Further results on the equipartition threshold in large nonlinear Hamiltonian systems

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Numerical simulations show the existence of an ergodicity threshold in the Fermi-Pasta-Ulam α model. This feature is common to a large class of nonlinear Hamiltonian systems.

In a recent paper[1] on the Fermi-Pasta-Ulam (FPU) β model, we reported the numerical evidence of the existence of an equipartition threshold in the case of large number N of degrees of freedom. The main result is that equipartition of energy is obtained when the energy density $\epsilon = E/N$ of the system is greater than a critical value ϵ_c which does not depend on the number N of degrees of freedom.

The persistence of the equipartition threshold for large values of N and for a very long, though finite time is a relevant physical result independent of the lack of knowledge on the infinite-time behavior. An important point is to understand if the results that we found are related to the particular functional form of the Hamiltonian of the FPU β model or are "generic" properties of nonlinear Hamiltonian systems with many degrees of freedom. A partial answer to this question can be found in Ref. 1 where we studied a FPU β model perturbed by random quenched fluctuations of the nonlinear coupling constant, i.e., given by the Hamiltonian

$$H = \sum_{i=1}^{N} \left[\tfrac{1}{2}\pi_i^2 + \tfrac{1}{2}(\phi_i - \phi_{i+1})^2 + \tfrac{1}{4}\beta_i(\phi_i - \phi_{i+1})^4\right] , \qquad (1)$$

where ϕ_i are the values of the discretized field, π_i the canonically conjugated momenta, and β_i a random quenched variable of given mean value equal to β. We found that the two systems with $\beta_i \equiv \beta$ and β_i random have the same statistical behavior.

The existence of stochasticity thresholds in other nonlinear Hamiltonian systems (such as discretized versions of nonlinear Klein-Gordon equations,[2] one- and two-dimensional Lennard-Jones lattices[3,4] β FPU,[5] etc.) is strongly hinting for a model independence of the results reported in Ref. 1 even though equipartition and stochasticity thresholds do not coincide.

In the present paper we report the results of a numerical investigation of the Fermi-Pasta-Ulam α model. The aim of this study is to test the model independence of the main result of Ref. 1. The FPU α model is described by the following Hamiltonian:

$$H = \sum_{i=1}^{N} \left[\tfrac{1}{2}\pi_i^2 + \tfrac{1}{2}(\phi_i - \phi_{i+1})^2 + \frac{\alpha}{3}(\phi_i - \phi_{i+1})^3\right] , \qquad (2)$$

where the symbols have the same meaning as in Eq. (1). We adopted periodic boundary conditions putting $\phi_1 = \phi_{N+1}$, and as initial conditions $\pi_i(0) = \dot{\phi}_i(0) = 0$ and

$$\phi_i(0) = \sum_{n=1}^{N/2} \left[A_n(0)\cos\left(\frac{2\pi n i}{N}\right) + B_n(0)\sin\left(\frac{2\pi n i}{N}\right)\right] , \qquad (3)$$

with the assumption that the only nonvanishing coefficients are those $A_n(0), B_n(0)$ with $n \in [\bar{n}, \bar{n} + (\Delta n - 1)]$. The initial conditions for ϕ_i are chosen in such a way that at $t=0$ the energy of the system is uniformly distributed only among Δn normal modes whose wave numbers are $\bar{n}, \bar{n}+1, \ldots, \bar{n}+(\Delta n - 1)$. During the time evolution of the system the mode-mode coupling due to the nonlinear potential in the Hamiltonian (2) yields an energy sharing between all the normal modes. If in a finite time it happens that each normal mode reaches the same average energy value $\sim 2E_0/N$ (E_0 being the energy at $t=0$) then equipartition of energy sets in and the system displays an ergodic behavior (fully developed stochasticity).

We observed that for low-energy density values nonequilibrium (i.e., far from equipartition) stationary states can be reached from generic initial conditions,[1] each nonequilibrium state displaying different spectral properties according to the initial conditions. On the contrary, the equilibrium spectrum $W_n^{\mathrm{eq}} = \langle A_n^2 + B_n^2 \rangle_{\mathrm{eq}}$, where $\langle\ \rangle_{\mathrm{eq}}$ indicates the microcanonical average, is unique so that we introduced a spectral entropy as equipartition indicator. To define this spectral entropy we use at any time the following Fourier decomposition:

$$\phi_i(t) = \sum_{n=1}^{N/2} \left[A_n(t)\cos\left(\frac{2\pi n i}{N}\right) + B_n(t)\sin\left(\frac{2\pi n i}{N}\right)\right] , \qquad (4)$$

so that the energy of each normal mode is

$$E_n(t)=\frac{1}{2}\{\dot{A}_n^2(t)+\dot{B}_n^2(t)+\omega_n^2[A_n^2(t)+B_n^2(t)]\} \ , \quad (5)$$

where $\omega_n=2\sin(\pi n/N)$. Now define $p_n(t)$ as

$$p_n(t)=\langle E_n(t)\rangle_T \Big/ \sum_{k=1}^{N/2} \langle E_k(t)\rangle_T \ , \quad (6)$$

where $\langle E_n(t)\rangle_T$ is the harmonic energy of the nth mode averaged in time as follows:

$$\langle E_n(t)\rangle_T=\frac{1}{T}\int_{t-T/2}^{t+T/2} dt'\, E_n(t') \ , \quad (7)$$

where T is chosen to be much greater than the lowest period of the harmonic part of the system to smear out short-time-scale fluctuations. We define the following spectral entropy

$$\mathcal{H}(t)=-\sum_{n=1}^{N/2} p_n(t)\ln p_n(t) \geq 0 \quad (8)$$

to obtain for each asymptotic stationary state a pure number $\mathcal{H}(\infty)$ which measures the degree of equipartition of the system. In fact, the quantity of Eq. (8) is maximum when all the weights p_n have the same value, that is, when equipartition of energy among the normal modes takes place and $\mathcal{H}(\infty)=\mathcal{H}_{\max}=\ln(N/2)$; on the other hand, when the system is completely harmonic $\mathcal{H}(\infty)=\mathcal{H}(0)$ is found. As we discussed in Ref. 1, $\mathcal{H}(\infty)$ can also provide a rough estimate of the dimension of the subspace of phase space that is spanned by the phase trajectories of the system; in a sense the effective number of degrees of freedom ("active modes") can be estimated as

$$\mathcal{N}_{\rm eff} \simeq \exp[2\mathcal{H}(\infty)] \ . \quad (9)$$

As we are interested in the behavior of the system at fixed energy density values as a function of N, we introduce a normalized spectral entropy

$$\eta(t)=[\mathcal{H}_{\max}-\mathcal{H}(t)]/[\mathcal{H}_{\max}-\mathcal{H}(0)] \ , \quad (10)$$

which no longer suffers the N dependence of the maximum value of $\mathcal{H}(\infty)$. η varies between 1, i.e., perfect harmonicity of the system, and 0, i.e., complete equipartition of energy.

Numerical simulations have been made for different values of the number of degrees of freedom, i.e., $N=64$, 128, 256; these values are powers of 2, thus allowing the use of a fast Fourier transform (FFT) to perform the computation of $A_n(t)$, $B_n(t)$, and consequently of $\eta(t)$.

Changing initial excitations we used $\bar{n}\propto N$ and $\Delta n \propto N$, so that the wavelength of the lowest excited mode was kept constant as well as the density $\Delta n/N$ of initially excited modes. The latter condition is introduced to simulate the usual thermodynamic limit of equilibrium statistical mechanics where the number of particles and the volume both become arbitrarily large at finite constant ratio.

The numerical integration algorithm used is the standard leapfrog algorithm:

$$\phi_i(t+\Delta t)=2\phi_i(t)-\phi_i(t-\Delta t)+(\Delta t)^2 F_i\{\phi_j(t)\} \ ,$$

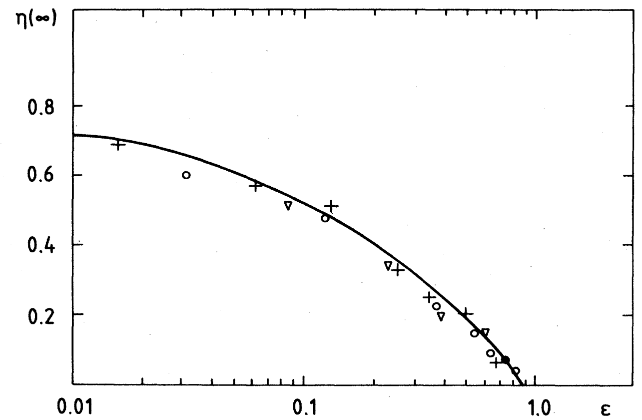

FIG. 1. Time asymptotic value of the spectral entropy vs energy density. The value of the coupling constant α has been set equal to 0.1. Circles stand for $N=64$, $\bar{n}=2$, $\Delta n=4$; crosses stand for $N=128$, $\bar{n}=4$, $\Delta n=8$; triangles stand for $N=256$, $\bar{n}=8$, $\Delta n=16$.

where $F_i=-\partial H/\partial\phi_i$.

The time integration step is $\Delta t=0.1$.

A typical relaxation time of $\mathcal{H}(t)$ to its time-asymptotic value is about 10^4, while in the worst situations, that is, when the energy density has a value which is close to the critical one, it can be as large as 4×10^4. The smoothing time T has been chosen equal to 3×10^3. In Fig. 1 we report the behavior of $\eta(\infty)$ vs $\epsilon=E/N$ which is obtained adopting $\bar{n}=N/32$ and $\Delta n=N/16$ and changing the number N of degrees of freedom. It is well evident that the different values found for $\eta(\infty)$ lie on the same curve independently of N so that the same critical energy density value ϵ_c is obtained as an equipartition threshold.

Thus, we have verified that the main result of Ref. 1 holds also for the FPU α model. In view of the results in the quoted references[1,2,3,5] and here reported, it seems reasonable to conclude that the existence of an ergodicity threshold is model independent. Another very important and still open question is the following: Have we observed at $\epsilon<\epsilon_c$ a true nonequilibrium state or rather a metastable situation with a very long relaxation time? It is evident that the answer can hardly be given with the aid of numerical simulations. It could happen that for $\epsilon<\epsilon_c$ and large N these nonlinear Hamiltonian systems behave similar to the amorphous systems[6] in which the equilibrium is reached only after very long times. Moreover, amorphous systems show a hierarchy of relaxation times according to the properties which are under consideration. This point deserves a more careful investigation which is now in progress.

The phase space structure of the nonergodic "phase" has been analyzed in more detail in Ref. 7.

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