Stability and chaos in Hamiltonian dynamics

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Numerical studies of integrable (Toda lattice) and nonintegrable (modified Toda lattice and Fermi-Pasta-Ulam model) Hamiltonian systems indicate the possibility of interpreting analogies and differences between the two in terms of dynamical stability properties. At large energy densities, according to Siegel's theorem, a small perturbation of an integrable system produces chaotic behavior and equipartition of energy. On the other hand, at low energy densities all the models we have considered show a similar ordered behavior and the absence of equipartition. In this region, soliton solutions of the corresponding continuum equations can provide a unified dynamical description of the properties of the discretized systems.

I. INTRODUCTION

Ergodicity and integrability are in a certain sense two opposite properties of nonlinear Hamiltonian systems; the former property is characterized by chaotic motions all over the phase space, with a rapid loss of any regularity in the evolution determined by the equations of motion; on the other hand, a regular or quasiperiodic motion is the typical feature of the latter. In the past, the main consequence of this double-faced situation led to different motivations and approaches in the study of these systems. As far as ergodicity is concerned, attention is concentrated on the behavior of a system of N particles interacting via a nonlinear potential; some fundamental theorems, e.g., the Kolmogorov-Arnold-Moser[1] (KAM) and the more recent Nekhoroshev[2] theorems, provide general criteria to investigate this behavior. Such an approach implies a wide use of numerical techniques (measure of the Lyapunov characteristic exponents, energy exchange among normal modes, Poincaré sections, etc.). The physical relevance of these studies relies upon the investigation of the nature of chaos in Hamiltonian systems and, more generally, on the possibility of obtaining a mechanical foundation of statistical mechanics.

As far as integrable models are concerned, only a few results are known for discrete systems and interest is focused on the class of continuum integrable equations, such as the Korteweg—de Vries equation. Their solutions are investigated by analytic techniques (e.g., the inverse scattering method), which, in general, reduce the equations to a set of linear problems; particular attention has been devoted to the study and classification of soliton solutions. The main area of interest in the study of these integrable systems has not been that of their stability with respect to perturbations in the Hamiltonian parameter space (structural stability).

The fundamental problem is to understand how the existence of integrable systems may be representative of some real physical situation and, on the other hand, what are the relations with the dynamics of a generic Hamiltonian system. From this point of view a first result is Siegel's[3] theorem which states that in the parameter space of analytic Hamiltonians, nonintegrable Hamiltonians are dense; i.e., integrable ones are rare, as rational numbers are among real ones; in this sense integrability appears to be an irrelevant feature in the study of Hamiltonian dynamics with many degrees of freedom.

In this paper we show the necessity of going beyond the concepts of integrability and ergodicity and concentrating our attention upon general stability criteria, which can reinterpret both aspects within a unified description.

A good candidate to perform a stability analysis is the famous Toda-lattice model,[4] which is fully integrable[5] and can also be studied by numerical methods:[6,7] a comparison with the properties of a class of nonlinear Hamiltonian models [including the Fermi-Pasta-Ulam (FPU) model[8]] will contribute significantly in clarifying analogies and differences.

Another interesting aspect of a stability analysis of integrable models is the study of spatial patterns at the onset of chaos: a simplified description in terms of a few degrees of freedom could be valid for some values of the control parameter (e.g., the energy density) and this could simplify the understanding of the region of transition to chaos.[9] This is probably true, for instance, for the Fermi-Pasta-Ulam model, where continuum soliton solutions are quasistable at low energy density.[10]

The structure of this paper is the following: in Sec. II we shall comment on the relevance of Siegel's theorem with respect to numerical simulations; in Sec. III we shall present and discuss the results of numerical simulations performed on the Toda lattice and on some perturbed versions of this model in comparison with the results for the FPU α model. Section IV will be devoted to some conclusions.

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II. MOTIVATION FOR A NUMERICAL STUDY OF INTEGRABILITY

Let us first recall the definition of completely integrable systems in Hamiltonian mechanics. Given the phase space Γ_{2N} with coordinates $\xi_i=(p_i,q_i)$, $i=1,\ldots,N$, the Hamiltonian $H(p,q)$ is called completely integrable if there exist N independent functions of the phase space $I_i(p,q)$ such that

$$\{H,I_i\}=0,\quad \{I_i,I_j\}=0;$$

the I_i are said to be in involution, due to the second property. This means, in other words, that any I_i generates Hamiltonian flow which has the same set of integrals of motion as H. Moreover, one can in principle find a change to "action-angle" variables[11]

$$(p_i,q_i)\rightarrow(I_i,\theta_i)\ .$$

In the new variables the equations of motion take the simple form

$$\dot{I}_i=\{H,I_i\}=0\ ,$$
$$\dot{\theta}_i=\{H,\theta_i\}=\omega_i(I)$$

so that the solution is

$$I_i=I_i(0),\quad \theta_i(t)=\omega_i t+\theta_i(0)\ .$$

The task of finding these variables is, in general, very difficult and in fact it has been accomplished only for a few models.

More often the study of the integrability has been approached by numerical simulations. For instance, some years ago Saito *et al.*[6] and Ford *et al.*[7] studied numerically some dynamical properties of the Toda lattice. The first authors analyzed the energy exchange among the Fourier modes and concluded that a "quasistochastic" behavior sets in as the energy density reaches a critical value. This was interpreted as evidence of the nonintegrability of the Toda lattice. Ford approached the numerical analysis of this model working with a few degrees of freedom and looking at the Poincaré surface of sections in the phase space.

Completely ordered structures, i.e., periodic motions, survived also in the "stochastic" region observed by Saito *et al.* The conclusion was that the Toda lattice was probably integrable. A few months later Henon and Flaschka[5] proved rigorously that the model was completely integrable and this, in a sense, solved the question.

The main justified consequence of this result was a quick change from numerical investigations to mathematical studies concentrated on the analytic properties of the "lattice soliton" solution of the Toda lattice.[12]

The interest in a detailed comparison between the dynamical properties of the Toda lattice and those of nonintegrable models (e.g., the FPU α model[8]) has been scarce.

Only when some particular continuum limits of these models were considered—e.g., the limit of the integrable KdV equation—it was realized that they were equivalent (see, e.g., Refs. 13 and 14). On the other hand, it is quite sensible from a physical point of view to accept the idea that, at least for small nonlinearities, these two models resemble one another, since the nonlinear potential of the FPU α model represents the leading term of the Taylor-series expansion of the Toda potential.

Since we are interested in the interpretation of all these aspects in a unified framework it is necessary to introduce a numerical technique able to describe chaotic as well as ordered dynamical behaviors. Anyway, the definition of a numerical technique suitable for the study of a generic nonlinear Hamiltonian problem is far from trivial and the above quoted failures show it.

Let us consider the Hamiltonian which describes a one-dimensional lattice composed of N particles, with periodic boundary conditions:

$$H\{p_i,q_i\}=\sum_{i=1}^{N}\frac{p_i^2}{2}+V(\{q_i\}),\quad q_1=q_{N+1} \tag{2.1}$$

where the $\{q_i\}$ are the displacements with respect to equilibrium positions and the $\{p_i\}$ are the conjugate momenta.

Hamilton's equations can be expressed in the form

$$\dot{\xi}=J\,\mathrm{grad}_{\xi}H\{\xi\}\ , \tag{2.2}$$

where $\xi=(\{q_i\},\{p_i\})$ and $J=\begin{pmatrix}0 & I\\ -I & 0\end{pmatrix}$, with I representing the $N\times N$ identity matrix. Let us make a transformation of variables $\xi'=f(\xi)$; then, $\dot{\xi}'=S\dot{\xi}$, where $S^{ij}=\partial\xi_i'/\partial\xi_j$. ξ' satisfies the equation

$$\dot{\xi}'=SJS^T\mathrm{grad}_{\xi}H\{\xi(\xi')\}\ , \tag{2.3}$$

where S^T is the transposed matrix. The transformation f maintains the Hamiltonian structure if and only if S is symplectic, i.e., $SJS^T=J$.

The numerical integration of Hamilton's equations can be performed by an approximate integration algorithm dependent on a finite time step Δt. This algorithm must be selected in such a way that it guarantees the local representation of a Hamiltonian flux, i.e., it maintains the symplectic structure of the theory.

In this respect a good fourth-order algorithm is Verlet's "leap frog" algorithm,[15] defined as follows:

$$\begin{aligned} q_i(t+\Delta t)&=q_i(t)+\Delta t D_i(t)\ ,\\ D_i(t+\Delta t)&=D_i(t)+\Delta t F(\{q_i(t+\Delta t)\})\ , \end{aligned} \tag{2.4}$$

where the auxiliary variables D_i (with $D_1=D_{N+1}$) approximate the momenta and $F(\{q_i\})=-\partial V(\{q_i\})/\partial q_i$. It can immediately be verified that such an algorithm satisfies the following desired properties:

(i) The map (2.4), after the identification $\xi'=(\{q_i(t+\Delta t)\},\{D_i(t+\Delta t)\})$ and $\xi=(\{q_i(t)\},\{D_i(t)\})$, is a symplectic transformation;

(ii) as a consequence $\det S=1$ and the map is volume preserving.

It is possible to generalize this algorithm to higher orders. It is also necessary to observe that the numerical integration of any differential equation produces an unavoidable numerical noise, which introduces an indetermination on the trajectories in the phase space.

For Anosov flows, which are characterized by chaotic motion, some theorems exist (e.g., Anosov-Bowen theorem)[16,17] which provide some general stability criteria. If the errors at each integration step are small enough, computations are reliable even for infinite time. On the other hand, for integrable systems we have Siegel's result.[3]

Let us consider the parameter space of all possible analytic Hamiltonians, i.e., the vector space of the coefficients of the convergent Taylor series of the Hamiltonians. Given a point $\widetilde{H}$ in this space, corresponding to an integrable Hamiltonian and a δ neighborhood of $\widetilde{H}$ with $||\delta||$ arbitrarily small, then in this δ neighborhood a point $\widetilde{H}'$ exists, which corresponds to a non integrable Hamiltonian (this is true in any "reasonable" topology). Then, even a little perturbation in principle is sufficient to destroy integrability.

On this basis one could conclude that the numerical noise makes numerical simulations unsuitable for studying integrable models. In spite of this we think that Siegel's theorem is inconclusive with respect to the problem of the stability of the features on an integrable motion. In fact, although the numerical noise modifies the integrability of the model, this does not necessarily imply that the dynamics described by the numerical algorithm cannot remain very close to the true one for extremely long integration time.

III. NUMERICAL STUDIES OF INTEGRABLE MODELS AND STRUCTURAL STABILITY

A. Integrability and equipartition

There is no apparent reason to investigate the Fourier decomposition of the Toda model. As the model is fully integrable and one knows how to pass to action-angle variables,[5] the natural coordinates in which one can study the properties of this model are the latter ones. There are, however, many reservations. First of all, the Fourier space is the most suitable for analyzing the transition to energy sharing among the degrees of freedom, when a small nonlinear term couples the modes of the Fourier decomposition. The method can be applied to any form of potential in the weak-coupling limit. Therefore, one can give a unified description of many models and of their dynamical properties; for instance, one can analyze, as we will, stability properties of integrable models in the space of the parameters which describe Hamiltonian systems.

Historically the Fourier decomposition of the Toda chain was studied[6] and no difference was found with respect to the Fermi-Pasta-Ulam model: an analogous transition to energy-sharing among the Fourier modes was clearly observed in numerical experiments. We shall clarify this point by introducing a distinction between "energy-sharing" and "equipartition."

We would like to point out that the knowledge of the action-angle representation does not help very much in the coprehension of the dynamical evolution in the "physical" phase space for a generic initial condition; this remains, in general, a difficult problem.[12]

The Hamiltonian of the Toda chain is the following:

$$H=\left[\sum_{i=1}^{N}\frac{p_i^2}{2}\right]+V(\{q_i\}),$$
$$V(\{q_i\})=\sum_{i=1}^{N}\frac{a}{b}(e^{-b(q_{i+1}-q_i)}-1)\;; \tag{3.1}$$

the corresponding equations of motion are

$$\dot{q}_i=p_i\;,$$
$$\dot{p}_i=a(e^{-b(q_i-q_{i-1})}-e^{-b(q_{i+1}-q_i)})$$
$$=F(\{q_i\})\;, \tag{3.2}$$

and we choose periodic boundary conditions

$$q_1=q_{N+1}\;. \tag{3.3}$$

We follow the time evolution of the real Fourier transform components $A_n(t)$ and $B_n(t)$ defined as follows:

$$q_i(t)=\sum_{n=0}^{N/2}A_n(t)\sin[k_n(i-1)]+B_n(t)\cos[k_n(i-1)] \tag{3.4}$$

with $k_n=2\pi n/N$. As a consequence of the conservation of total momentum the zero mode (B_0) is determined up to a constant and therefore the number of effective degrees of freedom is reduced to N. In order to apply the fast Fourier transform algorithm, our N's are always powers of 2.

We have chosen various initial conditions, but they are in general of the form

$$q_i(0)=\sum_{n=\bar{n}}^{\bar{n}+\Delta\bar{n}-1}A_n\sin[k_n(i-1)]+B_n\cos[k_n(i-1)]$$

corresponding to the excitations of a packet of Fourier modes. The initial momentum $\sum_i p_i(0)$ was always chosen to be zero as to avoid a systematic growth of the displacements.

Our first aim was to show, by direct Fourier analysis, the absence of an equipartition state in the Toda model. To study this we have used the "entropy," an equipartition indicator which has already proved powerful in the analysis of the equipartition transition in the FPU model.[18]

This entropy is defined in terms of the weight of the nth mode:

$$p_n(t)=E_n(t)/E,\quad E=\sum_{i=1}^{N/2}E_i,\quad 0\le p_n(t)\le 1\;, \tag{3.5}$$

where E_n is the linear energy in the nth mode,

$$E_n(t)=\tfrac{1}{2}[\dot{A}_n^2+\dot{B}_n^2+\omega_n^2(A_n^2+B_n^2)]\;, \tag{3.6}$$

$$\omega_n=2\sqrt{ab}\,\sin(\pi n/N),\quad n=1,\ldots,N/2\;. \tag{3.7}$$

Here we are selecting the information contained in the $N/2$ energies, leaving aside the equally interesting content of the $N/2$ phases.

The frequencies ω_n are those of the chain of coupled harmonic oscillators which is the small-amplitude (or $b\to 0$) limit of the Toda model. For this reason we have fixed a relation between the parameters a and b in (3.1) in order to obtain the coefficient $\frac{1}{2}$ in front of the quadratic term of the Taylor expansion of the Toda potential ($ab=1$).

Let us finally come to the definition of entropy $S(t)$, which follows the usual Boltzmann definition:

$$S(t)=-\sum_{n=1}^{N/2} p_n(t)\ln p_n(t) . \tag{3.8}$$

This quantity is bounded:

$$0\le S(t)\le \ln(N/2)=S_{\max} . \tag{3.9}$$

It reaches the upper limit when the system is at the equipartition ($E_n=$cost) and it is minimal when only one mode is excited. It is therefore a good parameter for establishing the degree of equipartition of the system.

First of all, we are interested in studying the long-time relaxation properties of $S(t)$, if they exist. In fact, we have already found in many models of coupled anharmonic oscillators[18] that $S(t)$ actually reaches an asymptotic value on available computer times, apart from fluctuations on time scales of the order of the periods t_n of the harmonic limit $\pi\le t_n\le[\pi/\sin(\pi/N)]\sim N$. The equations of motion (3.2) are integrated by the algorithm (2.4). We have chosen a time step $\Delta t=0.01$—0.05, which is 2 orders of magnitude smaller than the lowest harmonic period. This guarantees the conservation of energy and momentum up to 0.1% (other integrals of motion were not checked systematically and, in general, momentum was better conserved).

We have found these good relaxation properties of $S(t)$ also in the Toda model and Fig. 1 is an illustrative example of the behavior in time of $S(t)$: it already fluctuates around a mean value after a time of ~ 300 in natural units (number of integration steps $\times\Delta t$).

It is not surprising that for an integrable model the entropy grows from the initial value, which means that the evolution is towards a more disordered state. This can be understood for the Toda model in terms of solitons. In fact, if we initially excite a wave packet in Fourier space this corresponds to a superposition of solitons which then evolve in time.

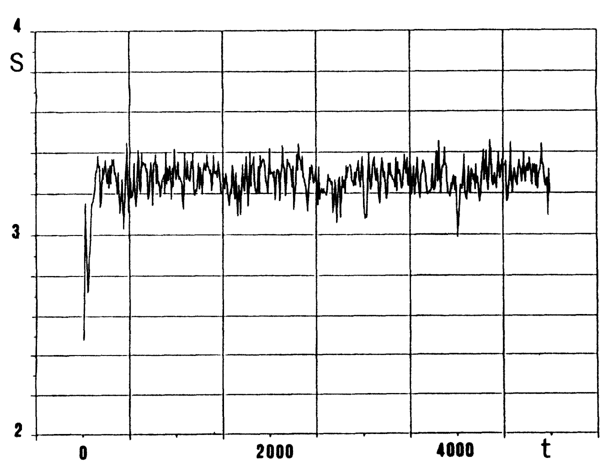

FIG. 1. $S(t)$ vs t for the Toda model ($a=5, b=0.2$): $\varepsilon=0.87$, $\Delta t=0.05$, $\bar{n}=4$, $\Delta\bar{n}=8$, $N=128$.

At any one time the Fourier transform of the solution corresponds to the excitation of all the Fourier modes and therefore, in general, it corresponds to a larger entropy. However, what should be noted is that $S(t)$ does not reach the maximum available value (in the case of Fig. 1, ln64).

In order to clear up the fluctuations we have performed a smoothing on the energy per mode E_n:

$$\overline{E_n(t)}=\frac{1}{T}\int_{t-T/2}^{t+T/2} E_n(t')dt' , \tag{3.10}$$

where T is larger than the largest typical time of the linear chain $[O(N)]$.

Since we are going to vary the number of degrees of freedom in our numerical simulations, we shall use the normalized quantity

$$\eta=[S_{\max}-S(t)]/(S_{\max}-S_{\min}) , \tag{3.11}$$

where $S_{\min}$ is the minimum value reached by $S(t)$. The bounds of η do not depend on N:

$$0\le\eta\le 1 . \tag{3.12}$$

η is zero when $S(t)$ reaches its maximum value, indicating that the system is at the equipartition, while its value is 1 when the energy is concentrated: a situation corresponding to the maximum order. With this definition η is the dual "order" parameter of the "disorder" parameter S.

In Fig. 2 we report the behavior of η_A [defined by (3.11) with $S(t)\to S_A$] as a function of the energy density $\varepsilon=H\{p(0),q(0)\}/N$ for the Toda model and for the FPU α model whose Hamiltonian is of the type (3.1) with the potential

$$V(\{q_i\})=\sum_{i=1}^{N}\left[\frac{(q_{i+1}-q_i)^2}{2}+\frac{\alpha}{3}(q_{i+1}-q_i)^3\right] . \tag{3.13}$$

The value of α was chosen such that the coupling constant in the cubic term of the potential of the α model coincides with the third-order coefficient of the Taylor-series expansion of the Toda model ($\alpha=-b/2$).

As ε is varied the FPU α model shows an evident transition to equipartition which is, on the contrary, absent in the Toda model. However, also in this case there is a clear tendency for the energy-sharing among the modes to increase as ε increases, but a plateau is reached at large values of ε.

In other words, energy-sharing is present also in the Toda model in a space which is not that of its proper modes (this is the phenomenon observed in Ref. 6), but, being that the model is integrable, it never reaches equipartition of the energy among the degrees of freedom.

It must be said that while for the α model the η_A curve is built up of many different initial conditions, this has not been done for the Toda model, for which the value of η_A may present a stronger dependence on the initial conditions. In all the simulations we have taken $\bar{n}$ and $\Delta\bar{n}$ both proportional to N, in such a way that the wavelength of the excited mode ($\sim\bar{n}/N$) was kept constant as well as

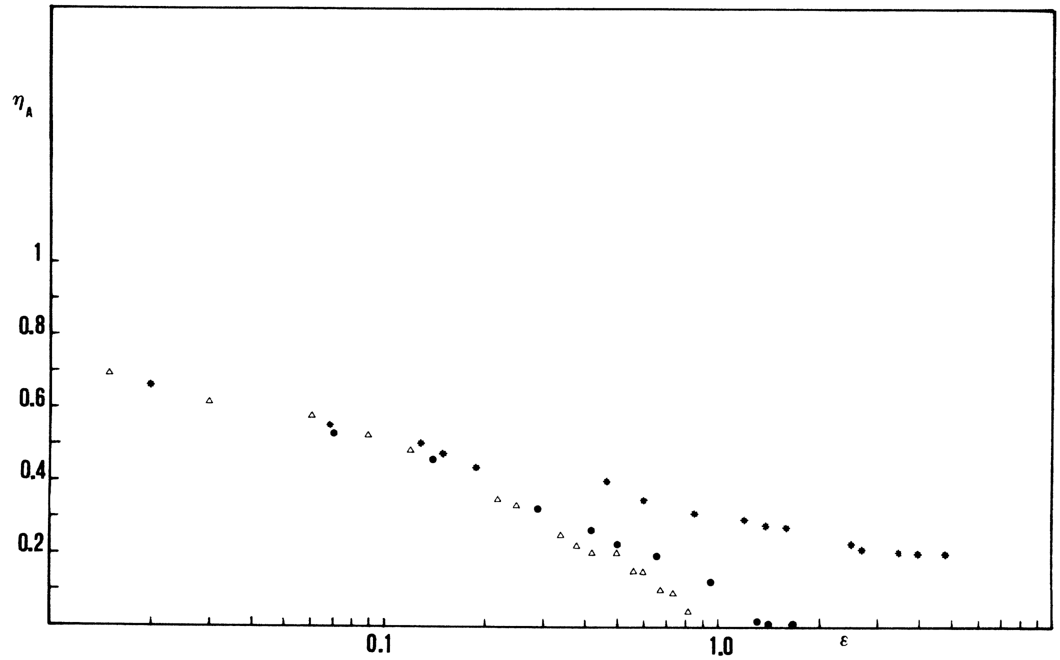

FIG. 2. η_A vs ε, $\bar{n}=N/32$, $\Delta\bar{n}=N/16$, with $N=64$ 128, 256 for the FPU α model (triangles), and the Toda model (stars) and its perturbed version (dots), see Eq. (3.14). A typical relaxation time of $\eta(t)$ to its asymtotic value η_A is $O(10^4)$.

the density ($\Delta\bar{n}/N$) of the initially excited modes (this is reminiscent of the thermodynamic limit).

B. Structural stability

Now, in order to study the stability of the Toda model in the space of the Hamiltonians, in the sense of Siegel's theorem (see Sec. II), we perturb it by adding a random quenched potential to Eq. (3.1),

$$V_{\text{pert}}(\{q_i\})=\sum_{i=1}^{N}\frac{\alpha_i}{3}(q_{i+1}-q_i)^3\ , \tag{3.14}$$

where α_i is a random process with zero mean value and whose distribution is uniform in the interval $(-0.1b,0.1b)$.

The effect is sizeable and quite evident if we look at the corresponding curve for $\eta_A(\varepsilon)$ (see again Fig. 2). The perturbation of the cubic term in the expansion of the ex-

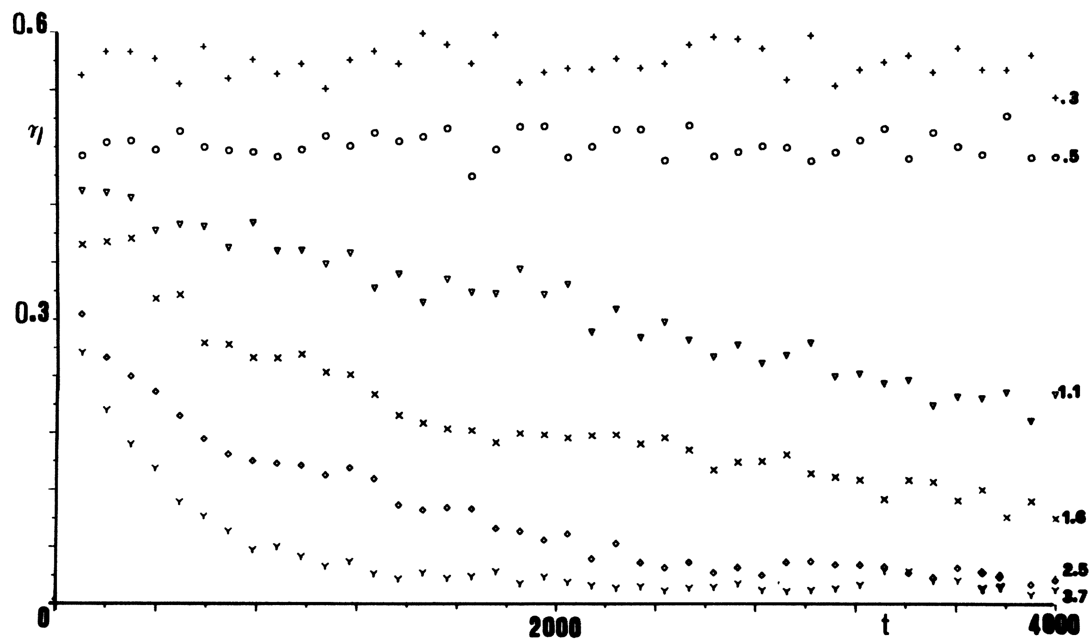

FIG. 3. η vs t for the modified Toda model with $N=64$ at different values of ε.

ponential potential drives towards the FPU α model as, intuitively, one would have expected.

We want to remark that the chosen perturbation explicitly breaks translation invariance and, therefore, momentum is no longer a conserved quantity. A similar perturbation of the α model does not cause any effect: the $\eta_A(\varepsilon)$ curve is the same as that of the unperturbed model.

One can also perturb the Toda model in a systematic way, without losing the momentum integral; for instance, one can subtract the cubic term in the development of the exponential. We do not report in this case the $\eta_A(\varepsilon)$ curve, but we show in Fig. 3 how η relaxes in time. One observes that, for small ε, η fluctuates around a mean value, different from zero, which it attains very early, while, for ε sufficiently high, $\eta \rightarrow 0$ in a time which shortens as ε increases.

The value of ε at which the relaxation properties of η change is in the region of the equipartition threshold of the FPU β model whose potential is.

$$V(\{q_i\})=\sum_{i=1}^{N}\left[\frac{(q_{i+1}-q_i)^2}{2}+\frac{\beta}{4}(q_{i+1}-q_i)^4\right] . \tag{3.15}$$

In this comparison one has to consider the control parameter R given by the mean value of the ratio between the nonlinear and linear parts of the potential (3.15) (Ref. 18),

$$R=\frac{\beta}{N}\sum_{i=1}^{N}(q_{i+1}-q_i)^2 . \tag{3.16}$$

For the modified Toda potential one considers only the first nonzero nonlinear term of the Taylor-series expansion. The critical value of the control parameter R_c, above which one has equipartition, is[18]

$$R_c \approx 0.03 . \tag{3.17}$$

It should also be noted that the change in the relaxation properties of η is very sharp at $R \sim R_c$: the relaxation time diverges very sharply at R_c. This suggests that this phenomenon cannot be understood in terms of perturbation theory and, moreover, it recalls some analogies with what happens at a phase transition.

C. Qualitative study of the dynamical properties

A deeper understanding of the dynamics of the models that we have introduced in the previous sections can be obtained by studying the "phase plane" $(\eta(t),\dot{\eta}(t))$,[19] where, now, the smoothing operation (3.10) is omitted and, therefore, the dynamics is followed at each time step. It should be noted that the choice of the $(\eta,\dot{\eta})$ variables is an alternative to the first step in the embedding in higher dimensions of the signal $\eta(t)$.

Clearly, $(\eta(t),\dot{\eta}(t))$ are not canonical variables, i.e., this phase plane is not connected by any canonical transformation to the proper phase space of the model. But $\eta(t)$ has other good features as an energy-sharing indicator; in particular, its dynamics can provide a qualitative description of the different dynamical behaviors in the Fourier space as the energy density varies. Regular motions in the $(\eta(t),\dot{\eta}(t))$ plane indicate the existence of recurrence times in the energy distribution among the normal modes, while irregular motions are interpreted as a relaxation of the system towards a thermal equilibrium state.

Let us observe that the integration of a harmonic chain produces a point in this plane:

$$(\eta(t),\dot{\eta}(t))=(1,0) . \tag{3.18}$$

Therefore, a motion different from this fixed point is due only to nonlinear effects.

At low energy densities the Toda model [Eq. (3.1)] and the FPU α model [Eq. (3.13)] both show the multiperiodic motion reported in Fig. 4. Figure 4(a) shows the Toda model, while Fig. 4(b) refers to the FPU α model integrated up to about half of the integration time of Fig. 4(a), in order to show the evolution. The orbits in the $(\eta,\dot{\eta})$ plane substantially coincide at fixed ε and for the same initial conditions. The return time near the initial condition, $(\eta,\dot{\eta})=(1,0)$, is more than 1 order of magnitude greater than the maximum harmonic period.

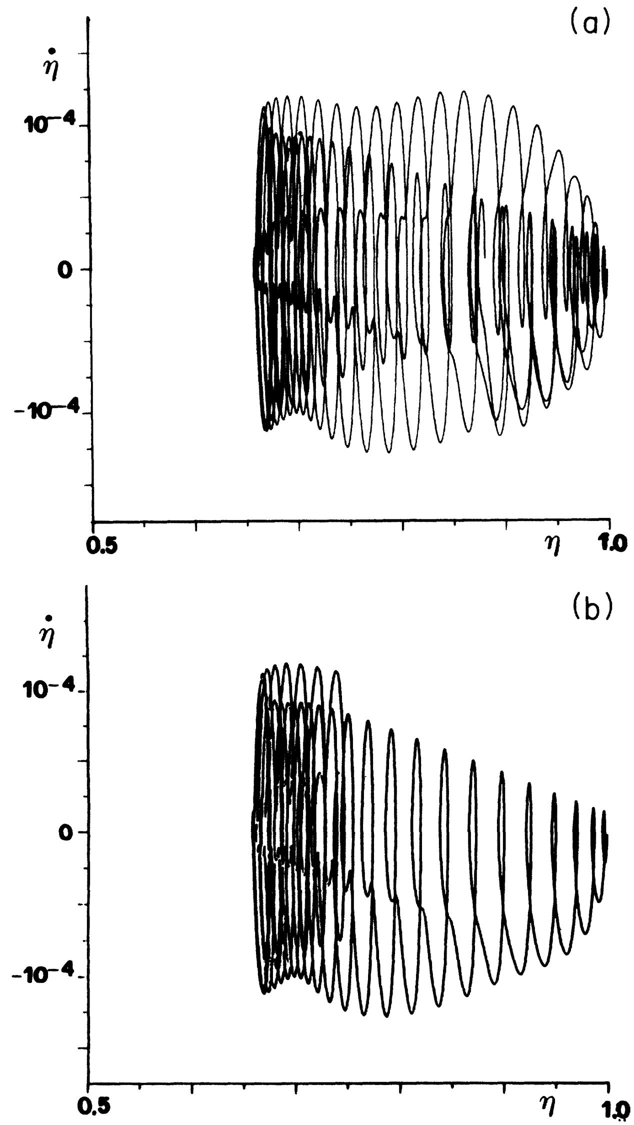

FIG. 4. The dynamics in the $(\eta,\dot{\eta})$ plane. (a) Toda model integrated up to $t_{\max}=400$, (b) FPU α model up to $t_{\max}=200$. In both cases we have chosen $\Delta t=0.01$, $\bar{n}=1$, $\Delta\bar{n}=1$, $N=16$, $\varepsilon=0.12$.

We could interpret this recursive phenomenon on the basis of the dynamic of solitons, whose configurations on the lattice are recurrent. The motion in Fig. 4 appears to be the projection on the plane $(\eta,\dot{\eta})$ of the motion on a bidimensional torus.

The most interesting effect, clearly shown in Fig. 5, is a transition to a qualitatively different motion when the energy density is increased above a certain threshold value, which is in the region of the equipartition transition $(\varepsilon_c \simeq 1)$ of the FPU α model.

For very long times the trajectory is no longer closed and it spends a long period in a region where the mean value of η is lower than the initial one $\eta = 1$. We call this qualitative change *breakdown phenomenon.* It is common to both an integrable model and a nonintegrable one and reveals the transition to energy-sharing which was already observed by Saito *et al.*[6]

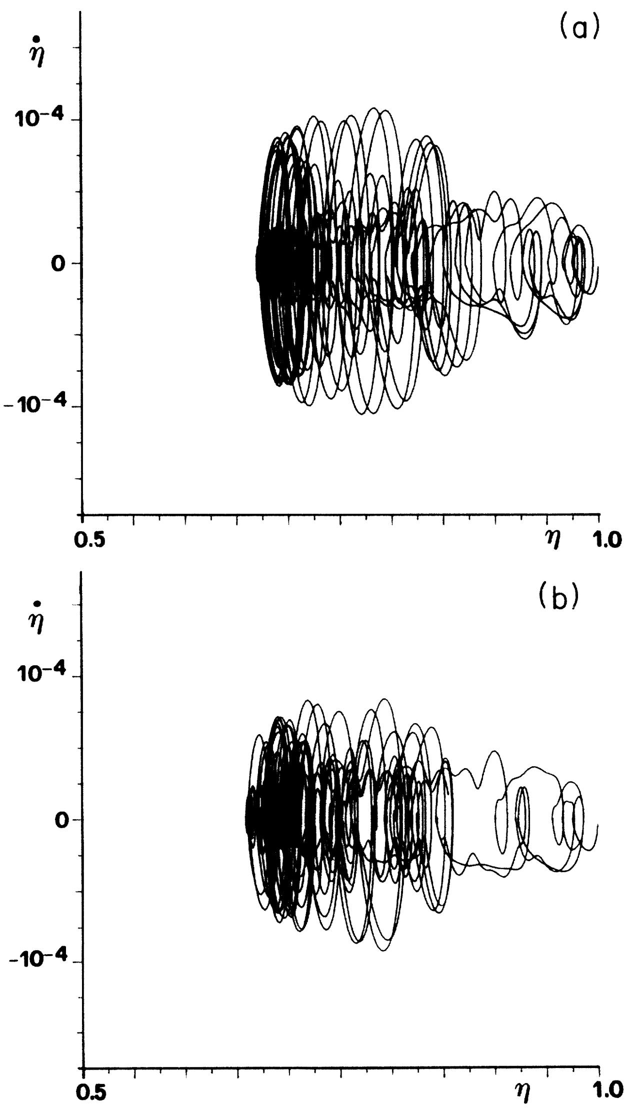

FIG. 5. The dynamics in the $(\eta,\dot{\eta})$ plane. (a) Toda model. (b) FPU α model. In both cases we have chosen $\Delta t = 0.01$, $\bar{n} = 1$, $\Delta\bar{n} = 1$, $\varepsilon = 1.8$, $t_{\max} = 400$.

The quantitative difference between the Toda and the α model can be observed at longer times and is clearly shown in Fig. 2: in the case of a nonintegrable model one observes the transition to equipartition $(\eta_A = 0)$ while for the Toda model η_A is bounded at values different from zero.

IV. CONCLUSIONS

Some authors[8] have shown the existence, at low energy densities, of solitons for the class of Hamiltonian models that we have studied in the previous sections. The common features of these models can be related to the fact that they are described by the same effective continuum equation. The best candidate is probably the *KdV* equation since it can be obtained as the continuum limit both of the Toda model and of the FPU α model.[13,14]

The periodicity of the orbits in the $(\eta,\dot{\eta})$ plane can be explained in terms of recurrences of configurations of solitons on the lattice. More precisely, at low energy density $(\varepsilon \rightarrow 0)$ the lattice can be considered a good approximation of the continuum (lattice spacing $h \rightarrow 0$) as far as its structurally stable properties are concerned.

One can imagine that at low ε the analyticity properties of solition solutions are well resolved by the lattice, just as a sampled signal is resolved when the sampling frequency is sufficiently high. As ε increases, at fixed h, solitons become more numerous and narrower and therefore they cannot be resolved by the lattice. This effect can explain the *breakdown phenomenon* of the discretized system and the transition to energy-sharing or equipartition.

Similar problems happen for the discretization of field equations when one studies the statistical mechanics of a continuum medium.[20] It can be easily proven[13,14] that our models give rise, at the lowest order in h, to hyperbolic equations, which can develop shock waves.[21] For instance, as far as the Toda and the α models are concerned, the corresponding hyperbolic equations produce a discontinuity in the derivative of the solution for times $t \sim O(1/\mu A)$ where $\mu = 2\alpha h$ for the α model and $\mu = bh$ for the Toda model, and where A is the amplitude of the initial condition.

The presence of energy-sharing or equipartition at large ε in the lattice models could be explained in terms of effective continuum equations which develop real singularities in a finite time. This is different from the soliton scenario at low ε. However, one should not forget that the Toda lattice maintains analytic solutions and integrability independent of ε.

Anyway, our numerical analysis in the Fourier space shows a *breakdown phenomenon* and a transition to energy-sharing also for the Toda lattice. The difference between the Toda lattice and a nonintegrable one is that for the latter the *breakdown phenomenon* leads to equipartition, while for the former it corresponds to a transition from a structurally stable situation to an unstable one. Above the transition a generic perturbation of the Toda model breaks integrability and leads to equipartition; this provides a confirmation of Siegel's theorem.

However, Siegel's theorem is inconclusive below the transition where integrable and nonintegrable systems show similar dynamical behavior. It seems that the presence of space-time patterns, such as solitons or "quasisolitons", is the relevant dynamical feature of a class of models.

Finally, let us remark that the description of a lattice model in terms of different effective continuum equations as ε varies cannot be restricted to the construction of some *ad hoc* limits. One must derive a sort of renormalization scheme coherent with the observed phenomenology.

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