. In the continuum limit the system is integrable in the whole high temperature phase. More precisely, the behavior $\lambda \sim N^{-1/3}$ is found numerically for $U > U_c$ and justified on the basis of a random matrix approximation. [S0031-9007(97)05121-1]

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Recently, the interest in phase transitions occurring in finite-size systems and the study of the related dynamical features has stimulated the investigation of the so far obscure relation between macroscopic thermodynamical properties and microscopic dynamical ones. In this respect several papers appeared in the recent literature in various fields ranging from solid state physics [1–7] to lattice field theory [8] and nuclear physics [9,10], where there is presently a lively debate on multifragmentation phase transition [9–13]. The general expectation is that there is a close connection between the increase of fluctuations at a phase transition and a rapid increase of chaoticity at the microscopic level. In several pioneering papers a different behavior of the largest Lyapunov exponent (LLE) λ was found, according to the order of the transition [3,7,8,10]. In particular, a well pronounced peak in LLE has been found for second order phase transitions, while a sharp increase has been seen for first order phase transitions. In the former case some universal features have also been found, i.e., different systems show the same behavior when properly scaled [10]. In order to connect dynamical properties of systems of size N to bulk phase transitions, one has to explore the continuum limit $N \to \infty$. This, unfortunately, is not always possible due to computer time limitations, and has been done very rarely. In this Letter we present numerical investigations of the N dependence of the LLE up to $N = 20\,000$, a size for which we already observe a certain convergence to the continuum limit. We have investigated a toy model consisting of N classical particles moving on the unit circle and interacting via long-range forces [5]. This model shows a second order phase transition from a clustered phase to a homogeneous one at $U_c = (E/N)_c = 0.75$ [5]. Some results for the LLE of systems of moderate sizes ($N \approx 100$) have already been published [6]. The model, though relatively simple, has very general properties which enable us to explore the connections between phase transitions and dynamical features in finite systems. In particular, it could be relevant for nuclear multifragmentation where one has 100–200 particles interacting via long-range (nuclear and Coulomb) forces [11]. In this latter case a very similar caloric curve has been observed [12] and critical exponents have been measured experimentally [13].

The main results of the Letter are as follows: (a) The system is strongly chaotic just below the canonical transition energy U_c. The peak in $\lambda(U)$, found in [6] for small systems, persists as $N \to \infty$. (b) The increase of the LLE is related to the increase of kinetic energy fluctuations. (c) For $U \to 0$, $\lambda \to 0$ as U^α where the exponent is found to be $\alpha = 0.5$. Essentially no dependence on the system size is observed in this regime. A similar result was found for other systems [10,14]. (d) For $U > U_c$, $\lambda \to 0$ as $N^{-1/3}$. This behavior is explained by means of a random matrix approximation [15]. (e) Long-lived quasistationary states are found in the critical region. These states look very similar to those recently obtained in [16] and simulate a discrepancy between the canonical and the microcanonical ensemble very similar to that one found in Refs. [17] and more recently by other authors [18–21]. The fact that they appear near a second order phase transition might be related to critical slowing down.

The Hamiltonian we consider is the following:

$$H(q,p) = K + V\,, \tag{1}$$

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where

$$K = \sum_{i=1}^{N} \frac{1}{2} p_i^2, \qquad V = \frac{\epsilon}{2N} \sum_{i,j=1}^{N} [1 - \cos(q_i - q_j)] \tag{2}$$

are the kinetic and potential energies. The model describes the motion of N particles on the unit circle: each particle interacts with all the others. One can define a spin vector associated with each particle $\mathbf{m}_i = (\cos(q_i), \sin(q_i))$. The Hamiltonian then describes N classical spins similarly to the XY model, and a ferromagnetic or an antiferromagnetic behavior according to the positive or negative sign of ϵ, respectively [5]. In the following we will consider only the ferromagnetic (attractive) case and in particular $\epsilon = 1$. Results concerning the case $\epsilon = -1$ will be discussed elsewhere [22]. The order parameter is the magnetization $\mathbf{M}$, defined as $\mathbf{M} = \frac{1}{N} \sum_{i=1}^{N} \mathbf{m}_i = (M_x, M_y)$. It is convenient to rewrite the potential energy V as

$$V = \frac{N}{2} [1 - (M_x^2 + M_y^2)] = \frac{N}{2} (1 - M^2). \tag{3}$$

The equations of motion can then be written as

$$\frac{d}{dt} q_i = p_i, \qquad \frac{d}{dt} p_i = -\sin(q_i) M_x + \cos(q_i) M_y. \tag{4}$$

In order to calculate the LLE one must consider the limit

$$\lambda = \lim_{t\to\infty} \frac{1}{t} \ln \frac{d(t)}{d(0)}, \tag{5}$$

with $d(t) = \sqrt{\sum_{i=1}^{N} (\delta q_i)^2 + (\delta p_i)^2}$ the metric distance calculated from the infinitesimal displacements at time t. Therefore, one has to integrate along the reference orbit the linearized equations of motion

$$\frac{d}{dt} \delta q_i = \delta p_i, \qquad \frac{d}{dt} \delta p_i = -\sum_j \frac{\partial^2 V}{\partial q_i \partial q_j} \delta q_j, \tag{6}$$

where the diagonal and off-diagonal terms are

$$\frac{\partial^2 V}{\partial q_i^2} = \cos(q_i) M_x + \sin(q_i) M_y - \frac{1}{N}, \tag{7}$$

$$\frac{\partial^2 V}{\partial q_i \partial q_j} = -\frac{1}{N} \cos(q_i - q_j), \qquad i \neq j. \tag{8}$$

Expression (7) can also be written for convenience as

$$\frac{\partial^2 V}{\partial q_i^2} = M \cos(q_i - \Phi) - \frac{1}{N}, \tag{9}$$

where Φ is the phase of $\mathbf{M}$. We have integrated Eqs. (4) and (6) using fourth order symplectic algorithms [23] with a time step $\Delta t = 0.2$, adjusted to keep the error in energy conservation below $\frac{\Delta E}{E} = 10^{-5}$. The LLE was calculated by the standard method of Benettin *et al.* [24]. The average number of time steps in order to get a good convergence was of the order 10^6. We discuss in the following numerical results for system sizes in between $N = 100$ and $N = 20\,000$.

In Fig. 1 we plot the caloric curve, i.e., the temperature as a function of U, and we compare it with the theoretical canonical prediction [5] (in the inset we show the magnetization). Simulations performed starting from equilibrated initial data, which are Gaussian in momenta at the given canonical temperature, agree very well with canonical predictions. In fact, it is possible to solve the stationary Vlasov equation, which represents the system in the $N \to \infty$ limit, and obtain, under the factorization hypothesis for the probability distribution, $P(q,p) = f(q)g(p)$, and assuming $g(p)$ to be Gaussian

$$f(q) = \frac{1}{2\pi I_0(M/T)} \exp\left(\frac{M\cos(q - \Phi)}{T}\right),$$

$$g(p) = \frac{1}{\sqrt{2\pi T}} \exp\left(-\frac{p^2}{2T}\right).$$

In the latter, I_0 is the modified Bessel function of zero order, and M the canonical equilibrium magnetization. The equilibrium probability distributions found numerically are in fair agreement with these theoretical predictions. However, around the critical energy, relaxation to equilibrium depends in a very sensitive way on the initial conditions adopted. When starting with "water bag" initial conditions, i.e., a flat probability distribution of finite width centered around zero for $g(p)$, and putting all particle positions q_i at zero, we find quasistationary (long living) nonequilibrium states. These states have a lifetime which increases with N, and are therefore stationary in the

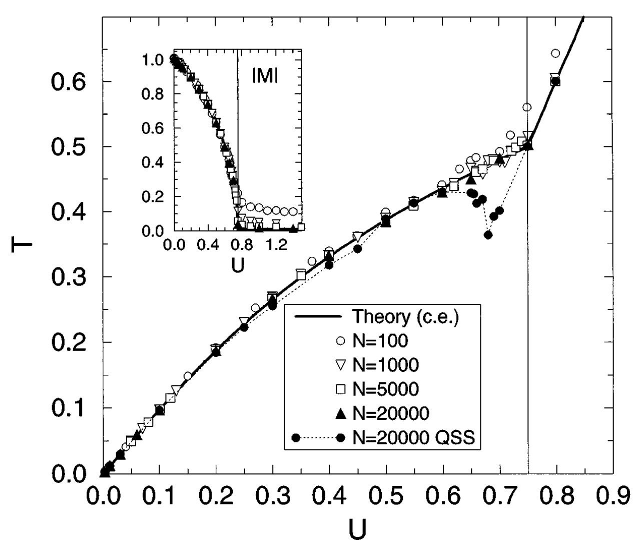

FIG. 1. Theoretical predictions in the canonical ensemble (full curve) for T vs U in comparison with numerical simulations (microcanonical ensemble) for $N = 100$, 1000, 5000, 20 000. The vertical line indicates the canonical critical energy $U_c = 0.75$. We plot also the microcanonical results for the quasistationary states (QSS) in the case $N = 20\,000$ (full circles). In the inset we show the magnetization vs U; again the full line is the canonical theoretical prediction.

continuum limit. We plot in Fig. 1 the caloric curve for these states in the case $N = 20\,000$. The points plotted are the result of an integration of 0.5×10^6 time steps. They are far from the equilibrium caloric curve around U_c, showing a region of negative specific heat and a continuation of the high temperature phase (linear T vs U relation) into the low temperature one. It is very intriguing that this out-of-equilibrium quasistationary states indicate a caloric curve very similar to that one found for first order phase transitions in Refs. [17–21]. In that case, however, the corresponding states are stationary also at finite N. The coexistence of different states in the continuum limit near the critical region is a purely microcanonical effect. It arises after the inversion of the $t \to \infty$ limit with the $N \to \infty$ one and could be considered as the typical signature of critical slowing down.

We have studied how finite-size effects influence the behavior of the LLE. In Fig. 2(a) we plot λ as a function of U for various N values. In the limit of very small and very large energies, the system is quasi-integrable, the Hamiltonian reducing to that of weakly coupled harmonic oscillators in the former case and to that of free rotators in the latter. In the region of weak chaos, for $U < 0.25$, the curve has a weak N dependence. Then λ changes abruptly and a region of strong chaos begins. In Ref. [5] it was observed that in between $U = 0.2$ and $U = 0.3$ a different dynamical regime sets in and particles start to evaporate from the main cluster. A similar regime was found in Ref. [10]. This behavior is also similar to that found in Ref. [3] at the solid-liquid transition. In this region of strong chaoticity we observe a pronounced peak already for $N = 100$ [6], which persists and becomes broader for $N = 20\,000$. The location of the peak is just below the critical energy at $U \sim 0.67$ and depends very weakly on N. At variance with what is suggested in Ref. [10] the peak does not grow with N.

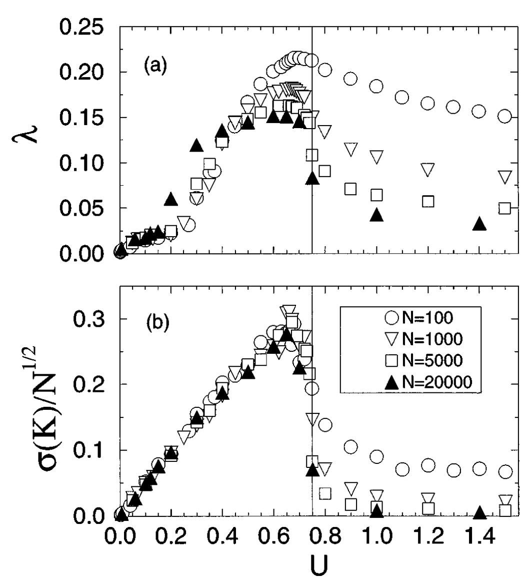

FIG. 2. (a) Numerical calculation of the largest Lyapunov exponent as a function of U for various system sizes: $N = 100$, 1000, 5000, and 20 000. (b) Kinetic energy fluctuations vs U. The vertical line indicates the canonical critical energy $U_c = 0.75$.

The standard deviation of the kinetic energy per particle $\sigma(K)/\sqrt{N}$ is plotted in Fig. 2(b). In the low energy region this quantity is in agreement with the canonical calculation $\sigma(K)/\sqrt{N} \propto U$. In correspondence to the Lyapunov peak, we observe also a sharp maximum of kinetic energy fluctuations, though finite-size effects are stronger for the LLE than for kinetic energy fluctuations. Thus, probes of chaotic behavior (LLE) and thermodynamical quantities (e.g., kinetic energy fluctuations) seem to be strongly related. We discuss here an intuitive interpretation of the relation between LLE and kinetic fluctuations. Each of the linearized equations (6) contains diagonal (7) and off-diagonal (8) terms. Since the off-diagonal terms result from a sum of incoherent terms, we can, in a first approximation, neglect them. The diagonal term is of order M^2 [see Eqs. (7) and (9)] and averages to $\langle M^2 \rangle = T + 1 - 2U$. If this term would be constant in time, the LLE would be zero. In fact, in this case one gets the equations for uncoupled harmonic oscillators. However, there are fluctuations, which give a nonzero coupling, whose standard deviation $\sigma(M^2)$ is related to the one of the kinetic energy $\sigma(M^2) = 2\sigma(K)/N$, considering the relationship $T = 2\langle K \rangle / N$. This indicates that the LLE is strictly related to kinetic energy fluctuations, but this relation is not simple and quite difficult to extract analytically (some indications in this sense were recently proposed also in Ref. [14]). In the low energy phase ($U < 0.25$) it is possible to work out a more stringent relation. In this case, the components of the tangent vector sum up incoherently to give for the average growth a term of the size $\sqrt{N}M^2$. It is then quite natural to associate the Lyapunov exponent to the inverse time scale given by the fluctuations of the average growth

$$\lambda^2 \sim \sigma(\sqrt{N} M^2) \sim 2 \frac{\sigma(K)}{\sqrt{N}} . \qquad (10)$$

Then, substituting the canonical estimation for kinetic energy fluctuations in Eq. (10), we get $\lambda \propto \sqrt{U}$. We have tested numerically this prediction [see Fig. 3(a)]. The $1/2$ power law at small U values is fully confirmed. We have checked numerically that off-diagonal terms (9) cannot be completely neglected—especially in the strong chaotic region. This latter important remark is also relevant for the application of a recently derived formula for the LLE [7] (see also [22,25]). A similar power law behavior was also found for other systems [26].

At variance with the N-independent behavior observed at small energy U, strong finite-size effects are present above U_c. In Fig. 3(b) we show, for $U > U_c$, how the LLE goes to zero as a function of N. We also plot in the same figure a calculation of the LLE using a random distribution of particle positions q_i on the circle in the equations for the tangent vector (6). The agreement

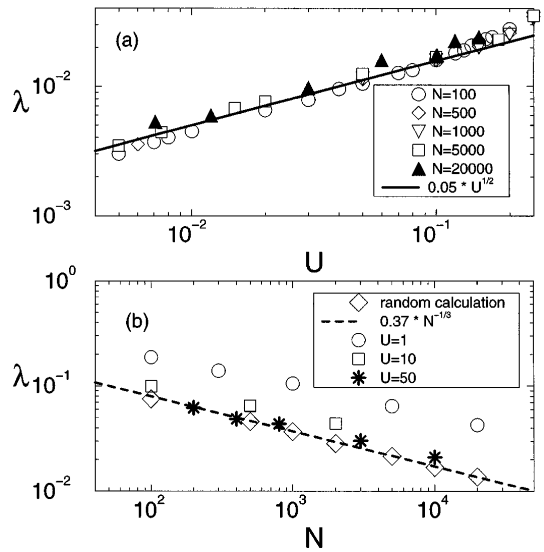

FIG. 3. Behavior of the largest Lyapunov exponent (LLE) for U much smaller (a) and much greater (b) than $U_c = 0.75$. In panel (a) LLE shows a universal law which can be fitted by a $1/2$ power law (full line). No N dependence is found. In (b) the LLE, for different N and energies, is compared with a calculation done with a random choice of particle positions (diamonds). The latter follow a power law with an exponent $-1/3$ (dashed line) (see text).

between the deterministic estimate and this random matrix calculation is very good. We find also that λ scales as $N^{-1/3}$, as indicated by the fit in Fig. 3(b). This can be explained by means of an analytical result obtained for the LLE of product of random matrices [15]. If the elements of the symplectic random matrix have zero mean, the LLE scales with the power $2/3$ of the perturbation. In our case, the latter condition is satisfied and the perturbation is the magnetization M. Since M scales as $N^{-1/2}$, we get the right scaling of λ with N. This proves that the system is integrable for $U \geq U_c$ as $N \to \infty$. This result is also confirmed by a recent, more sophisticated theoretical calculation [25].

In conclusion, we have investigated the Lyapunov instability for a system with long-range forces showing a second order phase transition. We found strong finite-size effects in the LLE. The LLE is peaked just below the critical energy, where kinetic fluctuations are maximal. Away from the transition region, the LLE goes to zero with universal scaling laws which can be explained by simple theoretical arguments. We think that this toy model contains all the main ingredients to understand the general behavior of the LLE in more realistic situations.

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