Journal of Statistical Physics, Vol. 76, Nos. 1/2, 1994

Equipartition Thresholds in Chains of Anharmonic Oscillators

Holger Kantz,[1] Roberto Livi,[2] and Stefano Ruffo[3]

Received July 29, 1993; final November 17, 1993

We perform a detailed numerical study of the transition to equipartition in the Fermi–Pasta–Ulam quartic model and in a class of potentials of given symmetry using the normalized spectral entropy as a probe. We show that the typical time scale for the equipartition of energy among Fourier modes grows linearly with system size: this is the time scale associated with the smallest frequency present in the system. We obtain two different scaling behaviors, either with energy or with energy density, depending on the scaling of the initial condition with system size. These different scaling behaviors can be understood by a simple argument, based on the Chirikov overlap criterion. Some aspects of the universality of this result are investigated: symmetric potentials show a similar transition, regulated by the same time scale.

KEY WORDS: Hamiltonian dynamics; equipartition threshold.

1. INTRODUCTION

The numerical experiment by Fermi, Pasta, and Ulam in 1954[1] was the first attempt to check the predictions of classical statistical mechanics in Hamiltonian systems. The result was a surprise: the expected ergodicity of the system was not observed for small excitation energies. In such a case initially excited harmonic modes turned out to be stable over the accessible computation time. More recently, Izrailev and Chirikov[2] showed that at sufficiently high energies the Hamiltonian models of Fermi, Pasta, and Ulam (FPU) relaxed to equipartition of the energy among the Fourier modes.

These results have inspired further numerical studies of the relaxation-

[1] Department of Theoretical Physics, University of Wuppertal, D 42097 Wuppertal, Germany.
[2] Dipartimento di Fisica, Università di Bologna, I-40126 Bologna, Italy, INFN and INFM.
[3] Dipartimento di Energetica, Università di Firenze, I-50100 Firenze, Italy, INFN and INFM.

0022-4715/94/0700-0627$07.00/0

to-equilibrium dynamics in various nonlinear Hamiltonian models with many degrees of freedom.[3,4] It is now well established that the transition from an integrable-like behavior to an ergodic one is a generic property of such models: around some finite value of a control parameter (e.g., the energy or energy density) one typically observes a transition region between a "regular" dynamics and a chaotic regime. Well above this "threshold" one can detect all the typical attributes of large-scale chaos such as an asymptotic distribution of positive Liapunov exponents, positive KS entropy,[5] and fast relaxation to equipartition of the energy.[6,7]

A deeper understanding of this phenomenon would demand a systematic study of the dependence of the threshold on the number of degrees of freedom N in the system, on the initial condition, and on the observation time t.

The guiding idea of this work is that this information can be arranged in a consistent framework if some scaling property with N characterizes all dynamical quantities in the transition region. More precisely, we show that for the FPU-β model a proper rescaling of the observation time and of the initial condition with N allows us to represent the spectral entropy[6] (i.e., the "probe" observable) as a quantity independent of N when plotted versus the total energy of the system. If only the observation time is rescaled with N, the spectral entropy has again a "universal" behavior if plotted versus the energy density.

These results extend to a wide class of nonlinear separable Hamiltonian models, thus improving significantly our knowledge about the stochasticity threshold in the thermodynamic limit.

The structure of the paper is the following. In Section 2 we introduce the normalized spectral entropy η. The dynamical properties of this quantity for the FPU-β model are analyzed in Section 3.

Section 4 is devoted to analyzing the dependence of η on the initial condition for fixed N. The decay of η toward zero allows us to locate the threshold of finite-size systems. The thermodynamic limit for large but finite values of time is investigated in Section 5. We consider the two cases where the initial conditions are rescaled or not with N. A simple argument identifies the dynamical mechanism at the origin of the scaling properties of η. This argument identifies also the proper control parameter (energy or energy density).

In Section 6 we extend this analysis to two classes of Hamiltonian systems. For the threshold behavior we show that all the symmetric potentials reproduce the properties of the FPU-β model. The more complex scenario obtained for the FPU-α model and for the Toda lattice[8] contributes to further clarifying the reliability of our analysis. Conclusions and perspective are contained in Section 7.

2. THE NORMALIZED SPECTRAL ENTROPY

In this paper we investigate the dynamical properties of FPU-like chains, i.e., 1D systems of N anharmonic oscillators with the Hamiltonian

$$H(\mathbf{p}, \mathbf{x}) = \sum_{i=1}^{N} \frac{p_i^2}{2} + \sum_{i=1}^{N} U(\Delta x_i) \tag{2.1}$$

where $\Delta x_i = x_{i+1} - x_i$ and we impose periodic boundary conditions, i.e., $x_{N+1} = x_1$. The nonlinear potential $U(\Delta x_i)$ is chosen in such a way that it is harmonic in the small-energy limit, where Fourier modes represent the normal modes of the chain. In this limit any solution of the Hamiltonian equations will remain close to the Fourier mode representation of the initial condition for a very long time. For high energy the nonlinear component of the potential favors the exchange of energy among the modes, possibly leading to the equipartition of energy. Therefore a natural approach to measure the effect of increasing energy is the one pursued in ref. 6, namely computing the spectral entropy $S(t)$. This is defined as follows:

$$S(t) = -\sum_{l=1}^{N/2} p_l(t) \log p_l(t), \qquad p_l(t) = \frac{E_l(t)}{\sum_l E_l(t)} \tag{2.2}$$

$E_l(t)$ is the energy in mode l at time t. Furthermore, we introduce the normalized spectral entropy $\eta(t)$:

$$\eta(t) = \frac{S_{\max} - S(t)}{S_{\max} - S(0)} \tag{2.3}$$

where $S_{\max} = \log N/2$ corresponds to an equal amount of energy in each mode (energy equipartition), and $S(0)$ is the entropy of the initial condition. Fourier mode analysis applies by substituting $x_j(t) = \sum_{l=0}^{N/2} u_l(t) \cos k_l j + v_l(t) \sin k_l j$ into (2.1). Because of periodic boundary conditions, one has $k_l = 2\pi l/N$. The energy E_l is given by

$$E_l = \frac{N}{4} [\dot{u}_l^2 + \dot{v}_l^2 + \omega_l^2 (u_l^2 + v_l^2)] \tag{2.4}$$

where $w_l = 2 \sin \pi l/N$. In our numerical simulations we compute u_l, v_l, $\dot{u}_l$, and $\dot{v}_l$ by applying a FFT routine to both space and momentum variables. To suppress fluctuations we average $\eta(t)$ over a finite time interval, which we fix to 256 time units in all the following numerical analysis (this choice amounts to averaging over high frequencies maintaining the relevant information for the long-time behavior).

According to Eq. (2.3), $\eta(t)$ is a positive quantity; moreover,

$$\eta(t) \leqslant \left(1 - \frac{\log \Delta l}{\log N/2}\right)^{-1}$$

where Δl is the number of initially excited modes, each one containing the same amount of energy. Energy transfer from the initially excited modes is detected by decreasing values of $\eta(t)$. Observe that η is unstable with respect to fluctuations of $S(t)$ when a large number of normal modes is initially excited [i.e., $\Delta l \approx O(N/2)$], since the denominator of Eq. (2.3) becomes very small. In such a case even the upper bound of $\eta(t)$ diverges. Nevertheless, since we are interested in studying relaxation to equilibriuim starting from far-from-equilibrium initial conditions, we shall choose Δl not too large such that η is a proper quantity. Finally, let us stress that the results of the following analysis may depend on the choice of the basis of normal modes underlying the definition of E_l in Eq. (2.4), as we discuss briefly in Section 6.

3. THE *N* DEPENDENCE OF TYPICAL TIME SCALES

Using η as our indicator for energy sharing among normal modes, we are faced with the problem of the dependence on three variables, namely the energy of the system E, the number of degrees of freedom N, and the observation time t. In principle one would be interested in investigating the time-asymptotic properties of η. However, in numerical simulations this limit cannot be always obtained on reasonable time scales. Lengthy numerical simulations on long time spans are avoided if one observes a scaling behavior of η in t when N is varied.

We have explicitly checked this conjecture in the FPU-β model,[4] where $U(\Delta x_i) = \frac{1}{2}(\Delta x_i)^2 + \frac{1}{4}\beta(\Delta x_i)^4$ and $\beta = 0.1$ in all our simulations. In Fig. 1 we show η as a function of the energy at different times. Its time dependence is characterized by three different regimes: For $E < 1$, $\eta(t)$ remains constant close to 1 with fluctuations of very small amplitude (an exponentially slow diffusion of η to 0 cannot be excluded according to the Nekhoroshev result[9]). For large values of the energy ($E > 100$) η decays rapidly to a limiting value, remaining constant with small fluctuations. It is evident that in both of these energy regions the long-time behavior is not affected by a rescaling of the time. The only part of the curve that can be

[4] For all numerical work we use the symplectic leapfrog integrator with a step width of $\delta t = 0.04/\sqrt{E}$. Thus from here on our unit of time t corresponds to $25 \cdot \sqrt{E}$ steps of the leapfrog integrator.

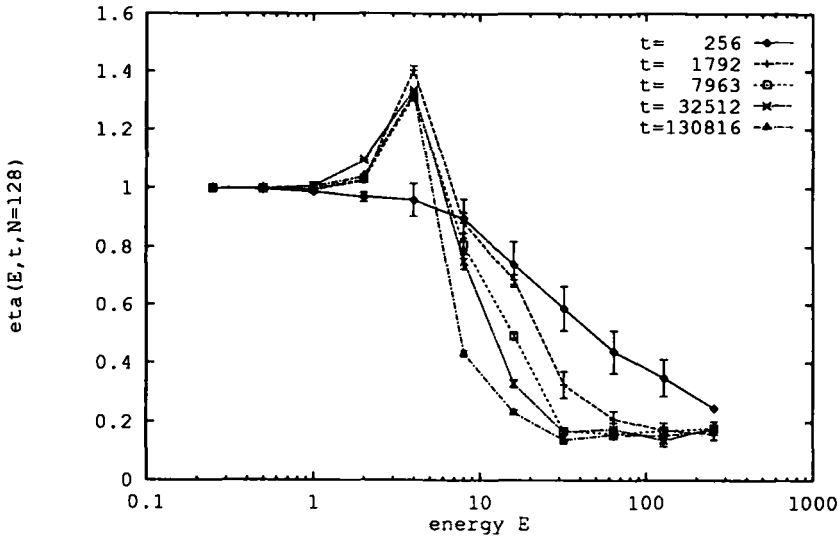

Fig. 1. Plot of η as a function of the energy after different times for the FPU-β model ($N = 128$, modes 4–19 are initially excited with the same energy). Plotted are the averages of η over the last 256 time steps, the errors bars indicating the fluctuations.

characterized by a nontrivial time dependence is the transition region between the previously mentioned regimes, i.e., $1 < E < 100$, where no asymptotic behavior can be easily obtained by numerical simulations.

In Fig. 2 we present the curves $\eta(E, \tau, N)$ at a fixed energy $E = 10$ for different N as a function of the rescaled time $\tau = t/N$. Initially all modes in the interval $[N/32, 3N/32[$ are excited with an equal amount of energy. Note that by this choice the central frequency of the initially excited packet is independent of N. We find evidence that the data collapse on the same curve, i.e., the typical time scale increases linearly with system size. We have obtained the same result for various values of E in the stochasticity threshold region.

Let us recall that η is defined in terms of the eigenmodes of the harmonic chain, whose eigenfrequencies are $\omega_l = 2 \sin(\pi l/N)$, $l \in [0, N/2]$. Since the relevant time scale for equipartition of the energy is set by those modes which are the slowest to gain energy, the observed scaling suggests that these are the low-lying modes, whose eigenfrequencies are approximately proportional to $1/N$. In fact, we have also checked numerically that the harmonic energies of the initially unexcited modes increase the more slowly, the lower is the mode number. This can be justified by observing that in the nonlinear terms of the equations of motion for mode amplitudes one can factor out the eigenfrequency of the mode.

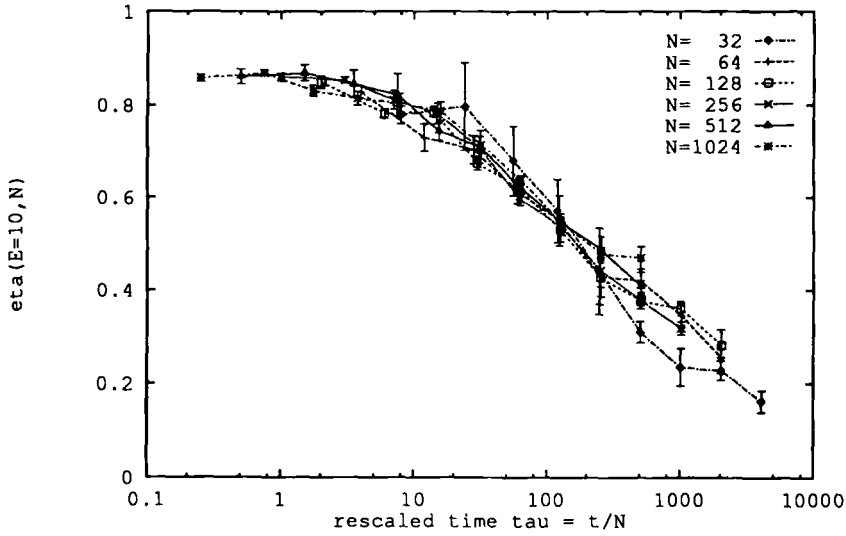

Fig. 2. Plot of η vs. the rescaled time $\tau = t/N$ for the FPU-β model with energy $E = 10$.

4. THE SHAPE OF THE THRESHOLD FOR FIXED *N*

Before we pass to our main goal, namely determining the asymptotic properties of η for large N, we study its dependence on initial conditions for fixed N. From this analysis we obtain important information about the threshold behavior of η.

We restrict our numerical work to the study of the relaxation properties of initial condition, where a packet of Fourier modes with equal amount of energy and random relative phases is excited. The initial values of the momenta are all set equal to zero. In Fig. 3 we present the results for different packet excitations. Each data point represents the average over $\eta(E,\ \tau = 80,\ N = 128)$ obtained from four different realization of the random phases. It turns out that the shape of the curves is determined only by the number of excited modes and not by their wave number (within the given errors). But let us analyze the curves in more detail.

As already shown in Section 3, the small-energy region corresponds to $\eta \approx 1$ independently of the initial conditions. There are very small fluctuations around this value, but no instability was detected in our numerical simulations up to $t = 10^6$ for $E \leqslant 1$ and $N = 128$.

In the high-energy limit η drops down to a small, almost constant value which depends on $\Delta I/N$ only. This is not an artifact of the numerical simulation, but also a consequence of the fluctuations of the mode energies

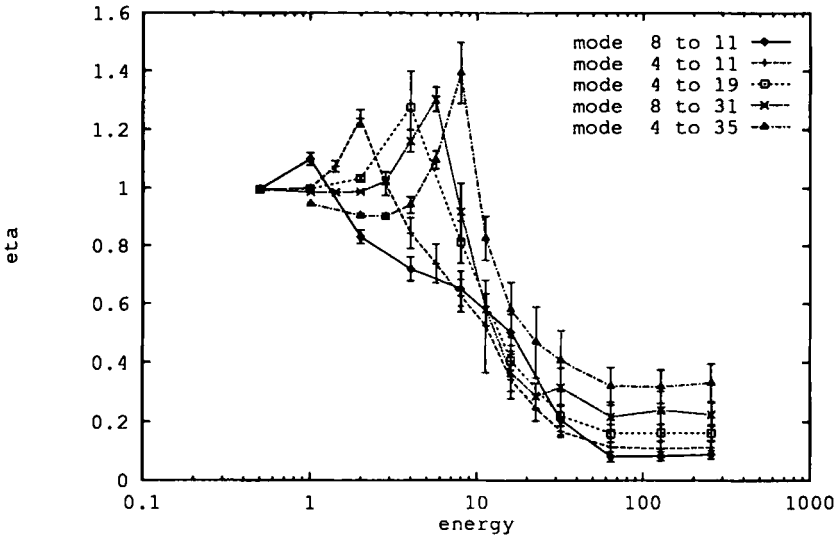

Fig. 3. Plot of $\eta(E, \tau, N)$ for $\tau = 80$ for different initial conditions (FPU-β model, $N = 128$). The indicated modes are excited with an equal amount of energy and random relative phases, each data point being an average over four different realizations. Note that the right part of all curves corresponds to the same entropy S, the differences in η originating in the normalization.

in the equipartition regime.[10] The calculation in ref. 10 is indeed done for a chain of harmonic oscillators under the assumption that a weak coupling between them causes ergodicity. In this case the distribution of energies is Boltzmannian, and using the partition function, one can compute, in the linear approximation, the value of η averaged over infinite time by averaging over the phase space. The result is $\eta_{\text{ergodic}} = (1 - C)/\ln(N/2\Delta l)$, where $C = 0.5772$ is the Euler constant and Δl is the number of initially excited modes. Numerically we find that η_{ergodic} is an upper bound to $\eta(E, \tau, N)$ for large values of E and τ (see Figs. 1 and 3). For instance, for $\Delta l/N = 1/16$, $\eta_{\text{ergodic}} \approx 0.2$, whereas we find 0.12. This disagreement may be due to nonlinear contributions to the partition function, which cannot be neglected for large energies. Nevertheless, the linear calculation correctly predicts the increase of η with Δl in the large-energy region.

The crossover between the low- and high-energy asymptotic regimes is first characterized by the region of energy where η becomes larger than 1. The origin of the "bumps" in Fig. 3 can be interpreted as an instability of the harmonic modes leading to a concentration of energy in fewer modes than the initially excited ones. The dynamics of η in this energy range (see Fig. 4) resembles quasiperiodic motion, the oscillations yielding an average

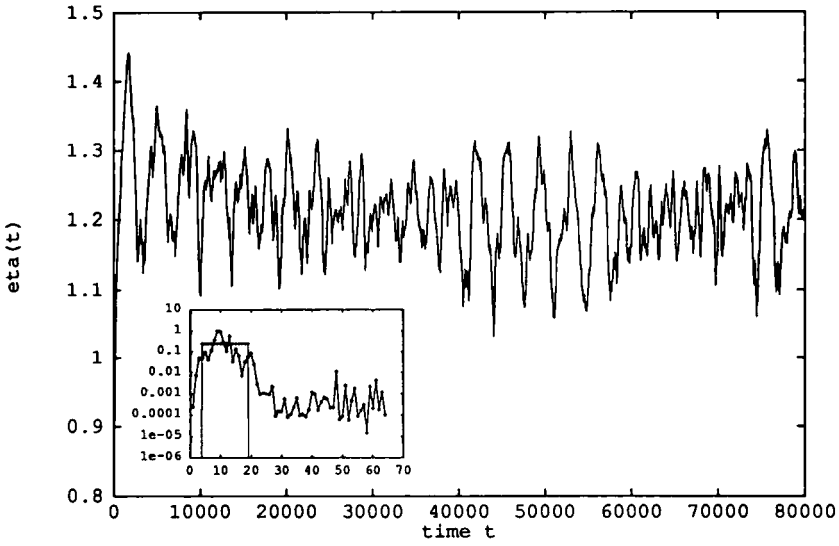

Fig. 4. The instantaneous value of η as a function of time, $N = 128$, $E = 4$, modes 4–19 initially excited. The insert shows the mode energies E_l versus mode number l at time $t = 0$ (broken curve) and $t = 53000$ ($\eta = 1.44$) (solid curve).

of η larger than 1. This behavior is maintained up to $t = 10^6$, thus excluding that we are in fact observing a transient behavior. The insert in Fig. 4 shows how the mode energies of a packet excitation have changed after $t = 53{,}000$. We argue that in the whole region with $\eta > 1$ the FPU-β model is close to some integrable nonlinear Hamiltonian, where a packet of initially excited harmonic modes is slightly deformed in a superposition of the stable nonlinear eigenmodes. It is reasonable to assume that there are two different mechanisms of destabilization of eigenmodes at the upper- and lower-energy boundaries of the $\eta > 1$ region. Nevertheless, we expect that both are related to the magnitude of the energy E_l of each initially excited harmonic mode and not simply to the total energy of the system. This is confirmed by the observation that the energy $E_{\max}$ at which η reaches its maximum is approximately proportional to Δl.

For energies larger than $E_{\max}$ the corresponding η curves decrease, reflecting a destabilization of the nonlinear eigenmodes. For energies larger than 20 the curves are characterized by a fast loss of memory of the initial conditions (see Fig. 4). This latter energy is quite close to $E_{\max} = 16$, which can be obtained extrapolating the linear behavior of $E_{\max}$ as a function of Δl to $\Delta l = 64$, the largest possible value for $N = 128$. Actually, for such an initial condition, corresponding to equipartition of the energy among the

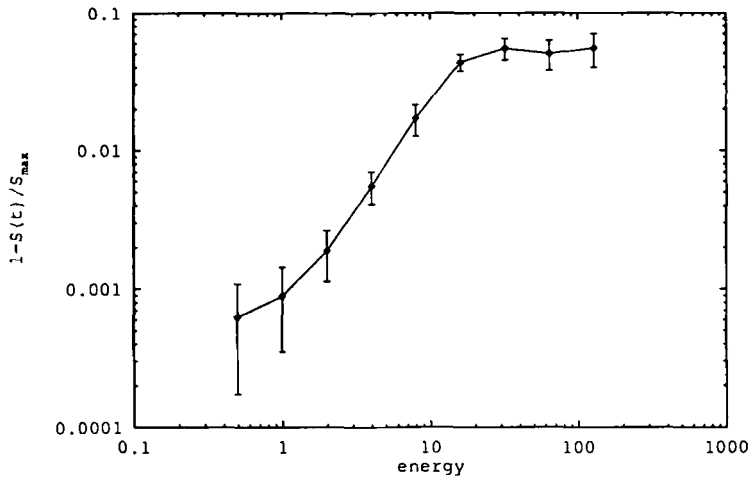

Fig. 5. Plot of $\tilde{\eta}$ for $\tau = 80$ as a function of the energy; $N = 128$ and $\Delta I = 64$).

Fourier modes, η is not a conveniently defined quantity. The effect of reduction of the entropy S in the bump region starting from this initial condition can be better detected by quantity $\tilde{\eta} = 1 - S(t)/S_{\max}$. As we show in Fig. 5, $\tilde{\eta}$ grows with a power law up to an energy $E_{\max} \sim 16$ and then saturates. This is further evidence that the equipartition state (corresponding to $\tilde{\eta} = 0$) is unstable below this energy and stabilizes, for higher values of the energy, to a value compatible with Gibbsian fluctuations (see Section 4).

5. THE THRESHOLD IN THE THERMODYNAMIC LIMIT AT FINITE TIMES

In this section we study the behavior of $\eta_\tau(E, N) \equiv \eta(E, \tau N, N)$ for different values of N. We have chosen $\tau = 16$, which allows numerical analysis up to $N = 1024$ on a Cray X-MP computer. In Fig. 6 we plot $\eta_{\tau=16}$ versus the energy E for different system sizes. All modes $l \in [N/32, 5N/32[$ are initially excited with the same amount of energy. Thus the number of excited modes is scaled with N to investigate thermodynamic limit properties.[5] Again, each data point in Fig. 6 is as average over four different initial conditions of the same modes excited with equal energies, but with different

[5] After the previous section we know that a different choice for the rescaled packet of modes would change the shape of the η curve in the region of the "bump," but not in the decaying part of the curve.

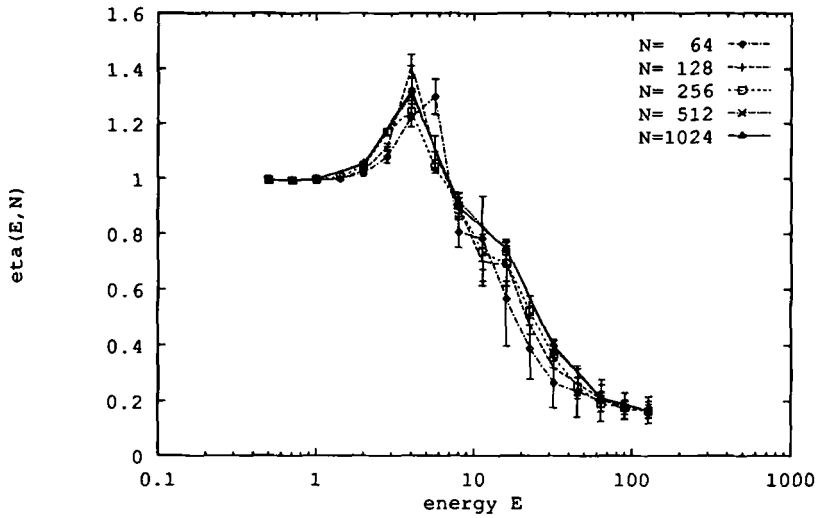

Fig. 6. Plot of $\eta(\tau = 16)$ as a function of the total energy E for different system sizes (β-model). Initially modes $l \in [N/32, 5N/32[$ are excited.

relative phases between the cosine and the sine waves. The error bars are the variance of these values. The data fall very nicely onto a common curve, confirming that the relevant control parameter for this kind of initial conditions is energy rather than energy density. This is true from 128 to 1024 degrees of freedom. For the $N = 64$ system we observe a small deviation at the "bump." The small number of excited modes together with finite-size effects are at the origin of these differences.

We have also studied the case of $l_0 = 1$ and $\Delta l = 3$ fixed independently of N. In this case the different η curves superpose if they are plotted as a function of the energy density, as shown in Fig. 7.

A simple argument can explain these two different results.[6] The Hamiltonian of our model can be expressed approximately in terms of the harmonic action variables $\mathbf{I} = (I_1, ..., I_N)$ as follows:

$$H = H_0 + \Delta H$$
$$H_0 = \boldsymbol{\omega} \cdot \mathbf{I}, \qquad \Delta H = \frac{\beta}{N} (\boldsymbol{\omega} \cdot \mathbf{I})^2 \tag{5.1}$$

The width of the lth resonance $\Delta\omega_l$ can be estimated by

$$\Delta\omega_l = \frac{\Delta H_l}{I_l} \approx \frac{\beta}{N} \omega_l^2 I_l = \frac{\beta}{N} \omega_l E_l \tag{5.2}$$

[6] The argument was suggested by D. Shepelyansky.

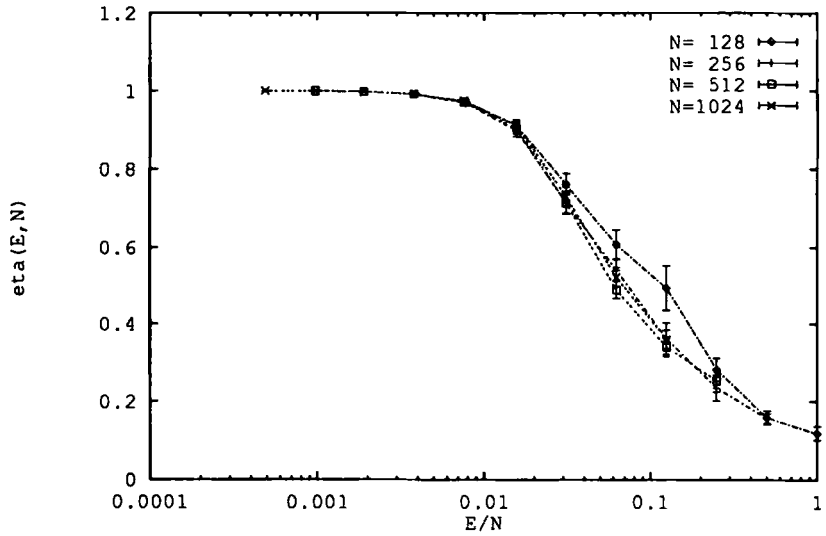

Fig. 7. Plot of η as a function of the energy density E/N for the FPU-β model with $\tau = 16$. Initially, the modes $l = 1, 2, 3$ are excited with equal energy.

where E_l is the energy of the lth mode. In the acoustic branch of the spectrum (small l values) the distance between nearby resonances is $\delta_l \sim 1/N$ (independent of l). According to the Chirikov criterion,[11] large-scale chaos sets in if $\Delta\omega_l \approx \delta_l$, i.e.,

$$\beta\omega_l E_l \sim 1 \tag{5.3}$$

For initial conditions where l increases proportionally to N, $\omega_l \sim l/N =$ const. is a finite value independent of N and the Chirikov criterion establishes a threshold value for the energy of the system

$$E_l^{\text{thres}} \sim \frac{1}{\beta} \tag{5.4}$$

while when fixing l_0 and Δ_l independent of N, $\omega_l \sim 1/N$ such that the threshold is determined by the energy density

$$\left(\frac{E_l}{N}\right)^{\text{thres}} \sim \frac{1}{\beta} \tag{5.5}$$

It is evident that the two cases discussed in this section correspond to the different ways of performing a thermodynamic limit. The first one is the correct way if one wants to describe the dynamics of an anharmonic crystal where the initially excited frequencies are defined as the relevant

physical quantities. The second case does not seem to have physical relevance in the thermodynamic limit, since any initially excited frequency would tend to zero; it can be physically interesting only for finite systems.

Let us summarize the results for the FPU-β model. For the type of initial conditions that we consider as physically relevant we find a double threshold in the energy, the first being a transition from linear to nonlinear stable eigenmodes, the second indicating equipartition of energy in the Fourier modes. Both threshold energies are independent of the system size and they are true thresholds in the sense that they are independent of the observation time (see Fig. 1). Nevertheless, the relevant time scale for the equipartition of energy among the Fourier modes is proportional to the system size.

6. THE UNIVERSALITY OF THE NORMAL MODE ANALYSIS

In this section we extend our analysis of the stochasticity threshold to various models defined in Eq. (2.1). Specifically, we compare the threshold behavior of the following potentials $U(\Delta x_i)$:

$$\frac{1}{2}\Delta x_i^2 + \frac{1}{3}\alpha\,|\Delta x_i|^3 \qquad \text{symmetrized FPU-}\alpha\text{ model} \tag{6.1}$$

$$\frac{1}{2b^2}\left(e^{b\Delta x_i} + e^{-b\Delta x_i} - 2\right) \qquad \text{symmetric Toda potential} \tag{6.2}$$

$$\frac{1}{2\beta}\left(1 - e^{-\beta\Delta x_i^2}\right) \qquad \text{Gaussian potential} \tag{6.3}$$

$$\frac{1}{2}\Delta x_i^2 + \frac{1}{3}\alpha\Delta x_i^3 \qquad \text{FPU-}\alpha\text{ model} \tag{6.4}$$

$$\frac{1}{a^2}\left(e^{a\Delta x_i} - \frac{1}{a}\Delta x_i - 1\right) \qquad \text{Toda potential} \tag{6.5}$$

The total energy is not an appropriate parameter for this comparison, because the energy scale of the anharmonic components (responsible for the threshold behavior) greatly varies with the model. A more reasonable quantity is the ratio between the energy of the anharmonic component of $U(\Delta x_i)$ and the harmonic one at $t=0$ (provided that we consider initial conditions with vanishing kinetic energy):

$$\varepsilon = \frac{\left|\sum_{i=1}^{N} U(\Delta x_i) - \frac{1}{2}\Delta x_i^2\right|}{\sum_{i=1}^{N} \frac{1}{2}\Delta x_i^2} \tag{6.6}$$

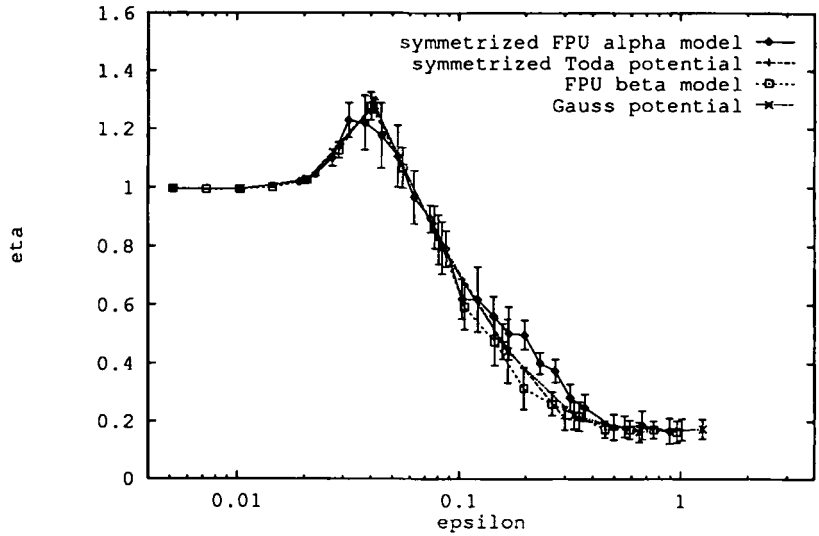

Fig. 8. Plot of η as a function of ε for different symmetric potentials, $N = 128$, $\tau = 40$, modes 4–19 initially excited.

In fact, for a fixed value of this extensive parameter the anharmonic energies of all the models have the same magnitude.[7]

For our numerical simulations we choose $N = 128$ and $\tau = 40$, which corresponds to roughly 1600 periods of the fastest harmonic and 40 periods of the slowest one. The η curves as a function of ε for the potentials in Eqs. (6.1)–(6.5) are shown in Figs. 8 and 9. Again, for all systems we have $\eta(\varepsilon \to 0) \approx 1$ and $\eta(\varepsilon \to \infty) = \text{const} \neq 0$.

The main differences occur in the transition region. The $\eta(\varepsilon)$ curves of the symmetric potentials superpose very nicely and exhibit a region where $\eta > 1$ (Fig. 8). The arguments used in Section 4 to explain the origin of the transition apply to all of these models. Actually, the transition region is located at $\varepsilon \approx 10^{-1}$, thus indicating that the quartic nonlinearity is the dominant one. On the other hand, also the symmetrized FPU-α model shows the same quantitative behavior. We have no analytical argument to interpret this result; nevertheless, it confirms that ε is a proper control parameter.

[7] A simpler choice would amount to rescaling the energy by a factor β (α^2) for potentials having $(\beta/4)\,\Delta x_i^4$ [$(\alpha/3)\,\Delta x_i^3$] as the leading nonlinear contribution in the Taylor expansion of U. Beyond the impossibility of applying this to model (6.1), this way of rescaling the energies becomes insignificant if high-order nonlinear terms dominate in the transition region.

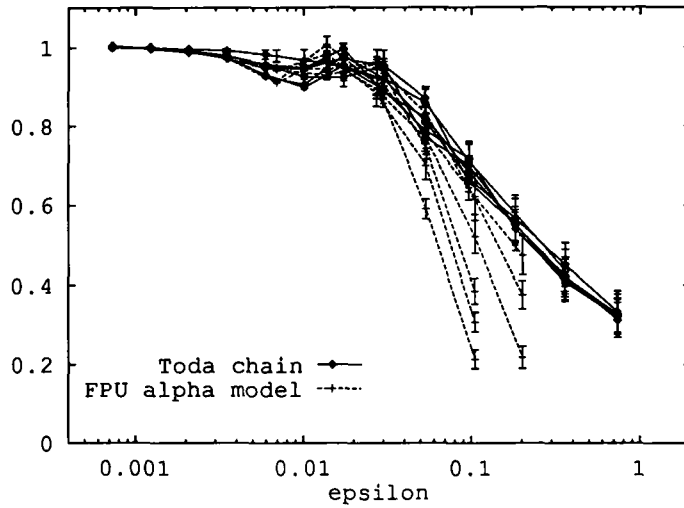

Fig. 9. Plot of η as a function of ε for the FPU-α model and the Toda chain after different times τ, ranging from $\tau = 2$ to $\tau = 1022$ and spaced by powers of 2 ($N = 128$, modes 4–19 excited). Plotted are the averages of η during the last 256 time steps, the error bars indicating the fluctuations. The curves for the FPU-α model terminate at $\varepsilon \leqslant 0.21$, since the trajectories eventually escaped due to the unboundedness of the potential. All points shown in this figure are taken for situations where the trajectory was well inside the bounded region such that the decay of η is not related to this possibility of escape.

For the FPU-α model and the Toda chain the scenatio is more complicated. Since the Taylor series expansions of the two models coincide up to third order, we expect a superposition of the $\eta(\varepsilon)$ curves for sufficiently small ε. This is what one can observe in Fig. 9 up to $\varepsilon \approx 0.05$ independent of time. In contrast to the symmetric models, no clear "bump" structure exists in both models. For larger values of ε the η curves of the Toda lattice remain time independent and decay slowly in ε, while in the FPU-α model η decays as time is increased. Thus we locate a time-independent threshold for the α model at $\varepsilon \approx 0.02$.[8] On the contrary, for the Toda model the smooth decay of $\eta(\varepsilon)$ independent of time does not allow us to define a threshold for the equipartition of energy. This is not surprising if one considers that the Toda lattice is an integrable model.[8] For large values of ε the eigenmodes of the Toda lattice are known to be solitons whose Fourier representation averaged in time spreads over a broad band, thus

[8] From Eq. (6.4) it is evident that the potential forms a well with a finite height. Thus for large ε a trajectory may escape from this well leading to unbounded motion and a numerical overflow.

leading to equipartition of the energy in Fourier space, if ε is large enough. This is in agreement with ref. 12, where it is shown that numerically computed time averages coincide with analytically computed ensemble averages. The numerical simulations in ref. 12 were done for energies ranging between 100 and 10^6, with $N = 1000$, corresponding to the range $0.2 < \varepsilon < 25$ for our class of initial conditions.

7. CONCLUSIONS

We present numerical evidence of some properties of the normalized spectral entropy η, which allows us to characterize the presence of a stochasticity threshold as a general feature of many-degrees-of-freedom Hamiltonian models. More precisely, we show that:

1. The relevant time scales behave proportionally to the system size N, i.e., systems with different N are "dynamically" equivalent at the rescaled time $\tau = t/N$.
2. For initial conditions where the number of excited modes and their mode numbers are rescaled proportionally to N the spectral entropy η depends only on the total energy and not on N.
3. The energy density is the correct control parameter when the mode numbers of the initially excited modes are kept fixed when varying N.

It is worth observing that for the rescaled initial conditions in the thermodynamic limit both the central frequency of the initially excited wave packet and the density of modes inside it are constant. This is the correct way to define the thermodynamic limit for a dynamical model of a physical system where quantities like the total energy are finite.

Another important result is that the class of Hamiltonian models having a quartic term as leading nonlinearity exhibit the same threshold behavior as the FPU-β model. This is far from trivial, because *a priori* there is no reason to conclude that the time scale associated to the quartic nonlinearity is responsible in any such model for the decay of the spectral entropy around the threshold value of the energy.

These results seemingly contradict previous findings reported in ref. 6, where the equipartition threshold of the FPU-β model was determined by plotting the "asymptotic" value of η as a function of the energy density, using the same type of rescaled initial conditions that in this paper show η depending only on the total energy. The disagreement derives from the fact that η values for larger N's in ref. 6 were obtained with shorter integration times and averaging over larger time intervals, due to the short

available computer time and to poor statistics. Thus, for larger values of N, η was not yet "asymptotic." For instance, considering Fig. 6 of this paper, if the data were plotted as a function of E/N, one would observe regularly shifted curves toward lower values of E/N. The integration times for larger N's are increasing linearly in N, while in ref. 6 they were decreasing with N, thus producing a superposition of data corresponding to different N's. One might still think that the data in ref. 6 suggest a scaling of the form $\eta = \eta(E/N, tf(N))$, with $f(N)$ increasing with N. This scaling form is not in contradiction with the one proposed in this paper, but, without any analytical input on the function $f(N)$, it is extremely hard to verify numerically.

Nonsymmetric potentials like the FPU-α model and the Toda lattice show some different features with respect to the symmetric case. Nonetheless, the former is still characterized by the presence of a stochasticity threshold which is again identified by a sudden decay of the time-rescaled spectral entropy η. Even the Toda lattice, which is known to be integrable, possesses a mechanism of energy sharing among the Fourier modes; its main peculiarity is that in broad range of energies η relaxes very fast to an asymptotic value $\eta(\varepsilon)$ different from the equipartition value, thus showing a smooth transition rather than a sharp threshold.

This means also that equipartition of energy among the eigenmodes is not necessarily approached on the same time scale when the basis is changed. For instance, the extreme situation is obtained when the initial condition in Fourier space is projected on the basis of the Toda nonlinear eigenmodes and the weights p_l in Eq. (2.3) are redefined in the new basis. It is obvious that in this case for the Toda chain $\eta(\varepsilon) = 1$ at any time, in the whole energy range.

Recently a similar scaling property for the relaxation to equipartition was proposed in ref. 13. Although there is not complete agreement concerning the scaling of time with the number of degrees of freedom, it is remarkable that also these authors show that the relaxation to equipartition is ruled by the total energy.

ACKNOWLEDGMENTS

We thank D. Shepelyansky for useful comments, and Y. Elskens and M. Pettini for discussions and a critical reading of the manuscript. We also acknowledge useful discussions with A. Lichtenberg. We thank INFN for financial support and the ISI Torino for hospitality during the realization of a part of this work. The work was started when H.K. was an EC follow of the Science Programme in Florence. CINECA is acknowledged for providing CPU time on the Cray-YMP under grant G4WFIZQ1.

REFERENCES

1. E. Fermi, J. Pasta, and S. Ulam, in *Collected Papers of E. Fermi* (University of Chicago Press, Chicago, 1965), Vol. 2, p. 78.
2. F. Izrailev and B. Chirikov, *Sov. Phys. Doklady* **11**:30 (1966).
3. B. V. Chirikov, F. U. Izrailev, and V. A. Tayurskij, *Comp. Phys. Comm.* **5**:11 (1973).
4. P. Bocchieri, A. Scotti, B. Bearzi, and A. Loinger, *Phys. Rev. A* **2**:2013 (1970) M. Casartelli, G. Casati, E. Diana, L. Galgani, and A. Scotti, *Theor. Math. Phys.* **29**:205 (1976); G. Benettin and A. Tenenbaum, *Phys. Rev. A* **28**:3020 (1983).
5. R. Livi, A. Politi, and S. Ruffo, *J. Phys. A* **19**:2033 (1986).
6. R. Livi, M. Pettini, S. Ruffo, M. Sparpaglione, and A. Vulpiani, *Phys. Rev. A* **31**:1039 (1985); R. Livi, M. Pettini, S. Ruffo, and A. Vulpiani, *Phys. Rev. A* **31**:2740 (1985).
7. H. Kantz, *Physica D* **39**:322–335 (1989); M. Pettini and M. Landolfi, *Phys. Rev. A* **41**:768 (1980); M. Pettini and M. Cerruti-Sola, *Phys. Rev. A* **44**:975 (1991).
8. M. Toda, *Phys. Rep.* **18**:1 (1975).
9. N. N. Nekhoroshev, *Russ. Math. Surv.* **18**:85 (1977); G. Benettin, L. Galgani, and A. Giorgilli, *Celestial Mech.* **37**:1 (1985); G. Benettin, L. Galgani, and A. Giorgilli, *Commun. Math. Phys.* **11W3**:87 (1987), **121**:557 (1989); L. Galgani, A. Giorgilli, A. Martinoli, and S. Vanzini, *Physica D* **59**:334 (1992).
10. C. G. Goedde, A. J. Lichtenberg, and M. A. Lieberman, *Physica D* **59**:200 (1992).
11. B. Chirikov, *Phys. Rep.* **52**:263 (1979).
12. G. A. Vinogradov, M. M. El'yashevich, and V. N. Likhachev, *Phys. Lett. A* **151**:515 (1990).
13. J. De Luca. A. J. Lichtenberg, and M. Lieberman, Time scale to ergodicity in the FPU system, preprint, University of California, Bekeley (1994).