The Fermi-Pasta-Ulam problem revisited: Stochasticity thresholds in nonlinear Hamiltonian systems

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The Fermi-Pasta-Ulam α model of harmonic oscillators with cubic anharmonic interactions is studied from a statistical mechanical point of view. Systems of $N=32$ to 128 oscillators appear to be large enough to suggest statistical mechanical behavior. A key element has been a comparison of the maximum Lyapunov coefficient $\lambda_{\max}$ of the FPU α model and that of the Toda lattice. For generic initial conditions, $\lambda_{\max}(t)$ is indistinguishable for the two models up to times that increase with decreasing energy (at fixed N). Then suddenly a bifurcation appears, which can be discussed in relation to the breakup of regular, solitonlike structures. After this bifurcation, the $\lambda_{\max}$ of the FPU model appears to approach a constant, while the $\lambda_{\max}$ of the Toda lattice appears to approach zero, consistent with its integrability. This suggests that for generic initial conditions the FPU α model is chaotic and will therefore approach equilibrium and equipartition of energy. There is, however, a threshold energy density $\epsilon_c(N)\sim 1/N^2$, below which trapping occurs; here the dynamics appears to be regular, solitonlike, and the approach to equilibrium—if any—takes longer than observable on any available computer. Above this threshold the system appears to behave in accordance with statistical mechanics, exhibiting an approach to equilibrium in physically reasonable times. The initial conditions chosen by Fermi, Pasta, and Ulam were not generic and below threshold and would have required possibly an infinite time to reach equilibrium. The picture obtained on the basis of $\lambda_{\max}$ suggests that neither the KAM nor the Nekhoroshev theorems in their present form are directly relevant for a discussion of the phenomenology of the FPU α model presented here. [S1063-651X(97)15105-4]

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I. INTRODUCTION

Few problems have been studied so extensively over recent decades as the one devised originally by Fermi, Pasta, and Ulam (FPU) in 1954 [1]. Their purpose was to check numerically that a generic but very simple nonlinear many-particle dynamical system would indeed behave for large times as a statistical mechanical system, that is, it would approach equilibrium. In particular, their purpose was to obtain the usual equipartition of energy over all the degrees of freedom of a system, for generic initial conditions. To their surprise, for the system FPU considered—a one-dimensional anharmonic chain of 32 or 64 particles with fixed ends, and in addition to harmonic, cubic (α model) or quartic (β model) anharmonic forces between nearest neighbors—this was not observed. A variety of manifestly nonequilibrium and nonequipartition behaviors was seen, including quasiperiodic recurrences to the initial state. In fact, a behavior reminiscent of that of a dynamical system with few degrees of freedom was found, rather than the expected statistical mechanical behavior. The duration of their calculations varied between 10 000 and 82 500 computation steps. These results raised the fundamental question about the validity or at least the generally assumed applicability of statistical mechanics to nonlinear systems of which the system considered by FPU seemed to be a typical example. Most of the attempts to clarify this difficulty have approached the problem as one in dynamical systems. These analyses have revealed many very interesting properties of the FPU system and uncovered a number of possible explanations for the resolution of the observed conflict with statistical mechanics. The classical explanations are (i) the survival of invariant tori in the phase space of a quasi-integrable system (KAM theory) [2], (ii) the existence of Zabusky and Kruskal's solitons in the KdV continuum limit [3,4], (iii) the existence of an order-to-chaos transition [5]. However, we do not believe that the problem has as yet been entirely resolved. In particular, it is the purpose of this paper to try to clarify the problem from a

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statistical mechanical point of view. That is, we will try to exhibit the reasons why this apparently *bona fide* statistical mechanical system did not behave as such and, in particular, what in our opinion the significance of this apparent failure is for the general validity of statistical mechanics.

There are a number of obvious questions related to the unstatistical mechanical behavior observed by FPU, which all address the generic nature of their results.

(a) Was their time of integration long enough?

(b) Was their dynamical system of $N=32$ or 64 particles in one dimension large enough, i.e., possessing a sufficient number of degrees of freedom, to qualify as a statistical mechanical system?

(c) Were the recurrence phenomena (to within 3%) observed by FPU, transient, or generic, i.e., possibly related to a Poincaré recurrence time?

The search for answers to these questions made the work of FPU very seminal, spawning many new developments and connections in the theory of nonlinear dynamical systems, such as the connection with continuum models based on the Korteweg–de Vries equation, leading to solitons [3], heavy breathers, etc., or with few degrees of freedom models, like the Hénon-Heiles and the Toda lattice [6]. For a recent review we refer to [7].

The approach to equilibrium of the FPU β model was studied extensively for various classes of initial conditions by Kantz *et al.* [8] and recently by De Luca *et al.* [9]. A very detailed picture has emerged from their work, as to the behavior of the FPU β model in its dependence on nonequilibrium initial conditions as well as the role played by low frequency and high frequency mode-mode couplings [10] during its time evolution. Two threshold energies were identified, but the connection of all the very interesting and detailed information obtained with the generic statistical mechanical behavior of the FPU β model remains unclear so far.

Thus, although the effort to resolve the so-called FPU problem has led to enormous advances in our understanding of nonlinear dynamical systems, it has not yet, in our opinion, led to a full evaluation of the statistical mechanical relevance of the FPU paradox, i.e., FPU's original question has not yet really been answered.

It is commonly asserted [7] that the KAM theorem provides the essential answer to FPU's observations, i.e., for sufficiently small nonlinearities and a class of initial conditions living on nonresonant tori, the FPU system behaves like an integrable system and is represented by deformed tori in phase space. With increasing strength of the nonlinearities, a progressive chaotic behavior appears, which would ultimately lead to the expected approach to equilibrium and equipartition [11].

Even though there are regular regions in phase space, the existing estimates based on the KAM theorem are qualitatively different from what we found, indicating that the physics of the FPU model is quite different from what is contained in these estimates. This makes us believe, on the basis of our numerical simulations, that it is the very special initial conditions chosen by Fermi and collaborators that make their system belong to a regular region of phase space. If they had chosen an initial excitation ten times larger, they could have observed equipartition. This takes place via a disappearance with increasing initial amplitude of a threshold, whose N dependence is entirely different from that estimated in the KAM theory framework. Hence the source of FPU's failure is the fortuitous choice of initial conditions in a regular region of phase space, below this critical energy.

Thanks to the power of modern computers, we have considerably extended the calculations performed in the past by various authors. We have been able to reconcile different, and sometimes contradictory, aspects of the FPU dynamics, finding that regular regions and a large ''chaotic sea'' can coexist in phase space. The lack of equipartition in the original FPU experiment is not representative of a global property of phase space: apparently regular, solitonlike structures, similar to those of Zabusky and Kruskal, have a very long, possibly infinite, lifetime below a stochasticity threshold, whereas, above the same threshold, they have only a finite lifetime.

By choosing more physically generic initial conditions, i.e., random positions and momenta, a threshold energy for the onset of chaos is detected, showing a rather strong tendency to vanish at an increasing number of degrees of freedom. Thus we have found strong evidence in support of the point of view that the so-called ''FPU-problem'' does not invalidate the (generic) approach to equilibrium and the validity of equilibrium statistical mechanics. On the other hand, the existence of long-living initial states far from equilibrium may well have interesting, nontrivial physical implications.

II. MODEL AND RESULTS

We have considered a one-dimensional lattice of unit mass particles interacting via nearest-neighbor forces with unit harmonic coupling constant, with fixed endpoints $(q_1=q_{N+1}=0)$ and described by the Hamiltonian

$$H(\mathbf{p},\mathbf{q})=\sum_{k=1}^{N}\left[\frac{1}{2}p_k^2+\frac{1}{2}(q_{k+1}-q_k)^2+\frac{\alpha}{3}(q_{k+1}-q_k)^3\right], \tag{1}$$

which is known as the FPU α model. We can think of Eq. (1) as the first anharmonic approximation to physical interatomic potentials of the Morse or Lennard-Jones type.

The cubic term is obviously responsible for the energy exchange among the normal modes of the harmonic part of Eq. (1). The normal mode coordinates, obtained by a standard orthogonal transformation, read

$$Q_k=\left(\frac{2}{N}\right)^{1/2}\sum_{i=1}^{N} q_i \sin\frac{ik\pi}{N} \tag{2}$$

and diagonalize the harmonic part of Eq. (1).

The Hamiltonian in these new coordinates becomes

$$H(\mathbf{P},\mathbf{Q})=\sum_{k=1}^{N}\left[\frac{1}{2}P_k^2+\frac{1}{2}\omega_k^2 Q_k^2 + \alpha\sum_{k',k''=1}^{N} C(k,k',k'')Q_k Q_{k'} Q_{k''}\right], \tag{3}$$

where $\omega_k = 2\sin(k\pi/2N)$ is the frequency of the kth normal mode and $P_k = \dot{Q}_k$ are the conjugated momenta. The natural unit of time with the choice of the units of Eq. (1) is given by the inverse of the fastest frequency of the harmonic part of Eq. (1): $T_{\min} = 2\pi/\omega_{\max} \equiv \pi$. In what follows $t = 1$ corresponds to $1/\pi$ of this fastest linear period.

We have numerically integrated this model by means of a very efficient third order bilateral symplectic algorithm [12] that ensures a faithful representation of a Hamiltonian flow and, with the adopted values of the rather large time step ranging from 0.01 to 0.1, keeps the total energy E constant within an average fluctuation level of $\Delta E/E \simeq 10^{-8}$ without drift. Such a high precision in numerical integration makes the outcome of the very long runs that are reported in the following reliable. The coupling constant was $\alpha = 0.25$. In order to give an idea of the computational effort that was necessary to obtain the results reported in this paper, let us mention that the computation of the largest Lyapunov exponents λ_1 at low energy typically required integration times in the interval 10^7–10^9 natural units of time: the longest runs lasted about 60 h of CPU time on an HP9000/735 computer (about the same CPU time would be necessary on a CRAY Y-MP computer). The CPU time amounted to about 4000 h on the following computers: HP 9000/735, HP 9000/715, Sun SPARC10, Sun SPARC5, Digital Alphaserver 2000 4/200.

For what concerns the initial conditions, we begin by choosing single mode excitations as Fermi and collaborators did in their original experiment, i.e., the initial displacements of the particles from their equilibrium positions are given by the fundamental mode

$$q_i(0) = A\sin\left(\frac{2\pi n i}{N}\right), \quad i = 1, \ldots, N, \tag{4}$$

and the initial momenta $p_i(0) = 0$ for $i = 1, \ldots, N$. Fermi *et al.* used $N = 32$, $A = 1$, and mode number $n = 1$.

Now the main question is, if we repeat the original experiment, do we have any chance to find equipartition or any clear tendency to it by using present-day fast computers?

To answer this question we cannot blindly make the longest integration of the trajectories of the Hamiltonian (1) that we can afford on a very fast computer: the absence of equipartition, even after a very long integration time, would not be by itself conclusive for the nonexistence of equipartition for this model. Rather, one should make an estimate of the equipartition time at $A = 1$ and $N = 32$, and determine the A dependence of this time for larger values of A: a large initial excitation amplitude makes the anharmonicity of the system larger, hence the mode-mode couplings stronger, so that a faster relaxation to equipartition can be expected.

A. Detecting energy equipartition

A possible method to numerically detect equipartition of energy makes use of the spectral entropy [13] defined by

$$\mathcal{S}(t) = -\sum_{k=1}^{N} w_k(t)\ln w_k(t), \tag{5}$$

where the weights w_k are given by the fraction of the total harmonic energy $E_k = \frac{1}{2}(P_k^2 + \omega_k^2 Q_k^2)$ in the kth normal mode [14],

$$w_k(t) = \frac{E_k(t)}{\sum_i E_i(t)} \tag{6}$$

so that $\mathcal{S}(t)$ reaches its maximum value when equipartition is attained. This entropy can be normalized as follows:

$$\eta(t) = \frac{\mathcal{S}(t) - \mathcal{S}_{\max}}{\mathcal{S}(0) - \mathcal{S}_{\max}}, \tag{7}$$

hence $\eta = 1$ detects a ''freezing'' of the initial condition and $\eta = 0$ detects equipartition.

By following the time relaxation of $\eta(t)$ we have obtained some estimates of the equipartition time τ_E at values of the initial excitation amplitude A ranging from 3 to 11. Note that A cannot be too large, since then the cubic part of the potential becomes repulsive and the phase space trajectories are ''runaway'' trajectories, nor can A be too small, since then the relaxation times become too large to be determined by our computations. However, two major difficulties arise with the η method: (i) contrary to previously investigated systems [15,16], the relaxation pattern of $\eta(t)$ does not show clearly when equipartition sets in, so that the equipartition time is a fuzzy quantity, (ii) if we somehow *define* the equipartition time by, for example, measuring the time needed for $\eta(t)$ to drop below a threshold value, say $\eta = 0.1$, we find that $\tau_E(\epsilon) \sim \epsilon^{-3}$ ($\epsilon = E/N$ is the energy density). For the FPU case ($A = 1$, $\epsilon = 0.002\,41$), we will show (see Sec. II B) that the equipartition time is far too long a time for numerical tests, since it would amount to about a year's CPU time.

B. Phase space trapping

We have been able to overcome these difficulties by focusing on the development of chaoticity in the time evolution of the system rather than on the attainment of equipartition.

The natural way of characterizing chaotic motions is to compute the largest Lyapunov exponent λ_1. Let us briefly remember its definition. Let

$$\dot{x}^i = X^i(x^1, \ldots, x^N), \quad i = 1, \ldots, N \tag{8}$$

be a given dynamical system, and denote by

$$\dot{\xi}^i = \sum_{k=1}^{N} \mathcal{J}_k^i[x(t)]\xi^k, \quad i = 1, \ldots, N \tag{9}$$

its tangent dynamics equation, $[\mathcal{J}_k^i] = [\partial X^i/\partial x^k]$ is the Jacobian matrix of $[X^i]$, then the largest Lyapunov exponent λ_1 is defined by

$$\lambda_1 = \lim_{t\to\infty} \frac{1}{t} \ln \frac{\|\xi(t)\|}{\|\xi(0)\|}. \tag{10}$$

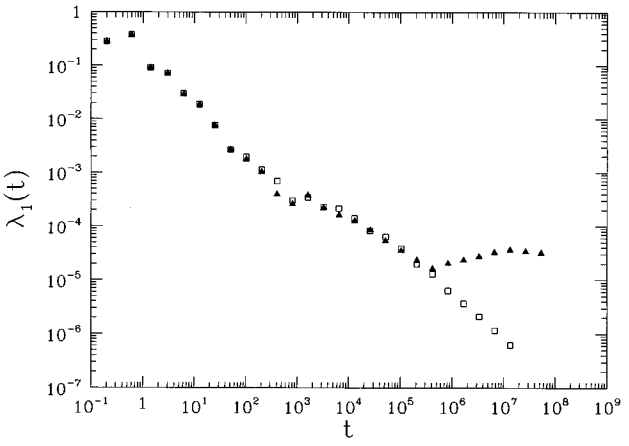

FIG. 1. $\lambda_1^{\mathrm{FPU}}(t)$ (solid triangles) and $\lambda_1^{\mathrm{Toda}}(t)$ (squares) are plotted vs time for $N=32$ and energy density $\epsilon=0.0217$ [which corresponds to an initial excitation amplitude $A=3$ in Eq. (4)]. Dividing t on the horizontal axis by π gives the time in units of the fastest period of the harmonic part of the chain, $T_{\min}=\pi$.

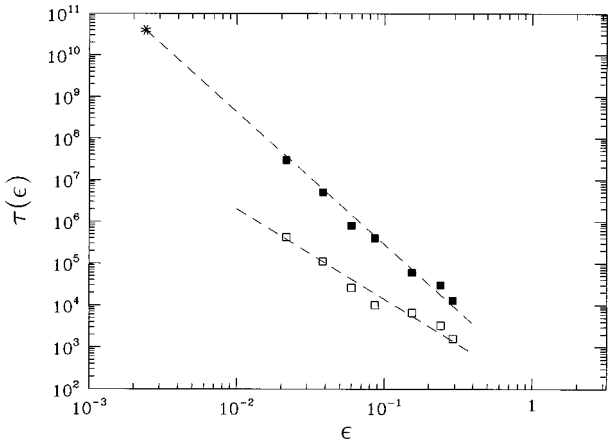

FIG. 2. The relaxation times to equipartition (full squares) and the trapping times (open squares) are plotted (for the FPU α model) vs the energy density ϵ for $N=32$ and the initial conditions of Eq. (4). The initial excitation amplitudes considered are, from left to right, $A=2,3,4,5,8,10,11$, respectively. The asterisk represents the extrapolation of the equipartition time to the case $A=1$ (FPU's original paper [20]).

By setting $\Lambda[x(t),\xi(t)]\equiv \xi^T\mathcal{J}[x(t)]\xi/\,\xi^T\xi=\xi^T\dot{\xi}/\,\xi^T\xi$ $=\frac{1}{2}(d/dt)\ln(\xi^T\xi)$, λ_1 can be formally expressed as a time average,

$$\lambda_1=\lim_{t\to\infty}\frac{1}{2t}\int_0^t d\tau\Lambda[x(\tau),\xi(\tau)], \tag{11}$$

which, in practice, is evaluated by computing [17]

$$\lambda_1(t_{\mathcal{N}})=\frac{1}{\mathcal{N}\Delta t}\sum_{n=1}^{\mathcal{N}}\ln\left(\frac{\|\xi(t_n)\|}{\|\xi(t_{n-1})\|}\right), \tag{12}$$

where $t_n=n\Delta t$ (Δt is some time interval), up to a final time $t_{\mathcal{N}}$, $n=\mathcal{N}$, such that $\lambda_1(t_{\mathcal{N}})$ has converged to a reasonably asymptotic value [18]. A positive asymptotic value of λ_1 obviously detects a chaotic dynamics, whereas $\lambda_1(t)\sim t^{-1}$ corresponds to a nonchaotic dynamics.

We have exploited the existence of an integrable model, the Toda lattice, close to the FPU α model. The Toda lattice Hamiltonian reads, in the same units as used in Eq. (1),

$$H(\mathbf{p},\mathbf{q})=\sum_{k=1}^{N}\left[\frac{1}{2}p_k^2+\frac{1}{4\alpha^2}\{\exp[-2\alpha(q_{k+1}-q_k)]+2\alpha(q_{k+1}-q_k)-1\}\right], \tag{13}$$

and the power series expansion of its potential coincides, up to third order, with the potential part of Eq. (1).

As the Toda lattice Hamiltonian describes an integrable system, the numerical computation of the time behavior of the largest Lyapunov exponent $\lambda_1(t)$ must reveal the nonchaotic property of its dynamics. In particular, one might wonder whether some information can be obtained by comparing $\lambda_1^{\mathrm{FPU}}(t)$ with $\lambda_1^{\mathrm{Toda}}(t)$ for the same initial conditions, i.e., $\{q_i(0),p_i(0)\}$, $i=1,\ldots,N$. This turns indeed out to be the case. In Fig. 1 we report, as an example, $\lambda_1^{\mathrm{FPU}}(t)$ and $\lambda_1^{\mathrm{Toda}}(t)$ in the case $N=32$ and $\epsilon=0.0217$ for an initial condition with $A=3$ in Eq. (4). Up until $t\simeq 2\times 10^5$ these two functions are so close to each other that the two are virtually indistinguishable. Then, suddenly, they separate at $t\geqslant 4\times 10^5$: $\lambda_1^{\mathrm{Toda}}(t)$ continues its decay toward zero, whereas $\lambda_1^{\mathrm{FPU}}(t)$ tends to converge to a nonvanishing value. This makes it possible to define clearly what a trapping time in a regular region of phase space is; moreover, its numerical determination is unambiguous, as it can be deduced by simply looking at Fig. 1. We attribute this dramatic difference to the untrapping of the FPU system from its regular region in phase space by escaping to the chaotic component of its phase space.

The peculiar behavior of $\lambda_1^{\mathrm{FPU}}(t)$ suggests therefore that nonintegrable motions, originated by one-mode initial excitations, after a transient, possibly long, trapping in a regular region of phase space, enter its chaotic component. The chaotic component of phase space, by the Poincaré-Fermi theorem [19], is connected, so that we may well expect that equipartition is eventually attained on a finite, albeit possibly very long, time scale.

The precise nature of the trapping mechanism is unclear to us. One could either think that the trajectories stick close to a KAM torus during the trapping time, or that, for example, they are geodesics of a bumpy manifold to which an N-torus has been differentiably glued by a tiny ''bridge;'' in that case a geodesic, originating at any point of the N-torus, is locally stable until it finds a path to escape from the torus. Another possible mechanism of trapping and escape is discussed in Sec. III under point (v), in light of the data discussed in the sequel of the present Section.

In conclusion, once we observe that a trajectory enters the chaotic component of phase space, we are allowed to think that equipartition will be eventually attained. In Fig. 2 the relaxation times to equipartition $\tau_E(\epsilon)$ and the trapping times $\tau_T(\epsilon)$, evaluated for the FPU α model, are shown. The results refer to $N=32$ and initial conditions given by Eq. (4). The initial excitation amplitudes A range from 3 to 11. The equipartition times appear to be between one and two orders of magnitude larger than the trapping times. If we extrapo-

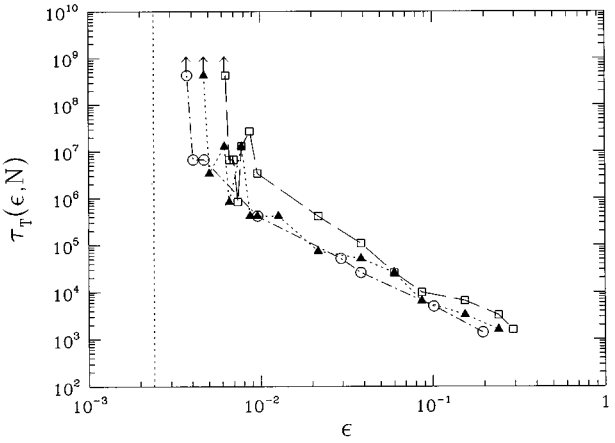

FIG. 3. The trapping times $\tau_T(\epsilon,N)$ at different values of energy density ϵ (i.e., at different values of the initial excitation amplitudes A), are reported. Open squares refer to the case $N=32$ (A ranges from 1.6 to 11), solid triangles refer to $N=64$ (A ranges from 1.4 to 10), open circles refer to $N=128$ (A ranges from 1.25 to 9), respectively. The endpoints of the broken lines are lower bounds for the trapping time (the cutoff of the integration time is at $t=4.3\times10^8$). The dotted vertical line at $\epsilon=0.002\,41$ corresponds to the initial excitation amplitude $A=1$ of FPU's original paper.

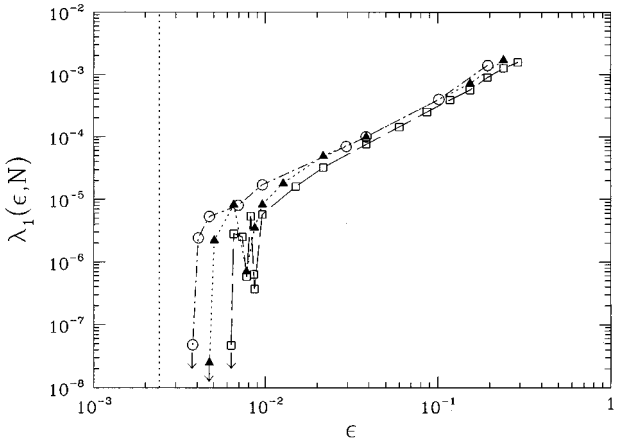

FIG. 4. The largest Lyapunov exponents $\lambda_1(\epsilon,N)$ are shown for different values of the energy density ϵ and a sine wave initially excited [Eq. (4)]. Open squares refer to $N=32$ and $n=1$, full triangles to $N=64$ and $n=2$, open circles to $N=128$ and $n=4$, respectively. The endpoints of the broken lines, marked by arrows, are upper bounds for the FPU Lyapunov exponents at $t=4.3\times10^8$ (cutoff of the integration time). The dotted vertical line at $\epsilon=0.002\,41$ corresponds to $A=1$ (FPU's original paper).

late [20] the equipartition time to the case of FPU, we find $\tau_E\simeq4\times10^{10}$ (as is indicated in Fig. 2 by an asterisk).

Since we can consider the FPU α model as a third order expansion of a Lennard-Jones potential around its minimum, we can tentatively extrapolate the equipartition times reported in Fig. 2 to a macroscopic system in three dimensions. As an example, we can roughly estimate what the physical equipartition time could be for a *classical* xenon crystal at zero temperature and only one normal mode initially excited. At $\epsilon=0.01$, $\tau_E\sim10^9$ proper times (see Fig. 2) corresponds to about 10^{-3} s, using as proper time, obtained with standard Lennard-Jones parameters for xenon, 2.4×10^{-12} s.

C. Stochasticity threshold

We have evaluated the trapping times $\tau_T(\epsilon,N)$ for the FPU α model at different values of both the energy density ϵ and of the number of degrees of freedom N. When N was varied, we kept the wavelength of the initial excitation constant [i.e., n in Eq. (4) is taken proportional to N: $n=1$ at $N=32$, $n=2$ at $N=64$, and $n=4$ at $N=128$], and we excited only one mode at $t=0$. The results are reported in Fig. 3. With decreasing ϵ, first τ_T tends to increase monotonically, then, abruptly, it displays an apparently divergent behavior. In fact, when reaching critical threshold values, a very small change in ϵ suddenly gives an extremely steep increase in τ_T. This very steep increase of τ_T with decreasing ϵ suggests at least a very narrow bottleneck in phase space, through which the system can only escape with great difficulty. We assume that this bottleneck is not an insurmountable barrier, and for that reason, as well as to conform with previous use, we will call it a *threshold*. This is consistent with the results of Fig. 4, where the largest Lyapunov exponents are reported for the same cases as in Fig. 3. We have used a cutoff of the integration time at $t=4.3\times10^8$. After such a long time, when ϵ was smaller than the threshold value, no separation between $\lambda_1^{\mathrm{Toda}}(t)$ and $\lambda_1^{\mathrm{FPU}}(t)$ has been observed: the values of λ_1^{FPU} at $t=4.3\times10^8$ (endpoints of broken lines in Fig. 4, marked by arrows) are taken as upper bounds for the FPU-Lyapunov exponents and $t=4.3\times10^8$ is taken as a lower bound for the trapping time of the FPU-phase point (endpoints of the broken lines in Fig. 3, marked by arrows). Both $\lambda_1(\epsilon,N)$ (from here on, by λ_1 we mean λ_1^{FPU}) and $\tau_T(\epsilon,N)$ strongly suggest the existence of an N-dependent threshold value of the energy (density), above which the motion is chaotic and below which the trajectories appear to be trapped in a regular region of phase space [*stochasticity threshold* (ST)].

The following approximate relationship between A and ϵ holds: $\epsilon\simeq0.002\,41A^2$, therefore the threshold amplitudes A_c leading to chaos are $A_c(N=32)\simeq1.62$, $A_c(N=64)\simeq1.42$, $A_c(N=128)\simeq1.28$, respectively.

The dotted line at $\epsilon=0.002\,41$ corresponds to the initial excitation amplitude $A=1$ of FPU's original paper. We see that Fermi and co-workers chose an initial condition well below this ST [20]. Figure 3 shows that if they had taken a ten times larger amplitude, they would have observed equipartition during the integration time they used. This appears to us to be the explanation of the lack of statistical mechanical behavior observed in the original FPU numerical experiment.

A few more comments on these results are as follows: (i) Fig. 3 suggests that with increasing N, $\tau_T(\epsilon,N)$ probably becomes less dependent on N [in fact the values of $\tau_T(\epsilon,N=64)$ are closer to those of $\tau_T(\epsilon,N=128)$ than to those of $\tau_T(\epsilon,N=32)$]; (ii) there is a narrow energy density interval where τ_T and λ_1 oscillate, suggesting the transition in phase space from chaotic behavior at large ϵ to regular behavior at small ϵ; (iii) the ST shows a weak but clear dependence on N (provided the wavelength of the initial excitation is kept constant). This is not surprising because if we combine two identical systems—each with the same initial excitation—the composite system will have new low fre-

quency modes that are absent in the separate subsystems, which can be expected to facilitate the mechanism of energy exchange among the normal modes.

As far as we are aware, the *direct* evidence given in Fig. 4 of the existence of a ST at $N \gg 2$, obtained through the behavior of the largest Lyapunov exponent, was never found before in nonlinear Hamiltonian systems. An *indirect* suggestion of its existence (through a ''freezing'' of the decay of the spectral entropy) has been given in [8] for the FPU β model.

D. Coexistence of order and chaos

A question now arises: does such a threshold refer to a global property of the constant energy surface Σ_E or is it, rather, a local property of Σ_E sensitive to the initial condition?

In order to answer this question, we have considered also the following initial conditions at $N=32$: (i) $A \neq 0$ [the fundamental mode—Eq. (4)—is excited with amplitudes ranging from $A=0.7$ to $A=5.5$] and $p_i(0) \neq 0$ $(i=1,\ldots,N)$ are Gaussian random numbers with zero mean and standard deviation (''temperature'') equal to 0.001; (ii) $A=0$, $q_i(0)=0$ $(i=1,\ldots,N)$, and $p_i(0)$ $(i=1,\ldots,N)$ are randomly chosen according to a Gaussian distribution.

In the first case, a fraction of the energy in the initial excitation is given to all the normal modes of the system: in so doing, we are displacing the starting point on Σ_E, proportional to the magnitude of the standard deviation of the noisy component of the initial excitation. This is intended to provide some information about the extension of the regular region(s) in phase space. If all, or almost all, the energy of the initial excitation is concentrated in one or a few modes, then we are dealing with a nonequilibrium initial condition; the existence of a ST entails then that a system, prepared in a nonequilibrium state below such a threshold, will appear never to attain equipartition of the energy of the initial excitation. The noisy component has a self-evident physical meaning related to the impossibility of preparing any physical system in a perfectly ordered initial state: at nonzero temperature some randomness in the initial conditions is unavoidable.

The second choice—completely random initial conditions—mimicks a physical situation that corresponds to a crystal prepared at an assigned temperature (i.e., mean kinetic energy per degree of freedom) at thermal equilibrium.

In Fig. 5 the effect of changing the initial conditions according to the above prescriptions is shown. Here $N=32$, the squares refer to $A \neq 0$ and no random component, the asterisks refer to only random initial excitations, and the starlike squares refer to $A \neq 0$ plus a random component.

In each case a threshold energy (or equivalently energy density, since N is fixed) is found. At $\epsilon > 0.01$, the uncertainties in the determination of λ_1 are of the order of the size of the symbols used; at $\epsilon < 0.01$, an estimate is difficult because of unpredictable fluctuations of $\lambda_1(t)$ that could be reduced only by prohibitively long integration times. Nevertheless, the information given by Fig. 5 is unambiguous. Down to $\epsilon \simeq 10^{-2}$ all the values of $\lambda_1(\epsilon)$, obtained with different initial conditions, crowd along the same line; below $\epsilon \simeq 10^{-2}$ the values of λ_1, obtained with different initial conditions,

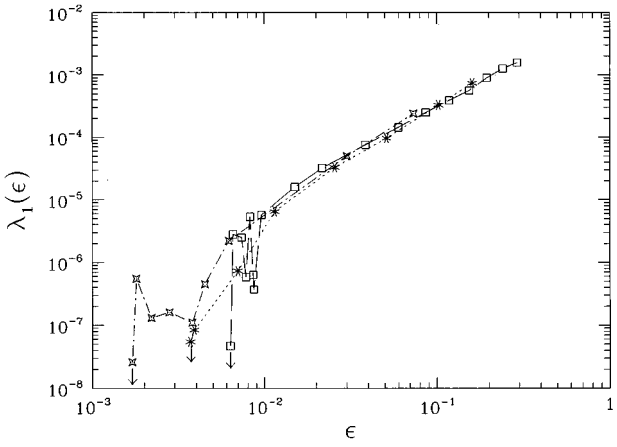

FIG. 5. The largest Lyapunov exponents $\lambda_1(\epsilon)$ are plotted, for $N=32$, at different values of ϵ and different initial conditions. Squares refer to the cases $A \neq 0$ and no random initial conditions, asterisks refer to the cases $A=0$ and random initial conditions, starlike squares to $A \neq 0$ and random initial conditions with zero mean and standard deviation 0.001. The endpoints of the broken lines, marked by arrows, are upper bounds for the FPU Lyapunov exponents at $t=4.3\times10^8$ (cutoff of the integration time).

separate and exhibit a coexistence of regular and chaotic regions on the constant energy surface in phase space, whose details depend on the initial conditions. Below $\epsilon \simeq 1.8\times10^{-3}$, even with only random initial conditions, the motions are regular (starlike squares).

This tells us that the phase space undergoes some important structural change as a function of the energy, in analogy with what is observed in two-degrees-of-freedom systems, like the Hénon-Heiles model [21], where fully developed chaos, a coexistence of regular and chaotic regions of phase space, or only regular trajectories, are observed, depending on the value of the energy.

E. N dependence of the stochasticity threshold

An important question is the stability or instability of the stochasticity threshold with N. To this end we have numerically determined $\lambda_1(\epsilon,N)$ at $N=8,16,32,64$ always choosing random initial conditions, i.e., $\{q_i(0)=0,\ p_i(0)=r_i\}$, $i=1,\ldots,N$, with r_i Gauss-distributed random numbers with zero mean and variance $\sqrt{2\epsilon}$ (after the assignment of the random values r_i, the momenta are adjusted, by rescaling them, in order to obtain a fixed initial ϵ).

In Fig. 6 the outcome of these computations is reported. The endpoints of the broken lines have the same meaning as already discussed above. At large ϵ there is a tendency of all the sets of points to join. This fact is most evident for $N=32$ and $N=64$ which have a line segment in common and then separate at small ϵ: the larger N, the smaller the ϵ at which the separation occurs.

At each N, we take as a rough estimate of the stochasticity threshold ϵ_c the value of ϵ at the midpoint between the two lowest points on each curve, because the lowest point (marked by an arrow) is presumably below threshold.

Figure 7 then shows that for these threshold values ϵ_c plotted vs N holds: $\epsilon_c(N) \sim 1/N^2$. This result is interesting for the following reasons.

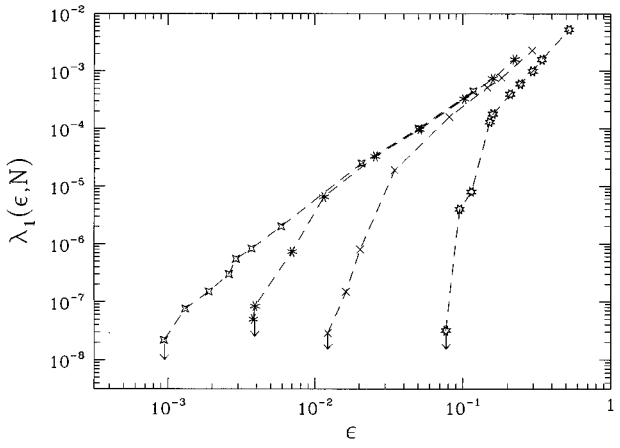

FIG. 6. The largest Lyapunov exponents $\lambda_1(\epsilon,N)$ are plotted vs the energy density ϵ, for different values of N. Random initial conditions are chosen. Starlike polygons refer to $N=8$, crosses to $N=16$, asterisks to $N=32$, starlike squares to $N=64$, respectively. The endpoints of the broken lines, marked by arrows, are upper bounds for the FPU Lyapunov exponents at $t=4.3\times10^8$ (cutoff of the integration time).

(i) The threshold values vanish sufficiently fast with increasing N, so that the existence of regular regions of phase space below ϵ_c does not constitute a problem for *equilibrium* statistical mechanics. In fact, it appears that $N=32,\ldots,128$ is not too small to obtain indications, if not ''confirmation,'' of the statistical mechanical behavior of the FPU α system.

(ii) Both the values of ϵ_c and the N dependence $\epsilon_c(N)\sim1/N^2$ can hardly be explained on the basis of the best available estimate of the perturbation amplitudes for which a positive measure of the regular KAM regions in phase space exists: $\mu<\mu_c\sim a\exp(-bN\ln N)$ [23], where μ measures the relative strength of the anharmonic to the harmonic part of a given Hamiltonian (μ depends on ϵ), μ_c is a threshold value, a and b are constants. There are also power-law estimates for $\mu_c(N)$, i.e., $\mu_c(N)\sim N^{-\delta}$, obtained in the context of KAM theory [24]; however, at present, δ is still very large: $\delta\simeq160$.

(iii) The bounds on the threshold value $1/4\alpha^2N\leqslant\epsilon_c\leqslant1/2\alpha^2N$ found by Enz *et al.* for the FPU α model [22] predict an N dependence which is in much better agreement with our results than the exponential drop with N mentioned in the preceding point.

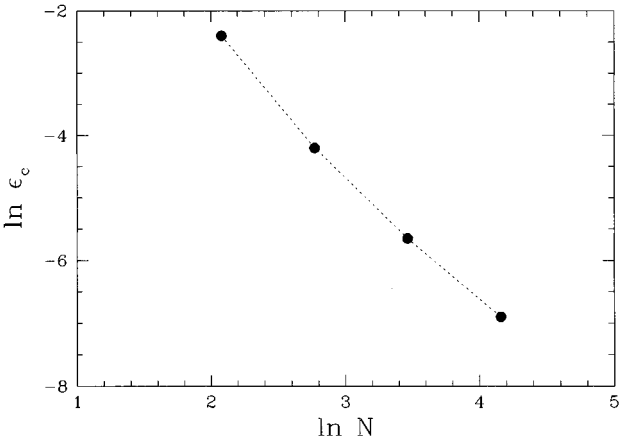

FIG. 7. The values of the stochasticity thresholds ϵ_c are plotted for different values of N (for the estimate of ϵ_c, see text).

III. DISCUSSION

We conclude with the following remarks.

(i) It is worth mentioning that recently the existence of an equipartition threshold vanishing at increasing N has also been reported for the FPU β model [8,25,26]. It is inappropriate to compare these results *quantitatively* with ours: our model is different and the evidence for a stochasticity threshold for the FPU β model has been obtained indirectly, through the opening of a local trap in phase space, which prevented equipartition. However, we can say that both results are in *qualitative* agreement: threshold effects, either concerning transient dynamics to equipartition of nonequilibrium initial conditions (studied through spectral entropy) or concerning the dynamics of equilibrium initial conditions [studied through $\lambda_1(\epsilon,N)$], vanish at increasing N.

A qualitative agreement about the vanishing with N of the critical energy to get chaos is reported in a recent paper on the FPU α model [27].

The question of how to explain the existence and the $1/N^2$ dependence of the stochasticity threshold reported here, remains open.

(ii) In this paper we report the existence of two interesting phenomena among others: the apparent existence of regular regions in the phase space of a nonintegrable Hamiltonian system as is the FPU α model and the existence of almost regular regions of phase space where the trajectories are trapped during long but finite times. These phenomena are reminiscent of the KAM and Nekhoroshev [28] theorems, respectively. We have already discussed throughout the paper why our results disagree with the present-day quantitative predictions of the KAM theorem. Similarly, the Nekhoroshev theorem does not seem to be able to provide an explanation of the observed phenomenology as well. In fact, without entering into the details of how a thorough comparison with our results could be made, Nekhoroshev's estimate of the lower bound of the ''trapping'' time T of a trajectory close to its initial condition is $T\simeq\exp(c/\mu)^{\gamma(N)}$, where c is a constant, μ has the same meaning as above, and $\gamma(N)\sim1/8N$ is the optimal N dependence [29] of the exponent. Hence for $N=32,64,128$, as is the case of the results of Fig. 3 for $\tau_T(\epsilon,N)$, the ''Nekhoroshev trapping'' time T is $O(1)$ independently of μ (thus of ϵ). Therefore, it appears that the physical mechanisms responsible for finite time trapping in phase space, which are behind the Nekhoroshev theorem and our numeric phenomenology, respectively, are different. Thus we emphasize the difference between, on the one hand, the approach to infinite time trapping (KAM theorem) and to finite time trapping (Nekhoroshev theorem) based on the description of the persistence of certain local properties of regular regions of phase space, and, on the other hand, our chaos-related approach, based on the comparison of $\lambda_1(t)$ for the FPU and Toda lattices (Fig. 1). The behavior of $\lambda_1(t)$ suggests that the sudden escape from the regular region occurs as if the trajectory would eventually find a ''hole'' in its boundary.

(iii) It is not out of place to note that while the ST drops

to zero as $N \to \infty$ in the FPU α model, there is another transition phenomenon that does not suffer this N dependence: it is the strong stochasticity threshold (SST) that concerns a transition from weak to strong chaos [15,16], which has been discovered in the FPU β model and in the lattice φ^4 model. Unfortunately, this SST cannot be investigated in the FPU α model because the cubic potential prevents working at too large energy. We note, however, that the stability with N of the SST makes the SST not only a dynamical phenomenon related to dynamical chaos, but also of potential interest to statistical mechanical phenomena.

(iv) The existence of special initial conditions that create nontrivial dynamical behavior, though irrelevant for *equilibrium* statistical mechanics because of their negligible measure, could be physically relevant for transient *nonequilibrium* statistical mechanics if we can conceive an operational method to prepare a real system in such a special initial state (see, for example, [30]).

(v) Let us comment about the classical explanation of the nonstatistical mechanical behavior of the FPU model proposed by Zabusky *et al.* [3,4], based on the existence of soliton solutions of the Korteweg–de Vries (KdV) equation, derived as a special continuum limit of the FPU α model. Their experiments were carried out over much shorter time scales than those that are possible nowadays. As we have seen above, thanks to very long numerical integrations, it turns out that, below a threshold, regular regions of phase space can coexist with chaotic ones. In light of our results, we can thus assert that the KdV soliton solutions belong to the regular region of phase space of the FPU system from which—after sufficiently long time—escape will occur to the chaotic component of phase space.

In Fig. 8 the patterns of the displacements q_i as a function of position i are shown at different times in the case $N=32$, $A=3$. For times t below the trapping time $\tau_T \simeq 4\times10^5$, they are looking as regular structures, apparently composed of a superposition of a small number of waves, which display a trapping and a solitonlike recurrence [see Fig. 8(b)], similar to that observed by Zabusky and Kruskal [3] and Tuck and Menzel [31], although we have fixed boundary conditions, as in FPU's original paper, rather than periodic boundary conditions as considered by Zabusky and Kruskal. For $t > \tau_T$ we observed a gradual untrapping or decay of these regular features due to more and more complicated structures consisting of a superposition of an increasing number of different waves (radiated by the decaying solitons [4]). Finally, for $t > 10^8$, an almost noisy pattern is attained [see Fig. 8(c)] as well as energy equipartition (detected through the spectral entropy). This demonstrates clearly the compatibility of the existence of trapping, i.e., very long-lived regular solutions, and the attainment of equipartition, albeit after possibly very long times. It is still an open question whether, at fixed N, below the stochasticity threshold, i.e., at energy density such that the largest Lyapunov exponent seems to vanish for any initial condition, the lifetime of regular solutions might actually diverge.

However, we have found that this threshold energy density drops to zero as $\sim 1/N^2$. Therefore it appears to us that at sufficiently large N the existence of KdV solitons does not hinder a good statistical mechanical behavior of the FPU system.

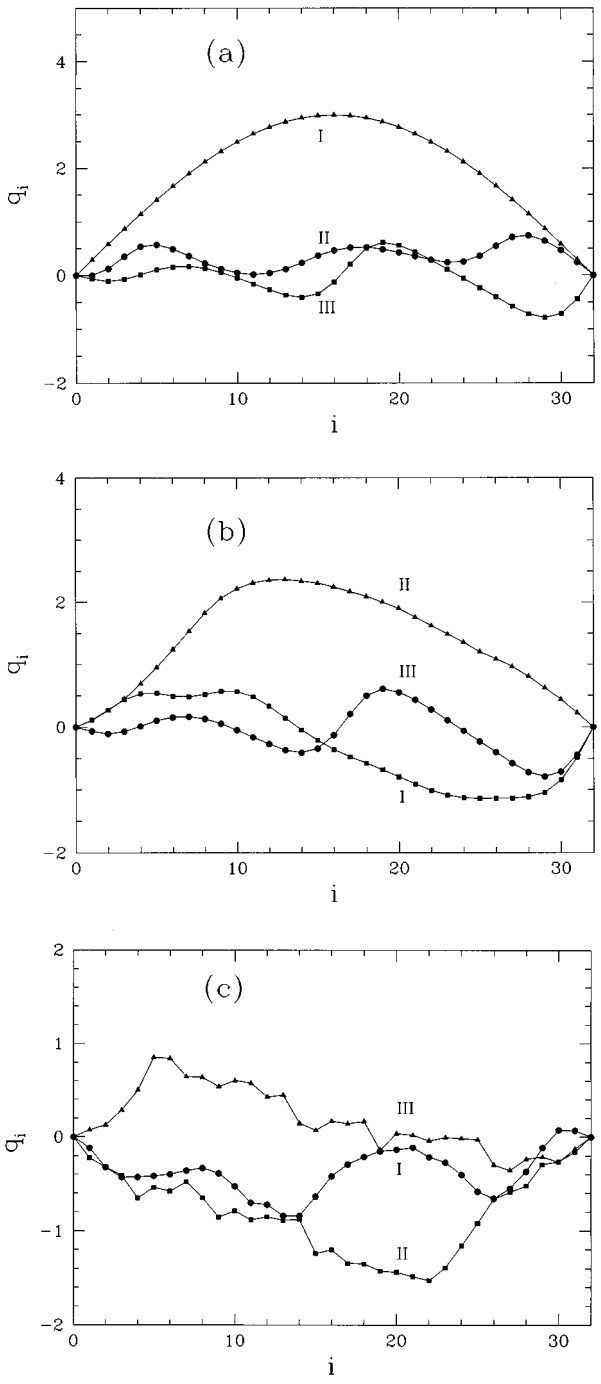

FIG. 8. Snapshots of the displacements q_i of 32 FPU α particles as a function of position i along the chain shown at different times. Here the initial amplitude is $A=3$—as in Fig. 1—for a sine wave [see Eq. (4)]. (a) Ordered configurations at $t=0$ (I), 10^4 (II), and 5×10^4 (III); (b) Ordered configurations at $t=10^5$ (I), 2×10^5 (II), and 4.2×10^5 (III); note the almost recurrence at $t=2\times10^5$; (c) $t=1.6\times10^6$ (I), 5.4×10^7 (II), and 2×10^8 (III). Note the increasing disorder of the configurations in (c), corresponding to the onset of a chaotic dynamics in the system, due to the breakup of regular solitonlike structures, and to its approach to equipartition.

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