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Relaxation to different stationary states in the Fermi-Pasta-Ulam model

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The Fermi-Pasta-Ulam model has been studied following the time evolution of the space Fourier spectrum through the numerical integration of the equations of motion for a system of 128 nonlinearly coupled oscillators. One-mode and multimode excitations have been considered as initial conditions; in the former case, an approximate analytic technique has been applied to describe the "short-time" behavior of the system, which fits well the experiment. The main result in both cases is the presence of different stationary states towards which the system is evolving: a $1/k^2$ spectrum (corresponding to the equipartition of energy) or an exponential spectrum can be reached, depending on the value of some parameter, which takes into account the relative weight of the nonlinear to the linear term of the equations of motion.

I. INTRODUCTION

In recent years there has been a considerable effort in the study of nonlinear Hamiltonian systems. Only a general analytical result is available: the Komolgorov-Arnol'd-Moser (KAM) theorem,[1] which states the regularity of most phase trajectories of a Hamiltonian system with a finite number of degrees of freedom when the nonlinear term is sufficiently weak.

A great number of studies have been devoted to these problems using numerical techniques. Historically the first attempt in this direction goes back to the famous work by Fermi, Pasta, and Ulam (FPU)[2]; they integrated with the aid of one of the first electronic computers the equations of motion of a chain of oscillators nonlinearly coupled by a derivative potential (for mathematical details see Sec. II). Their result showed "... very little, if any, tendency toward equipartition of energy among the degrees of freedom."[2] From then on several authors attempted to investigate numerically the ergodic behavior of nonlinear Hamiltonian systems, sometimes using analytical approximations.[3-7]

It has been shown with great accuracy the presence of a stochasticity threshold in systems with a few number N of degrees of freedom ($N=2$–10). Usually the energy E is the control parameter[8]: If E is lower than some "critical" value E_c, the motion is ordered; on the contrary, if it is higher than E_c, some phase-space regions show a "chaotic" motion. However, if one considers the measure $\mu(E)$ of the regions of ordered motions in the phase space as a function of the energy, one realizes that the threshold is not very sharp and, moreover, chaotic regions are present also below E_c and disappear only in the limit $E \to 0$ (see, e.g., the study of the Hénon-Heiles model[8]).

In the case of a system with a great number of degrees of freedom (as the FPU model) even the presence of a stochasticity threshold is still an open problem. E_c can hardly be determined by the usual techniques as, e.g., the study of Poincaré maps, which would lead to a huge number of phase-space sections.

Some authors studied numerically the FPU model,[6] the case of a Lennard-Jones potential,[9] and a $\lambda\phi^4$ model.[10] In all these cases they claim to find some evidence that the stochasticity threshold is still present in the limit $N \to \infty$ and, moreover, that $E_c \sim \omega_{\text{exc}}$, where ω_{exc} is the frequency of the initially excited mode. On the other hand, Izrailev and Chirikov,[3] studying the FPU model by an analytic approach based on the Bogoliubov-Krylov resonance technique, obtain $E_c \to 0$ as $N \to \infty$, when high-frequency modes are excited. At present, numerical confirmation of this result is not available. In a recent work[7] involving some authors of this paper, a discretized version of the $\lambda\phi^4$ model ($N=64$ and 128) has been studied numerically. An analytic approach has been also proposed, based on a technique first introduced by Frisch and Morf.[11] It has been shown that the system, at least for sufficiently high values of the coupling constant λ and of the energy E, approaches the equilibrium with a characteristic long-time scale which is a smooth function of the initial conditions. As will be clearly shown in this paper, this conclusion can be hardly extended to the range of small values of λ and E for which the system reaches a stationary state which does not correspond to the equipartition of energy.

Apart from the usual problem of choosing a good numerical algorithm in the integration of the system of differential equations, a much more relevant question is present when one wishes to study the transition to chaotic motion.

What is the quantity one has to compute to reveal whether the system is in the "chaotic phase" and is relaxing to equilibrium? Galgani and collaborators suggest the use of two kinds of "stochasticity parameters": (i) $p_k=(E_k^{\max}-E_k^{\min})/E_k^{\max}$, where $E_k^{\max}$ and $E_k^{\min}$ are, respectively, the maximum and the minimum of the energy E_k of the group of initially excited modes and (ii) λ_M, the maximal Lyapounov exponent.[12]

The use of such parameters shows the chaotic transition but hardly permits a direct intuition of the physical situation under analysis for systems with a great number of degrees of freedom. For instance, a large p_k does not necessarily imply that equipartition has set in: It may happen that the initially excited modes give the neighboring modes energy while the system is not globally involved in the chaotic behavior. A similar argument is valid for λ_M: $\lambda_M>0$ does not necessarily mean that all the degrees of freedom have a chaotic behavior. For instance, $\lambda_M>0$ does not necessarily imply ergodicity; it may happen that the energy surface is divided into invariant components, each with $\lambda_M>0$ (see an example in Ref. 9). It may happen that a portion of the accessible phase space is "chaotic" while the remaining part shows an ordered motion.

Another proposal, recently advanced by Benettin and Tenenbaum,[13] is to use time correlation functions of carefully chosen observables, for instance, the $E_k(t)$ autocorrelation and cross correlation functions. Also this method allows a precise determination of the chaotic transition, but does not give a global information on the phase space. The criticism addressed to microcanonical time correlation functions[14,15] does not apply to this approach because the authors of Ref. 13 consider time averages over single trajectories.

Apart from such difficulties there is also another point: The above-mentioned stochasticity parameters, excluding the last one, have been introduced with the implicit assumption of dynamical equilibrium, while the system may be in a state of slow relaxation toward it (as shown in the paper by Fucito *et al.*[7] for the $\lambda\phi^4$ theory). The choice of a good parameter is consequently crucial to reach a physical understanding of the approach to equilibrium of the system.

We are led from our analysis to the use of a parameter which (i) does not suffer the limitation of being "local" in the k space (as the p_k and λ_M), (ii) takes into account possible nonstationary situations, and (iii) is quite easy to compute. As in Refs. 7 and 16 we have used a parameter which directly measures the "degree of equipartition" of energy and also its variation in time. It is the slope $S(t)$ of the power spectrum W of the field $\phi(x,t)$ (see Sec. II),

$$W(k,t)\sim\exp[-S(t)k] \quad \text{as } k\to\infty \ .$$

It is evident that the main limit of the use of $S(t)$ is related to the assumption that the spectrum is exponentially shaped, but there are valid analytical evidences and also numerical indications to consider such a shape universal, at least when the first modes are excited (see Sec. III). In Sec. II we shall introduce the model and present an analytic approximation of the short-time behavior of the system. Section III will be devoted to the numerical results and to the phenomenological analysis of the long-time behavior and of different initial conditions.

II. DESCRIPTION OF THE MODEL AND ANALYTICAL STUDY OF THE SHORT-TIME BEHAVIOR

The model we consider in this paper is the celebrated Fermi, Pasta, and Ulam β model (FPU) whose Hamiltonian is[17]

$$H=\sum_{i=1}^{N}\left[\frac{1}{2}\pi_i^2+\frac{1}{2}v^2\left[\frac{\phi_i-\phi_{i+1}}{a}\right]^2+\frac{1}{4}\beta\left[\frac{\phi_i-\phi_{i+1}}{a}\right]^4\right], \tag{1}$$

representing a chain with spacing a of N nonlinearly coupled oscillators. π_i is the moment conjugate to ϕ_i (i.e., in this case $\pi_i=\dot{\phi}_i$) and v is the velocity of sound in the limit $\beta\to 0$. We choose periodic boundary conditions, $\phi_1=\phi_N$. From the Hamiltonian (1) one obtains the equation of motion

$$\ddot{\phi}_i=\frac{v^2}{a^2}(\phi_{i+1}+\phi_{i-1}-2\phi_i)+\frac{\beta}{a^4}[(\phi_{i+1}-\phi_i)^3-(\phi_i-\phi_{i-1})^3]\ , \tag{2}$$

which in the limit $a\to 0$ (Ref. 18) gives

$$\frac{\partial^2}{\partial t^2}\phi(x,t)=v^2\frac{\partial^2}{\partial x^2}\phi(x,t)+\beta\frac{\partial}{\partial x}\left[\frac{\partial}{\partial x}\phi(x,t)\right]^3 . \tag{3}$$

Our purpose is the investigation of the energy transfer among the different wave numbers; consequently, we introduce the space Fourier transform of the field $\phi(x,t)$ on the interval $I=Na$ ($N\to\infty$ so that Na remains finite) as follows:

$$\tilde{\phi}(k_n,t)=(2\pi)^{-1/2}\int_{[I]}dx\,\exp(-ik_nx)\phi(x,t)\ , \tag{4}$$

where $k_n=2\pi n/Na$ and where $n\in\mathbf{Z}$. The equations for the field $\tilde{\phi}(k_n,t)$ are of the form

$$\frac{\partial^2}{\partial t^2}\tilde{\phi}(k_n,t)=-v^2k_n^2\tilde{\phi}(k_n,t)+3\beta\sum_{k_{n'}k_{n''}} k_{n'}^2(k_{n''}-k_{n'})(k_n-k_{n''})\tilde{\phi}(k_{n'},t)\tilde{\phi}(k_{n''}-k_{n'},t)\tilde{\phi}(k_n-k_{n''},t) , \tag{5}$$

which shows that the effect of the nonlinear term is to couple different wave numbers. The way in which the excitation of the modes proceeds in time ($t\rightarrow t+\epsilon$) once a given set of modes is already excited is described by Eq. (5). If the arguments of the cubic term on the rhs of Eq. (5) are labeled by the index n of the wave number and refer to the excited modes n'_{exc}, n''_{exc}, n'''_{exc}, one derives by summing the arguments

$$n(t+\epsilon)=n'_{\text{exc}}(t)+n''_{\text{exc}}(t)+n'''_{\text{exc}}(t) . \tag{6}$$

From this relation it is easy to obtain that if a single mode labeled by $\bar{n}$ is excited at $t=0$, the resulting excitation involves the modes satisfying the relation

$$n_m=(2m+1)\bar{n} , \tag{7}$$

where $m=1,2,\ldots,$. We shall refer to the excited modes which satisfy the relations (6) and (7) as "resonant" modes. As far as the analytical analysis is concerned we shall restrict to initial conditions of the type

$$\begin{aligned}\phi_0&=\phi(x,0)=A\sin(k_{\text{exc}}x) ,\\ \dot{\phi}_0&=\frac{\partial}{\partial t}\phi(x,t)\,|_{t=0}=0 .\end{aligned} \tag{8}$$

We are interested in the time evolution of

$$W(k,t)=|\tilde{\phi}(k,t)|^2 \tag{9}$$

in the region $k\gg k_{\text{exc}}$.

If the distribution were of Boltzmann type at long times, we would have the following asymptotic value of $W(k,t)$ for large k:

$$\langle W(k,t)\rangle\sim k^{-2} , \tag{10}$$

where the brackets stand for a smoothing in time.

A typical $\phi(x,t)$ corresponding to the behavior of W in Eq. (10) would be nondifferentiable in x. Now $\phi(x,0)$ is an analytic function of x and one can show that the solution $\phi(x,t)$ will also remain analytic. Equation (10) can only be valid for infinite time.

If at finite times the extension into the complex plane $\Phi(z,t)$ of the field is analytic and we neglect a possible prefactor such as $(k)^{-\alpha}$ (where α depends on the nature of the singularity), the k behavior will be given by

$$\begin{aligned}&W(k,t)\sim\exp[-S(t)k] ,\\ &S(t)=2y_s(t) ,\end{aligned} \tag{11}$$

where y_s is the imaginary part of the nearest singularity to the real axis of the analytic continuation of the function $\phi(x,t)$ in the complex plane: for instance, if the singularity is a simple pole (or a branch point) y_s is the imaginary part of the pole (or branch point).

It is clear that this singularity can only be at $y_s=\infty$ at $t=0$ if the initial condition is the analytic continuation of (8). We shall see that the singularities set in at finite y_s as time increases.

We shall present in this section an heuristic analytic evaluation of the function $S(t)$ which will be compared with the numerical simulations of Eq. (2) in the following section. We shall investigate the "short-time" evolution of the system; the meaning of "short" will be clearer when we discuss the numerical results.

The singularities of the analytic continuation $\Phi(z,t)$ of the solution $\phi(x,t)$ of Eq. (3) are certainly not poles, by naive power counting. On the other hand, the correct identification of the nature of the singularities is beyond the aims of this paper, since we are interested in simple spectral properties of the field. However, it is possible to estimate the variable $S(t)$ in Eq. (11) at short times, at least for initial conditions given by Eq. (8), exploiting the following idea.

We approximate Eq. (3) with an "effective" field equation whose singularities are poles and we study the motion of these poles as in Ref. 7. It is clear that this procedure can only work at short times and with this particular choice of the initial conditions. If we rewrite Eq. (3) in terms of the field $\psi(x,t)=(\partial/\partial x)\phi(x,t)$, we obtain

$$\frac{\partial^2}{\partial t^2}\psi(x,t)=\frac{\partial^2}{\partial x^2}[v^2\psi(x,t)+\beta\psi^3(x,t)] . \tag{12}$$

Once the initial condition (8) is inserted in the rhs of Eq. (12), it reduces to

$$c_1\psi(x,0)+c_2\psi^3(x,0) , \tag{13}$$

where $c_1=-k_{\text{exc}}^2(v^2-6\beta k_{\text{exc}}^2A^2)$ and $c_2=-9\beta k_{\text{exc}}^2$. If we assume that the form (13) still holds at $t=0^+$, then the equation of motion (12) becomes simpler,

$$\frac{\partial^2}{\partial t^2}\psi(x,t)=c_1\psi(x,t)+c_2\psi^3(x,t) . \tag{14}$$

We shall deal with the modified problem (14) which is an approximation of problem (12) at short times. An easy way of extracting the spectrum of $\psi(x,t)$ is to solve Eq. (14) by an extension of the method due to Frisch and Morf.[11] The method consists of the analytic continuation of the field $\psi(x,t)$ and then in solving the equations

$$\begin{aligned}&\frac{\partial^2}{\partial t^2}\Psi_R=c_1\Psi_R-c_2(\Psi_R^3-3\Psi_R\Psi_I^2) ,\\ &\frac{\partial^2}{\partial t^2}\Psi_I=c_1\Psi_I+c_2(\Psi_I^3-3\Psi_R^2\Psi_I) ,\end{aligned} \tag{15}$$

where $\Psi=\Psi_R+i\Psi_I$. The force field associated with Eqs. (15) shows the presence of a pair of unstable points located on the imaginary axis at $\Psi_I=\pm(c_1/c_2)^{1/2}$. This is the origin of the development of the singularities of the field Ψ. Following the analysis developed for the ϕ^4 theory, we may assume that these singularities are simple poles, whose location in the complex plane can be determined by computing the time T needed to reach infinity starting from a given point on the imaginary axis $\text{Im}\Psi_0$ corresponding to the chosen initial condition

$$T(\Psi_0)\simeq c_2^{-1/2}\,|\text{Im}\Psi_0|^{-1} , \tag{16}$$

when $\text{Im}\Psi_0 \gg (c_1/c_2)^{1/2}$. The initial condition (8) yields in the complex plane

$$\Psi_0(x+iy) = Ak_{\text{exc}}[\cos(k_{\text{exc}}x)\cosh(k_{\text{exc}}y) - i\sin(k_{\text{exc}}x)\sinh(k_{\text{exc}}y)] \,. \quad (17)$$

Therefore for large y one obtains

$$\text{Im}\Psi_0 \propto Ak_{\text{exc}}\exp(k_{\text{exc}}|y|) \,. \quad (18)$$

By combining Eqs. (16) and (18), according to the hypothesis of the presence at finite times of only pole singularities located at $z_s = x_s + iy_s$, we obtain

$$|y_s(t)| \propto -\frac{1}{k_{\text{exc}}}\ln(\beta^{1/2}Ak_{\text{exc}}^2 t) \,. \quad (19)$$

This behavior has also been found for the ϕ^4 and ϕ^6 theories, suggesting that such a law is universal for bounded polynomial or derivative potentials, whenever it is possible to perform the above-discussed approximations which lead to "effective-pole" singularities. In the case of a ϕ^4 theory these singularities (poles) have been located by Padé approximant methods[19] and they move following the predicted law in Ref. 7.

III. NUMERICAL RESULTS

The Fourier transform of the discretized field ϕ_i obeying Eq. (2) is defined in our case as

$$\phi_j(t) = (2\pi)^{-1/2}\sum_{n=1}^{N/2}\left[a_n(t)\cos\left[\frac{2\pi n}{N}(j-1)\right] + b_n(t)\sin\left[\frac{2\pi n}{N}(j-1)\right]\right], \quad (20)$$

where $a_n(t)$ and $b_n(t)$ are, respectively, the cosine and sine Fourier integral of $\phi_i(t)$. The constant term is not present because of the initial conditions we have chosen and of the invariance of Eq. (3) with respect to parity $x \to -x$.

The spacing a is taken equal to 1, so that the length of the chain is N.

The interesting quantity $W_n(t)$ is defined as

$$W_n(t) = |a_n(t)|^2 + |b_n(t)|^2 \,, \quad (21)$$

we have performed simulations for $N = 128$. The integration of Eqs. (2) was made by means of the leap-frog algorithm

$$\phi_i(t+\Delta t) = 2\phi_i(t) - \phi_i(t-\Delta t) + (\Delta t)^2 F_i(\{\phi_i(t)\}) \,, \quad (22)$$

where the discretized force is given by

$$F_i(\{\phi_i\}) = (\phi_{i+1} + \phi_{i-1} - 2\phi_i) + \beta[(\phi_{i+1}-\phi_i)^3 - (\phi_i - \phi_{i-1})^3] \,. \quad (23)$$

In the limit $\Delta t \to 0$ Eq. (3) is recovered up to $O(\Delta t^2)$. The initial condition $\dot{\phi}_i = 0$ is imposed by $\phi_i(-\Delta t) = \phi_i(0)$. Equations (2) have been integrated numerically using a VAX-750 and a CDC-CY76 computer in double precision and the coefficients $W_n(t)$ have been evaluated with a fast-Fourier-transform code.

To improve the statistics we perform a smoothing operation of the spectrum $W_n(t)$ centered around the time t,

$$\langle W_n(t)\rangle = \frac{1}{T}\int_{t-T/2}^{t+T/2} dt' W_n(t') \,, \quad (24)$$

the slope $S(t) = 2|y_s(t)|$ at any time t is given by the following relation:

$$\langle W_n(t)\rangle \sim \exp[-k_n S(t)], \quad k_n = \frac{2\pi n}{N} \,. \quad (25)$$

The exponential tail of the spectrum is in very good agreement with the results of the numerical experiments performed with low modes initially excited; a typical example is shown in Fig. 1. Several initial conditions have been analyzed.

A. One-mode excitations

For an integration time $t < 10$ ($\Delta t = 10^{-4} \approx 3\times 10^{-5}$ T where $T = \pi$ is the smallest period of the harmonic chain) the law described by Eq. (19) is very well verified by the numerical results at fixed k_{exc}, as is shown in Fig. 2. As far as the k_{exc} dependence is concerned we have verified the prediction of Eq. (19) as it is reported in Fig. 3. As the system further evolves in time (we have taken $\Delta t = 0.1$ from now on) the law (19) modifies into some different behaviors, depending on the values of β, A, and k_{exc}.

Roughly we observe at small βA^2 (< 10) a decoupling of the β dependence from the t dependence. The law seems to be

$$S \sim a_1\left[\ln\left[\frac{t}{\tau}\right]\right]^{1/2} + a_2\ln\left[\frac{\beta A^2}{\eta}\right], \quad (26)$$

where a_1, a_2, η, τ are dimensional constants. This kind of behavior is shown in Figs. 4(a) and 4(b).

A different situation appears for larger values of βA^2, where the slope seems to behave as

$$S \sim a_3\ln\left[\frac{1}{a_4}(\beta A^2)^{\alpha_1}t^{\alpha_2}\right] \quad (27)$$

as shown in Figs. 5(a) and 5(b). The departure from the

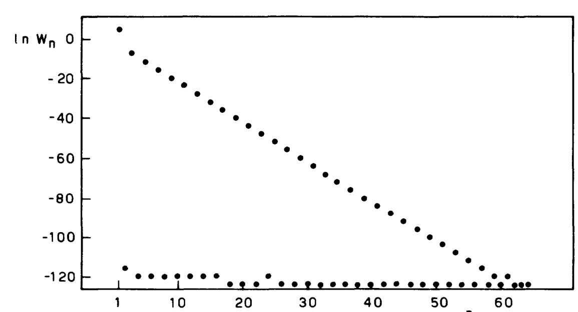

FIG. 1. Typical exponential spectrum at $t = 4000$ for $n_{\text{exc}} = 1$ [$k_{\text{exc}} = (2\pi/N)n_{\text{exc}}$]; $\beta = 2$ and $A = 1$; the integration time step of the equations of motion is $\Delta t = 10^{-1}$.

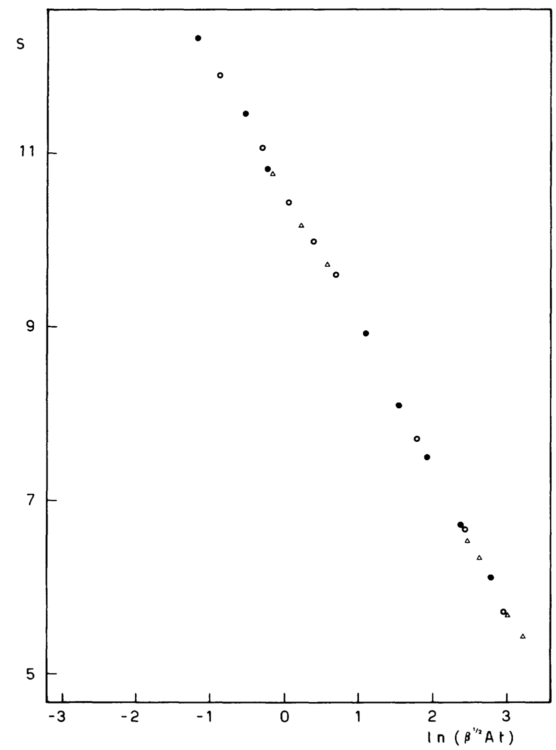

FIG. 2. Short-time dependence of the slope $S(t)$ of the exponential spectrum. The solid circles correspond to $\beta=1$, $A=5$; the open circles to $\beta=1.5$, $A=5$; and the triangles to $\beta=2$, $A=1$. For all these points $n_{\mathrm{exc}}=1$, $\Delta t=10^{-4}$, and t is up to ~ 10.

time regime described by Eq. (19), where the evolution of the slope scales with respect to the nonlinear characteristic time $\tau_{\mathrm{NL}}=(\beta^{1/2}Ak^2)^{-1}$, i.e., the nonlinear term dominates, is due to the influence of the linear term of the differential equation (3). In the case of strong nonlinearity this effect amounts to a slight modification of the time scale of Eq. (19), determining the new behavior given by Eq. (27). Instead, for weak nonlinearities the situation is more complicated resulting into a drastic modification of the time dependence from $\ln t$ to $(\ln t)^{1/2}$. In general, one can say that this intermediate-time region is no longer characterized by the universal features which we have met for the short-time regime that is dominated by the nonlinear term for large values of S, while for smaller values of S a competition between the linear and nonlinear term

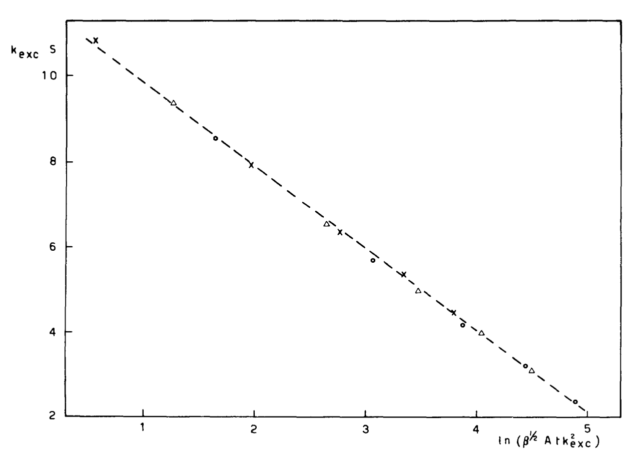

FIG. 3. k_{exc} dependence of the slope at short times; $\beta=0.5$, $A=5$ with $n_{\mathrm{exc}}=1,\ldots,5$ and $\Delta t=10^{-4}$. The crosses refer to $t=0.5$, the triangles to $t=1$, and the open circles to $t=1.5$.

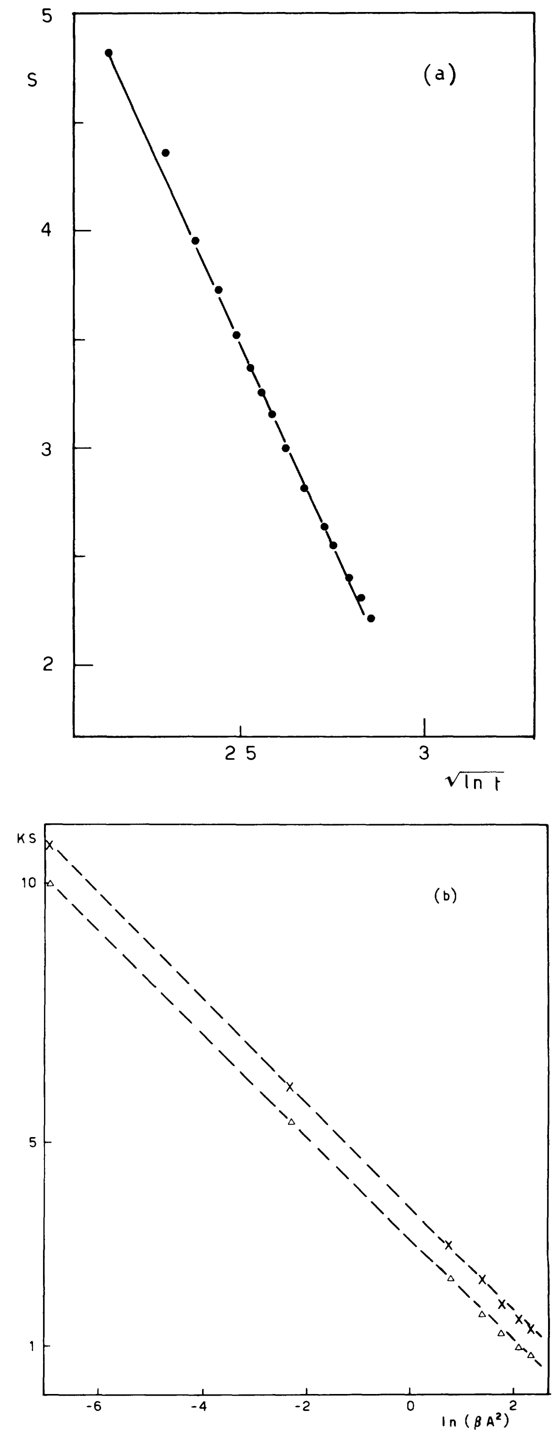

FIG. 4. (a) S as a function of $\ln t$ in the intermediate-time regime for $\beta A^2 \lesssim 10$: $n_{\mathrm{exc}}=1$, $\beta=2$, $A=1$, $\Delta t=10^{-1}$. (b) S as a function of $\ln(\beta A^2)$ in the intermediate-time regime for $\beta A^2 \lesssim 10$: $n_{\mathrm{exc}}=1$, $\Delta t=10^{-1}$; the crosses correspond to $t=100$ and the triangles to $t=300$.

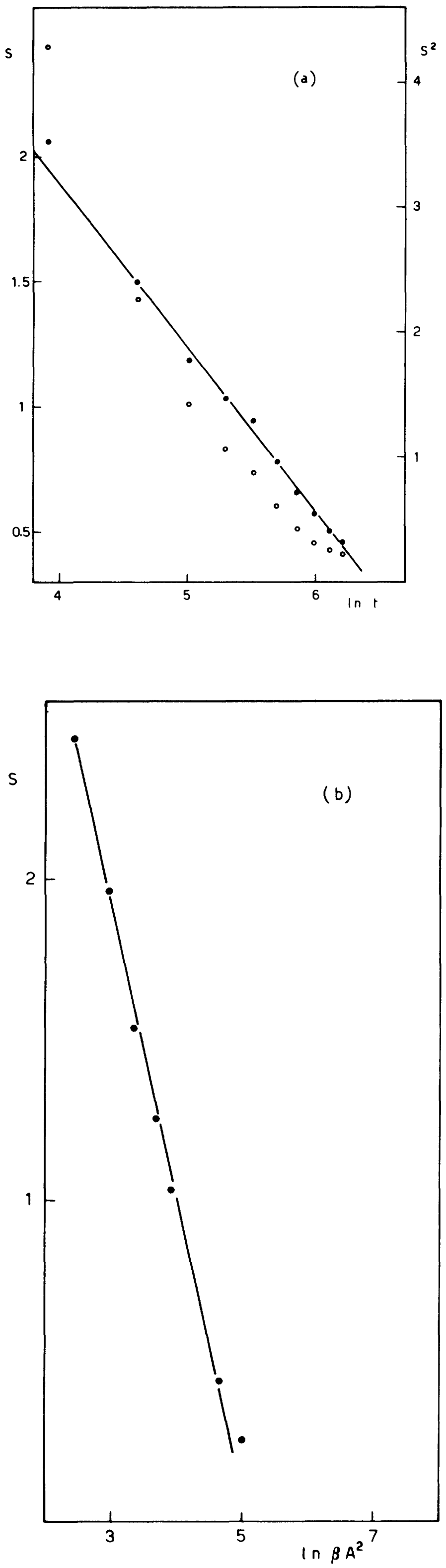

FIG. 5. (a) S vs $\ln t$ in the intermediate-time regime for $\beta A^2 \gtrsim 10$ (solid circles) with $\beta=50$, $A=1$, $n_{\rm exc}=1$, and $\Delta t=10^{-1}$. Also the dependence $S^2 \sim \ln t$ has been shown to rule out this behavior (open circles). (b) S vs $\ln \beta A^2$ in the intermediate-time regime for $\beta A^2 \gtrsim 10$ with $n_{\rm exc}=1$, $t=200$, $\Delta t=10^{-1}$.

and among different singularities leads to a less clear behavior.

It should be evident at this point that a crucial role is played by the relative weight of the nonlinear to the linear term of the equation of motion. This relation can be expressed by the introduction of some sort of "Reynolds" number:

$$R=\left\langle \frac{\beta \partial_x^2 \phi (\partial x \phi)^2}{v^2 \partial_x^2 \phi} \right\rangle = \frac{\beta}{v^2} \langle (\partial_x \phi)^2 \rangle \ , \tag{28}$$

where the angular brackets stand for an average over space. The time dependence of R must not be surprising, since we are studying the evolution toward equilibrium. A qualitative estimate of R in the case of one-mode excitations [see Eq. (8)] is

$$R \simeq \frac{\beta}{v^2}\frac{A^2}{L^2} \ , \tag{29}$$

where L is the typical length scale of variation of ϕ and L is a function of time (at $t=0$, $L=2\pi/k_{\rm exc}$).

The study of the long-time behavior of the spectrum $W(k,t)$ is sharply dependent on the value of R, i.e., on the value of the coupling constant β and on the intensity of the initial excitation A. We have found that for β and A sufficiently large ($\beta A^2 > 10$):

(i) The shape of the spectrum is exponential up to a certain time $\bar{t}$, which strongly depends on the value of βA^2, e.g., $\bar{t}=300$ for $k_{\rm exc}=2\pi/N$ and $\beta A^2=100$.

(ii) The equipartition of energy, i.e., $W(k) \sim k^{-2}$ (large k) is reached after the exponential regime of the spectrum in a time which decreases as βA^2 increases. We are led by these "experimental" results to parametrize the spectrum as

$$W(k,t) \sim \frac{1}{k^2} \exp[-S(t)k] \quad \text{as } k \rightarrow \infty \ . \tag{30}$$

As $t \rightarrow \infty$, $S(t) \rightarrow 0$ for the values of βA^2 under consideration.

The asymptotic power law for the spectrum is shown in Fig. 6. A completely different situation is found for values of βA^2 in the range $\beta A^2 \lesssim 10$.

(i) The shape of the spectrum is *always* exponential for long periods of time, e.g., $t \cong 70\,000$ for $k_{\rm exc}=2\pi/N$ and $\beta A^2=0.1$.

(ii) The slope $S(t)$ has a peculiar behavior, shown in Fig. 7 for $k_{\rm exc}=4\pi/N$, $\beta A^2=2.5\times 10^{-4}$. A similar curve is observed also for other $k_{\rm exc}$. It is evident that the slope damps to a nonvanishing value $S(\infty)$, which we consider as an asymptotic value since the oscillations with respect to it sharply decrease.

Our conclusion is that the system tends to a stationary equilibrium state which has a spectrum different from the Boltzmann spectrum.

If one plots $k_{\rm exc}S(\infty)$ as a function of $R \propto \beta A^2$, an impressive logarithmic law is obtained,

$$k_{\rm exc}S(\infty) \sim -\gamma_1 \ln R + \gamma_2 \ , \tag{31}$$

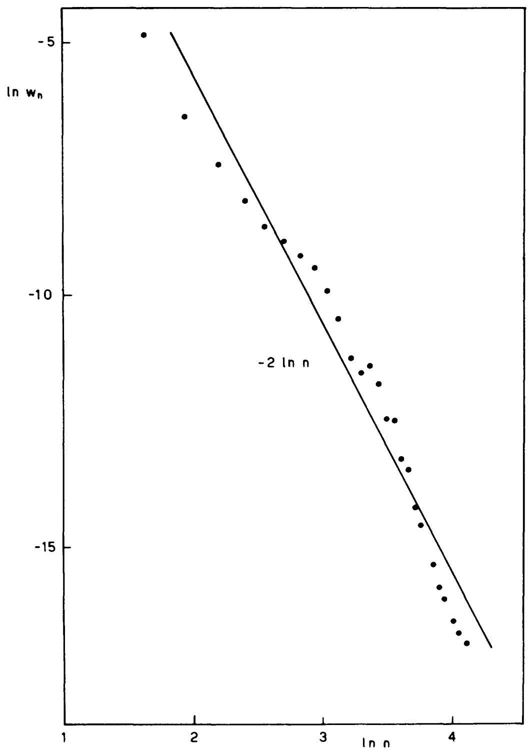

FIG. 6. Logarithm of the spectrum as a function of the serial number of modes n at $t=250$, $\beta=150$, $A=1$, $\Delta t=10^{-1}$. The experimental points are compared with the power law $W_n \simeq 1/n^2$ (straight line).

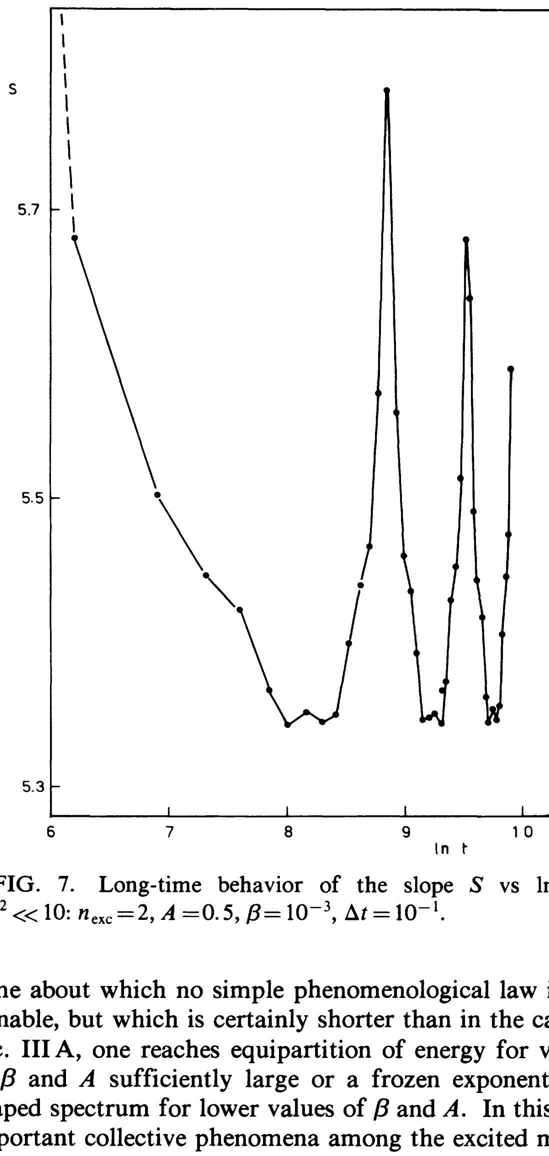

FIG. 7. Long-time behavior of the slope S vs $\ln t$ for $\beta A^2 \ll 10$: $n_{\rm exc}=2$, $A=0.5$, $\beta=10^{-3}$, $\Delta t=10^{-1}$.

as shown in Fig. 8. The value of $S(\infty)$ extrapolates to zero for $\beta A^2 \sim 10$. It should be observed that the law (31) is a direct consequence of laws (26) and (27) if the time dependence dies out through some damping factor in the coefficients, which is, on the other hand, evident in Fig. 7.

The numerical results that we have described in the present section yield to the interesting conclusion that a threshold value of R exists, below which the equipartition of energy is never reached. We want to stress that the parameter R takes into account not only the strength of the initial excitation A, whose value determines the total energy of the system when β and $k_{\rm exc}$ are small ($E \sim v^2 k_{\rm exc}^2 A^2 + \beta k_{\rm exc}^4 A^4$), but directly also the coupling constant, which would play a negligible influence if one considers the total energy as the control parameter for the transition to stochastic motion.

B. Multimode excitations

At variance with what happens in the case of one-mode excitations, the typical spectra of many modes excitations are much more complicated. First of all, even in the case of the excitation of the first modes, the spectrum is no longer a simple exponential one, although the amplitudes $|\phi_k|^2$ still fit into an exponential scale and consequently it is reasonable to define a sort of averaged slope $\bar{S}$. In principle it is possible to repeat the analysis of Sec. III A using $\bar{S}$, but the phenomenology which appears in this case is richer. The short-time behavior of $\bar{S}$ still reveals a logarithmic dependence on t and after an intermediate regime about which no simple phenomenological law is obtainable, but which is certainly shorter than in the case of Sec. III A, one reaches equipartition of energy for values in β and A sufficiently large or a frozen exponentially-shaped spectrum for lower values of β and A. In this case important collective phenomena among the excited modes become sizable. As an illustration of these phenomena see Fig. 9, which shows that a transfer of energy toward the higher modes is more efficient when a greater number of initial modes is excited at fixed energy. Another example is the response of the chain when two nonresonant modes

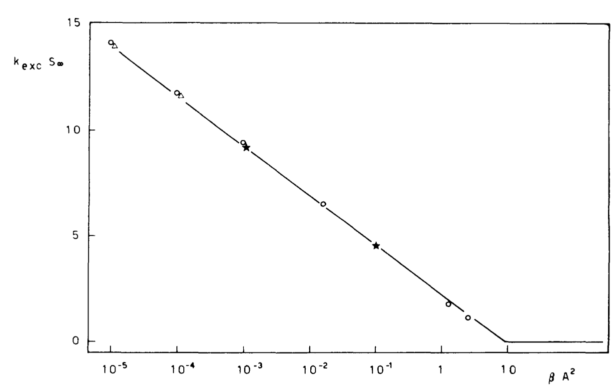

FIG. 8. Asymptotic behavior of $k_{\rm exc}$, S vs $\ln\beta A^2$: $n_{\rm exc}=1$ (stars), $n_{\rm exc}=2$ (open circles), $n_{\rm exc}=3$ (triangles).

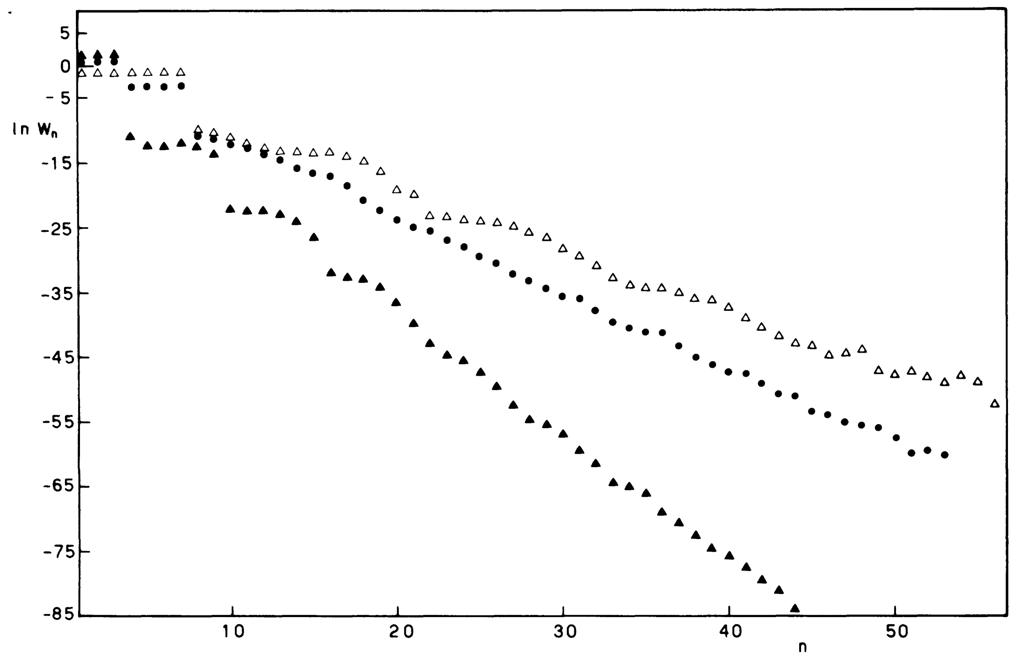

FIG. 9. Logarithm of the spectrum vs the serial number of modes n at $t=200$, $\Delta t=10^{-1}$, for different initial conditions: the solid triangles refer to $n_{exc}=1,\ldots,3$, $b_n(0)=0.5$, $\beta=0.1$ ($E=0.27$); the open triangles to $n_{exc}=1,\ldots,7$, $b_n(0)=0.15$, $\beta=0.1$ ($E=0.24$); the solid circles to $n_{exc}=1,\ldots,3$, $b_n(0)=0.49$; $n_{exc}=4,\ldots,7$, $b_n(0)=0.05$, $\beta=0.1$ ($E=0.28$).

are excited. If they are far away from each other, the spectrum is practically the superposition of the two corresponding one-mode excitation spectra, but if the wavelengths are closer, one notes also the excitation of modes which are not resonances of the two separate spectra.

A sensible way of showing up this cooperative effect in the case in which the spectrum freezes is to plot the $\bar{S}(\infty)$ as a function of the energy E, at *fixed* β, increasing the number of excited modes. The result is in Fig. 10, where one verifies that $\bar{S}(\infty)$ still scales quite well with respect to $\log E$. Now one can properly speak of a critical energy E_c which the experiment shows to slightly decrease as the number of initially excited modes is increased.

Also in the case of these "more physical" excitations two different equilibrium spectra are found separated by a threshold value of the same parameter R defined in Eq. (28) but for which the simple expression (29) does not hold any longer. Below this threshold [i.e., β and $b_n(0)$ suitably small] we have verified, even by very long runs ($\sim$700 000 integration steps with $\Delta t=0.1$), that the spectrum really remains frozen and exponentially shaped.

The excitation of a wave packet in the intermediate region of the spectrum produces a much more complicated but very peculiar situation. A typical spectrum is shown in Fig. 11 where the modes $\{n_{exc}\}=\{9,10,11\}$ are excited.

The spectrum can no longer be characterized by a single $\bar{S}$; it shows bumps corresponding to the resonances of the central excited wavelengths at $n=30$, 50 which still have an exponential shape on their sides.

Moreover, the spectrum still freezes quite soon if β and

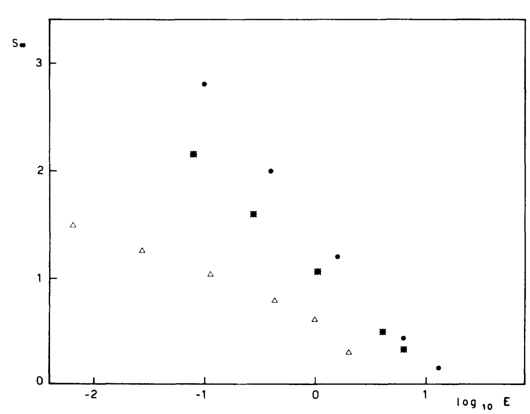

FIG. 10. Asymptotic value of the slope vs $\log E$ at fixed $\beta=0.1$: $n_{exc}=1,2$ (triangles), $n_{exc}=1,\ldots,3$ (stars), $n_{exc}=1,\ldots,7$ (dots).

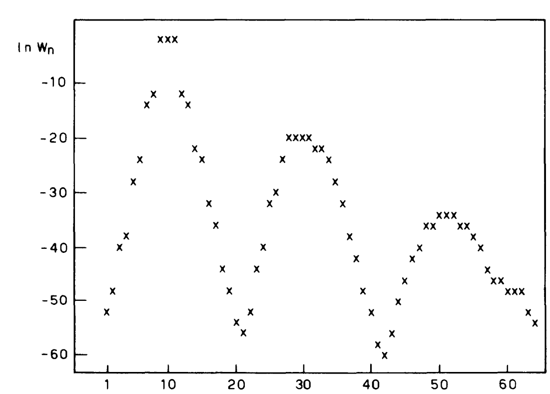

FIG. 11. Logarithm of the spectrum vs the serial number of modes n for $n_{exc}=9,10,11$ at $t=400$, $\beta=0.1$, $A=0.1$, and $\Delta t=10^{-1}$.

$b_n(0)$ are sufficiently small, while it is driven toward equipartition for higher values of these parameters. At present the lack of a proper stochasticity parameter does not allow a more careful investigation of this behavior.

IV. CONCLUSIONS

We have proposed an analytic approach to study the short-time behavior of the FPU model. The resulting time dependence of the slope of the exponential spectrum appears to be universal for a large class of polynomial and derivative potentials, but is probably not discriminating between integrable and nonintegrable models.

The most interesting results concern the long-time behavior of the spectrum. We have found, without ambiguity, the presence of a stochasticity threshold as the control parameter R, defined in Eq. (28), crosses a "critical" value R_c. R_c may depend, in general, on the number of the initially excited modes and on the number N of oscillators of the chain. It is therefore crucial to study how R_c varies as N is increased. This can be done at a fixed number of initially excited modes to get a comparison with the results of Ref. 4, or at a fixed density of initially excited modes. The latter initial condition is expected to give a better insight in the thermodynamic limit, but implies the definition of more refined parameters than the average slope of the spectrum.

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[1]A. N. Kolmogorov, Dokl. Akad. Nauk. SSSR 98, 527 (1954); V. I. Arnol'd, Russ. Math. Surv. 18, 9 (1963); J. Moser, Nachr. Akad. Wiss. Göttingen Math. Phys. Kl. 2, 1, 15 (1962).

[2]E. Fermi, J. Pasta, and S. Ulam, in Enrico Fermi, Collected Papers (Chicago Ill.), 978 (1965).

[3]F. M. Izrailev and B. V. Chirikov, Dokl. Acad. Nauk SSSR 166, 57 (1966) [Sov. Phys. Dokl. 11, 30 (1966)].

[4]P. Bocchieri, A. Scotti, B. Bearzi, and A. Loinger, Phys. Rev. A 2, 2013 (1970).

[5]G. Casati, B. V. Chirikov, and J. Ford, Phys. Lett. 77A, 91 (1980).

[6]B. Callegari, M. C. Carotta, C. Ferrario, G. Lo Vecchio, and L. Galgani, Nuovo Cimento 54B, 463 (1979).

[7]F. Fucito, F. Marchesoni, E. Marinari, G. Parisi, L. Peliti, S. Ruffo, and A. Vulpiani, J. Phys. (Paris) 43, 707 (1982).

[8]M. Henon and C. Heiles, Astron. J. 69, 73 (1964).

[9]L. Galgani and G. Lo Vecchio, Nuovo Cimento 52B, 1 (1979). The same model in two dimensions was studied by G. Benettin, G. Lo Vecchio, and A. Tenenbaum, Phys. Rev. A 22, 1709 (1980).

[10]P. Butera, L. Galgani, A. Giorgilli, A. Tagliani, and H. Sabata, Nuovo Cimento 59B, 81 (1980).

[11]U. Frisch and R. Morf, Phys. Rev. A 23, 2673 (1981).

[12]G. Benettin, L. Galgani, and J. M. Strelcyn, Phys. Rev. A 14, 2338 (1976); G. Benettin, L. Galgani, A. Giorgilli, and J. M. Strelcyn, Meccanica 15, 9 (1980); 15, 21 (1980).

[13]G. Benettin and A. Tenenbaum Phys. Rev. A 28, 3020 (1983).

[14]G. Casati, F. Valz-Gris, and I. Guarnieri, Physica D 3, 644 (1981).

[15]F. Marchesoni, M. Sparpaglione, S. Ruffo, and P. Grigolini, Phys. Lett. 88A, 113 (1982).

[16]F. Fucito, F. Marchesoni, M. Sparpaglione, and A. Vulpiani, J. Phys. A 16, 117 (1983).

[17]Fermi, Pasta, and Ulam studied a variety of models with different nonlinear terms, some of which correspond in the continuum limit to integrable equations of motion.

[18]This limit is clearly not unique and depends on the way in which the coupling constants v^2 and β scale with a.

[19]B. Bassetti, P. Butera, M. Raciti, and M. Sparpaglione (unpublished).