Journal of Statistical Physics, Vol. 57, Nos. 3/4, 1989

Probes of Equipartition in Nonlinear Hamiltonian Systems

D. Thirumalai[1] and Raymond D. Mountain[2]

Received April 21, 1989

The time scales for equipartition to be reached are studied using a generalization of the recently introduced measure of ergodicity in liquids. The β-Fermi-Pasta-Ulam model is chosen as an illustration. The measures are constructed by following the evolution of the systems using two independent initial conditions. The time-averaged property of an observable is calculated using the two dynamical trajectories. The measure is essentially the norm in the space of the observable obtained from the two trajectories. We show that the time-dependent behavior of the measure is a good indicator of the equipartition in large nonlinear systems. The numerical results show that equipartitioning critically depends on the initial conditions, and even when adequate mode mixing occurs the time scales appear to be extremely long.

KEY WORDS: Equipartition; ergodic measures; stochasticity.

1. INTRODUCTION

Several numerical experiments on large nonlinear Hamiltonian systems suggest that even in the thermodynamic limit, i.e., when the number of degrees of freedom tends to infinity, there exists an energy threshold for equipartition to be obtained.[1-4] The presence of a stochasticity threshold E_c^s for systems with a few degrees of freedom has been well established (see, e.g., ref. 5). However, the presence of E_c^s, or, more precisely, an equipartition threshold energy E_c^e for nonlinear systems with infinite degrees of freedom comes as a surprise. Below E_c^s (sometimes referred to as the nonergodic phase) the structure of the phase space is extremely complicated.[6]

[1] Department of Chemistry and Biochemistry and Institute for Physical Science and Technology, University of Maryland, College Park, Maryland 20742.

[2] Thermophysics Division, National Institute of Standards and Technology, Gaithersburg, Maryland 20899.

0022-4715/89/1100-0789$06.00/0

The phase space is broken into a union of several disjoint subspaces, whose number increases as the total energy E increases. Above a critical value of the total energy, which may correspond to the equipartition energy, the subspaces merge into a unique stochastic region. The physical implication of this finding is that the phase space structure decomposes into disjoint invariant regions on the same constant-energy surface. This implies that the particular invariant region the system may be locked into critically depends on the initial conditions. The situation encountered in these examples clearly violates the ergodic hypothesis, which states that phase space averages become equal to the time averages irrespective of the initial condition used in the dynamics.[7] The existence of many disjoint invariant subspaces suggests that ergodic behavior can be obtained only by averaging the results of time-average properties of observables over all possible initial conditions.[3]

There are two different suggestions concerning the existence of E_c^e in the thermodynamic limit for nonlinear Hamiltonian systems. Izrailev and Chirikov suggest that $E_c^e \sim 1/N$ as $N \to \infty$, implying that in the thermodynamic limit the KAM theorem is not relevant.[9] Callegari *et al.*[10] have argued that E_c^s/N is related to the energy of the centrally excited mode. Numerical experiments on several large nonlinear systems strongly suggest that E_c^e/N is nonzero.[1–4] The analysis of the phase space structure in the "nonergodic" phase and the estimation of the dependence of E_c^e on N have been made by introducing various probes of stochasticity. Livi *et al.*[4] have used the spectral entropy as an indicator of equipartition. The normalized value of the spectral entropy (defined below) η vanishes in the ergodic phase and remains nonzero in the nonergodic phase. Thus, η serves as a global order parameter. They found that E_c^e is nonzero when $N \to \infty$ for both the α and β versions of the Fermi–Pasta–Ulam model. Similar conclusions were reached by Bennetin and Tenenbaum[11] in their work on two-dimensional Lennard–Jones systems. These authors used fluctuation spectra of the energies of normal modes of the system as a probe of equipartition of energy.[11]

In this paper we use the recently introduced measure of ergodic behavior to investigate the equipartitioning of energy in the β model of the FPU chain of oscillators.[12,13] The primary objective of our previous study was to devise a simple enough measure that can be used to probe the time scales needed for ergodic behavior to be obtained in large Hamiltonian systems.[12] The measure can be introduced by considering the dynamics of a system with a Hamiltonian $H(p, q)$ on a constant-energy surface. Let **a**

[3] Similar results have been found in complex systems such as mean-field spin glasses. See, e.g., ref. 8.

be a point in the phase space, which means specifying the coordinates and the momenta of all the degrees of freedom. Let $f^{\mathbf{a}}$ be the time-averaged property of an observable,

$$f^{\mathbf{a}}(p, q) = \frac{1}{t}\int_0^t f^{\mathbf{a}}[p(s), q(s)]\, ds \tag{1.1}$$

The superscript **a** denotes that the initial condition for the trajectory corresponds to the point **a** in the phase space. Let $f^{\mathbf{b}}(p, q)$ be the time-averaged property of $f[p(s), q(s)]$, which is computed using Eq. (1.1) with **b** as the initial condition. A metric can be constructed using $f^{\mathbf{a}}(p, q)$ and $f^{\mathbf{b}}(p, q)$ as

$$d_f(t) = [f^{\mathbf{a}}(p, q) - f^{\mathbf{b}}(p, q)]^2 \tag{1.2}$$

In the context of supercooled liquids and glasses we had chosen f to be the sum of the kinetic energy and one-half the potential energy of the ith particle.[12] The resulting energy metric (summed over all the particles in the system) was shown to obey a simple dynamical scaling law. More importantly, we showed that if the free energy hypersurface (which is more appropriate for liquids and glasses) partitioned into different valleys with any two valleys being separated by a bottleneck, then the metric $d_{\mathscr{E}}(t)$ could be an indicator of such partitioning. Furthermore, the scaling behavior of $d_{\mathscr{E}}(t)$ could be used to estimate approximate time scales for mixing of two phase points **a** and **b** belonging to two different valleys. The major purpose of this article is to use similar ideas to assess the approximate time scales for equipartition in large nonlinear Hamiltonian systems. Our technique should serve as complementary to the already cited methods for numerically studying stochastic behavior in these systems.[4,10]

We would like to comment on the limitations of numerical studies in establishing the stochasticity threshold in nonlinear Hamiltonian systems with (essentially) infinite number of degrees of freedom. The transition times between two valleys on the constant-energy surface can be extremely long, and can easily exceed the time scales of the computer experiments. For example, the time τ needed for probing the entire allowed configurations on the constant-energy surface can scale as $\exp(\text{const}\, \Delta E)$, where ΔE is the average barrier height between two valleys. Thus, although equipartition could be established when $t \gg \tau$, for all practical purposes one essentially has a breakdown of ergodicity. Consequently, numerical calculations alone cannot be used to establish with certainty the existence of E_c^s, but they can serve as a useful guide for the approach to equipartition. It is this aspect that we wish to study using the above mentioned probes of stochasticity.[12,13]

2. THE MODEL AND NUMERICAL DETAILS

The model consists of a chain of N nonlinearly coupled oscillators whose Hamiltonian is given by[14]

$$H=\sum_{i=0}^{N}\left[\frac{V_i^2}{2}+\frac{1}{2}(X_i-X_{i-1})^2+\frac{\beta}{4}(X_i-X_{i-1})^4\right] \tag{2.1a}$$

We assume that the ends of the chain are clamped, i.e.,

$$X_0\equiv X_N\equiv 0 \tag{2.1b}$$

This choice of boundary conditions is different from the periodic boundary conditions used by Livi *et al.*[4] It is obvious that the precise boundary condition should have no bearing on any relevant results for $N\to\infty$. However, for finite N we find some significant differences. The unit of time is taken to be $\tau=(m/\mu)^{1/2}$, where m is the mass of an oscillator and μ is the harmonic coupling constant. All these quantities have unit value in Eq. (1). The coupling constant β has the value of 0.4.

The classical equations of motion obtained from the Hamiltonian in Eq. (2.1) were integrated either by the Beeman algorithm or a fifth-order Runge-Kutta algorithm. The time step for the Beeman algorithm was $\Delta t\leqslant 0.01$ and the time step for the Runge-Kutta algorithm was $\Delta t\leqslant 0.025$. In all cases $N=32$. The choice of initial condition for our purposes is of particular interest. If equipartitioning is to be obtained, then this should happen regardless of the particular initial condition used to generate the trajectory. Although the precise structure of the constant-energy phase space is hard to predict, the symmetry of the Hamiltonian can be utilized to suggest that the phase space is partitioned into three disjoint parts. The potential terms involving particle j and particle $k=N-j$ are equivalent because $l=N/2$ defines the midpoint of the chain. This means that if initial conditions satisfy

$$X_j=\pm X_{N-j},\qquad V_j=\pm V_{N-j},\qquad j=1,2,\ldots,N/2 \tag{2.2}$$

then the symmetry [given by $(+)$ in Eq. (2.2)] or the antisymmetry [given by $(-)$ in Eq. (2.2)] of the initial conditions with respect to the midpoint of the chain will be preserved for all future time. The third part of the phase space (M) is associated with initial conditions which do not satisfy either a symmetric $(+)$ or an antisymmetric $(-)$ initial condition. It is clear that these initial conditions do in fact characterize three disjoint parts of phase space. The further partitioning of phase space within the symmetry-allowed region depends on the value of the total energy, and in fact the dynamics of the system is a way to probe the phase space structure. Notice that the

phase space partitioning based on parity operation about the midpoint of the chain is not applicable when periodic boundary conditions are used.

The partitioning based on the grounds of symmetry leads to an interesting selection rule for the flow of energy.[15] This is easily seen by expressing the Hamiltonian in terms of the normal mode coordinates defined as

$$X_i(t) = \left(\frac{2}{N}\right)^{1/2} \sum_{j=0}^{N} A_j(t) \sin\left(\frac{ij\pi}{N}\right) \tag{2.3}$$

In terms of the normal mode amplitudes, the quartic terms in the Hamiltonian which couple the various modes become

$$\frac{\beta}{4} \sum_{i=1}^{N} \sum_{j=1}^{N} \sum_{k=1}^{N} \sum_{l=1}^{N} A_i A_j A_k A_l \mu_{ijkl} \tag{2.4a}$$

with

$$\mu_{ijkl} = \frac{1}{2N} \omega_i \omega_j \omega_k \omega_l (B_{ijkl} + B_{ijk-l} + B_{i-jkl} + B_{ij-k-l} + B_{i-j-kl} + B_{i-jk-l} + B_{i-j-k-l}) \tag{2.4b}$$

where

$$\omega_j = 2 \sin(j\pi/2N) \tag{2.4c}$$

and

$$B_{ijkl} = \begin{cases} 1 & \text{if } i+j+k+l=0 \\ -1 & \text{if } i+j+k+l = \pm 2N \\ 0 & \text{otherwise} \end{cases} \tag{2.4d}$$

The vanishing of coefficients μ_{ijkl} leads to the partitioning of phase space discussed above.

The lack of mixing of the symmetric and antisymmetric regions implies that if initially a certain mode corresponding to the S region is excited, then equipartition can be expected to be obtained only among the symmetric modes. The system is expected to behave in an ergodic manner if the allowed configurations belong to the restricted phase space. The selection rule implied in Eq. (2.4) can be used as a successful test of the stability of the algorithm used in integrating the equations of motion. This is particularly important in assessing the ergodic behavior of long, finite chains by numerical methods. Recent numerical studies have suggested that

"roundoff errors" are sufficient to mix the various regions.[15],[4] We have found that if the symmetric/antisymmetric initial condition is imposed at the machine representation level and if the algorithm used to integrate the equations of motion faithfully preserves the symmetry of the Hamiltonian, then these three regions of phase remain truly disjoint. We have shown this to be the case using both the Beeman algorithm and the fifth-order Runge-Kutta algorithm. Thus, we believe that numerical roundoff errors do not contribute to the time dependence of the various quantities computed.

3. NUMERICAL RESULTS

In order to study the ergodic properties of the clamped oscillator chains, we have used the measures discussed in the Introduction. One can in principle probe the onset of stochasticity by computing the Lyapunov exponents.[5] However, the indicators we have used give more detailed information about the dynamics of the trajectories in phase space. Furthermore, our measures can be easily computed for systems with a large number of degrees of freedom.

In our numerical experiments we considered three different initial excitations of the normal modes. The first corresponds to the excitation of all the symmetric modes (S), which are labeled $n = 1, 3, 5, \ldots$. In the second case all the even-numbered modes were excited, and this corresponds to the antisymmetric (A) case. The last case studied was the one in which all modes were excited, and this is the mixed (M) case. In all cases the total energy is approximately 18.327, and initially this energy is distributed equally among five modes. Two separate classes of modes were chosen for the initial distribution of the total energy. In the first case the five lowest modes were excited, and this was labeled **a**. We also studied a second case, labeled **b**, in which five of the intermediate modes were initially excited. By following the dynamics of the system using the two different initial conditions **a** and **b** the metric was constructed using Eq. (1.2). The initial momenta were set to zero, and the normal mode amplitudes at $t = 0$ were adjusted so that the desired total energy is obtained.

In order to assess the approach to equilibrium and the approximate time scales needed for exploring the allowed phase space (if ergodicity is obtained) we have used the following measures:

[4] While we cannot claim to understand why the calculations reported in ref. 15 suggest between the symmetric and antisymmetric regions, it is reasonable to suggest that the machine level representation of the initial conditions used by them was neither fully symmetric nor fully antisymmetric with respect to the center of the chain.

(i) A measure $d_{\mathscr{A}}(t)$ corresponding to the variable A is computed using Eq. (1.2), i.e.

$$d_{\mathscr{A}}(t)=\frac{1}{N}\sum_{j=1}^{N}[\mathscr{A}_j^{(\mathbf{a})}(t)-\mathscr{A}_j^{(\mathbf{b})}(t)]^2 \tag{3.1a}$$

where

$$\mathscr{A}_j^{(\mathbf{a})}(t)=\frac{1}{t}\int_0^t ds\,[A_j^{(\mathbf{a})}(s)]^2 \tag{3.1b}$$

and the normal mode amplitude $A_j(t)$ is given by

$$A_j^{(\mathbf{a})}(t)=\left(\frac{2}{N}\right)^{1/2}\sum_{j=1}^{N}X_j^{(\mathbf{a})}(t)\sin\left(\frac{ij\pi}{N}\right) \tag{3.1c}$$

This corresponds to the definition of the metric given in Eq. (1.2), where the observable $f(p, q)$ is made from the time-averaged value of the square of normal mode amplitudes. The labels (**a**) and (**b**) in Eq. (3.1a) refer to the initial conditions for the two different trajectories.

(ii) A metric similar to Eq. (3.1a) for the energy variable was used. This is obtained from the variables $E_j(t)=\omega_j^2\mathscr{A}_j(t)$, and is given by

$$d_{\mathscr{E}}(t)=\frac{1}{N}\sum_{j=1}^{N}[E_j^{(\mathbf{a})}(t)-E_j^{(\mathbf{b})}(t)]^2 \tag{3.2}$$

The properties of $d_{\mathscr{A}}(t)$ [or $d_{\mathscr{E}}(t)$] can be easily inferred. If the system is ergodic (on the time scale of the numerical experiment, τ_{exp}), then $d(t)$ should vanish for long times. This is because for time τ_{exp} the system explores all the allowed phase space, and consequently $\mathscr{A}_j^{(\mathbf{a})}(\tau_{\text{exp}})=\mathscr{A}_j^{(\mathbf{b})}(\tau_{\text{exp}})$. The nonvanishing (or, more precisely, any lack of decay) of the ergodic measures can be used to infer nonergodic behavior in Hamiltonian systems. The asymptotic time dependence indicates the approximate time scales needed for ergodicity to be established. The arguments presented above form the physical basis for using $d(t)$ as appropriate measures for inferring ergodic behavior.

(iii) Following Livi *et al.*,[4] we also computed the spectral entropy $H(t)$

$$H(t)=-\sum_{j=0}^{N_A}p_j(t)\ln p_j(t) \tag{3.3}$$

with $p_j(t) = E_j(t)/\sum_{i=0}^{N} E_i(t)$ and N_A is the number of modes allowed by symmetry conditions discussed in Section 2. For our example, $N_A = N/2$ for the symmetric case, $N_A = N/2 - 1$ for the antisymmetric case, and $N_A = N$ for the mixed case. Notice that our definition of $H(t)$ differs from that used by Livi *et al.*[4] The spectral entropy is zero when only one mode remains excited for all times. When equipartitioning is reached, then $p_j = 1/N_A$, and thus the maximum value of the spectral entropy is $H_{\max} = \ln N_A$. In our numerical example $H_{\max} = 2.78$ for the symmetric case, $H_{\max} = 2.71$ for the antisymmetric case, and $H_{\max} = 3.47$ for the mixed case. The results for the three cases are presented below.

3.1. Mixed Case

The behavior of $d_{\mathscr{A}}(t)$ and $d_{\mathscr{E}}(t)$ as a function of t is presented in Fig. 1. The two independent initial conditions were **a** and **b** corresponding to the two different initial excitations discussed earlier. The behaviors of $d_{\mathscr{A}}(t)$ and $d_{\mathscr{E}}(t)$ are very similar. For times greater than about 10^4 both the ergodic measures decay in time. The decay is characterized by the same

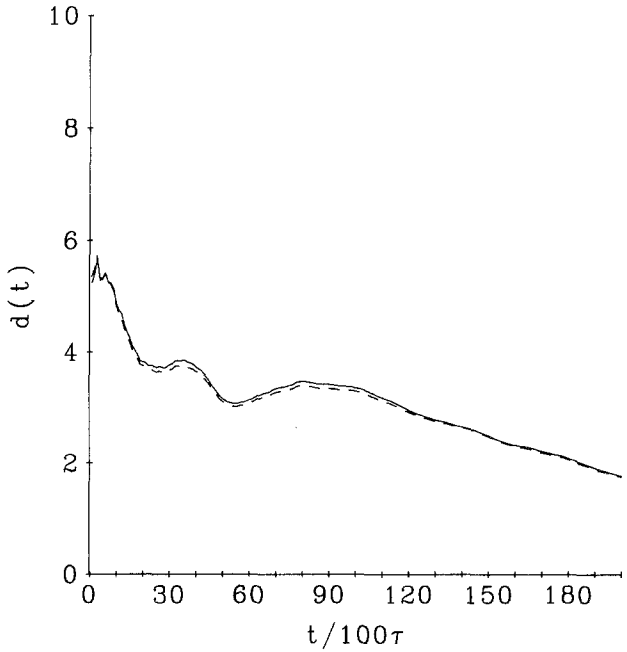

Fig. 1. Plot of $d_{\alpha}(t)$ ($\alpha = \mathscr{A}$ or $\mathscr{E}$) as a function of time for the mixed (M) case. The solid line corresponds to $d_{\mathscr{A}}(t)$ and has been reduced by a factor of 100. The dashed line shows $d_{\mathscr{E}}(t)$. The total energy $E = 18.237$.

functional form that we had found earlier in supercooled liquids and liquids near the glassy state.[12] The time dependence of $d(t)$ (for both $\mathscr{A}$ and $\mathscr{E}$) has the scaling form

$$d_\alpha(t) \sim f(tD_\alpha) \qquad (\alpha = \mathscr{A} \text{ or } \mathscr{E}) \tag{3.4a}$$

with

$$f(x) \sim 1/x, \qquad x \gg 1 \tag{3.4b}$$

The single parameter D_α is a generalized diffusion constant which characterizes the rate of exploration of the configuration space. Notice that the form suggested in Eq. (3.4) is valid only for times larger than a system-dependent characteristic time. For the present problem D_α is extremely slow, and only for times much larger than 2×10^4 does one expect ergodic behavior to be established.

In order to further assess the relaxation of the different normal modes, we analyzed the contribution to $d_{\mathscr{A}}(t)$ arising from all the modes. We found that both $d_{\mathscr{A}}(t)$ and $d_{\mathscr{E}}(t)$ appear to be dominated by the lowest mode, which in this case corresponds to $j = 1$. This implies that on the time scale τ_{exp} all the other modes essentially exchange energy easily and one expects equipartitioning between these modes.

Figure 2 is a plot of $H_{\max} - H(t)$ as a function of time. For the mixed case, $H_{\max} = 3.43$. The two curves a and b refer to the two different initial excitations. For both these cases $H(t) \sim H_{\max}$ at long times. However, the approach to $H_{\max}$ is faster when the initial excitation corresponds to **a**, namely when at $t = 0$ the total energy is distributed evenly between the lowest five normal modes. It is interesting that the $H_{\max}$ is approached from below. This is because, with time, more of the configuration is explored, and consequently the spectral entropy grows with time. The curves in Fig. 2 can be adequately described (for long times) by

$$H(t)/H_{\max} \sim (1 - A/t^\beta) \tag{3.5}$$

where β appears to be between 1 and 2. This form is not inconsistent with the form exhibited by Eq. (3.4). More careful numerical work is needed to determine precisely the value of β. Our experience with ergodic measures and suggestions that a generalized central limit theorem seems applicable for several indicators we have used in other contexts lead us to believe that $\beta = 1$.

3.2. Symmetric and Antisymmetric Case

In Fig. 3 we show a plot of $d_{\mathscr{E}}(t)$ for the S and the A cases as a function of t. The allowed modes for the S case are 1, 3, 5, etc., while only the

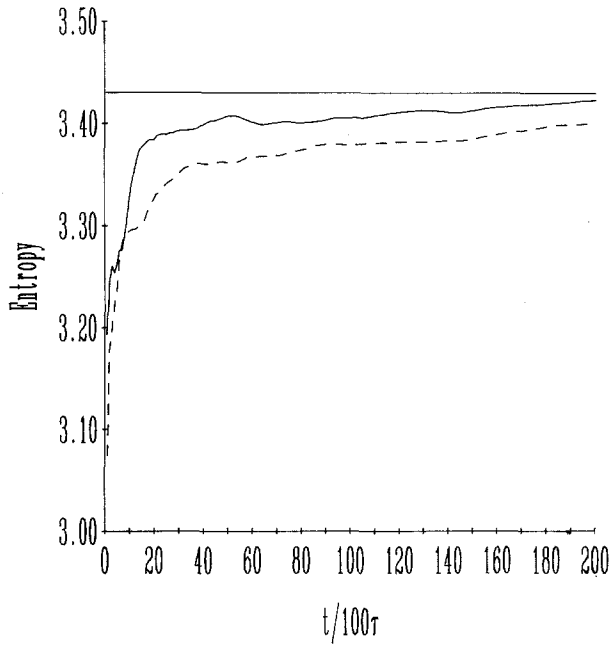

Fig. 2. Spectral entropy $H(t)$ for the mixed case as a function of time. The solid constant line parallel to the time axis corresponds to H_{max}, the maximum value expected if equipartitioning is to be obtained. The solid curvy line corresponds to the case when the total energy is initially distributed among the low modes and the dashed line shows $H(t)$ when the initial excitation corresponds to the intermediate modes. The total energy is the same as in Fig. 1.

even modes are allowed for the A case. It is clear that for neither of the two cases do we find the decrease in $d_{\mathscr{E}}(t)$ for long times—a characteristic of ergodic systems. Thus, we conclude that, based on the dynamics suggested by our probes of stochasticity, the β-FPU system appears to be nonergodic when only the modes corresponding to either the symmetric or the antisymmetric modes are excited. For these two cases we also computed the spectral entropy. The maximum value H_{max} is expected to be 2.78 (S) or 2.71 (A) if equipartitioning of energy is obtained.[4] The asymptotic value of $H(t)$, H_∞, is found to be about 2.55. A plot of $H(t)$ versus t indicates that $H(t)$ saturates at H_∞ for t greater than about 12,000. The saturation of $H(t)$ at a value less than H_{max} is an indication that the system under these conditions is not ergodic.

It has been suggested that H_∞ gives an estimate of the number of excited degrees of function which corresponds to the number of modes among which equipartition of energy is obtained.[4] Thus, one can write $H_\infty \sim \exp(N_{eff})$, where N_{eff} is the number of "degree of freedom" exhibiting

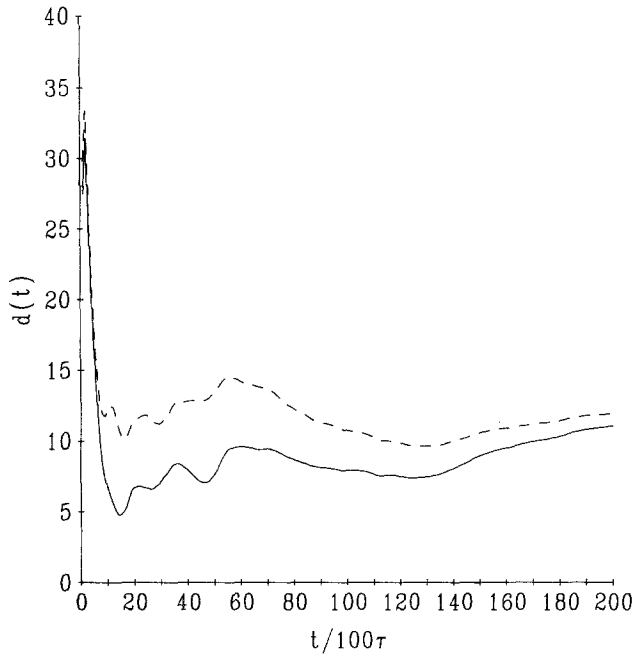

Fig. 3. Same as Fig. 1, except for the symmetric (S) case.

ergodic behavior. For our problems we estimate $N_{\text{eff}} \sim 14$. There are essentially one or two modes which do not exchange energy with others, leading to the breakdown of equipartition. We decompose $d_{\mathscr{E}}(t)$ into contributions from the different modes, and we find that $d_{\mathscr{E}}(t)$ is essentially dominated by the lowest frequency case. Thus, the mode 1 for the symmetric case and mode 2 for the antisymmetric case do not exchange energy with other modes asymptotically. The lowest frequency mode appears to be "frozen" or isolated. The freezing of the low-frequency modes suggests that the dynamics of the system is confined to lesser dimensional phase space than the allowed value—based on symmetry grounds and conservation of energy.

It is interesting that the mixed case appears to exhibit the behavior characteristic of ergodic systems, while both the symmetric and antisymmetric cases do not show energy sharing between the low-frequency modes and the high-frequency modes. Qualitatively one can rationalize this in terms of the resonance overlap criterion due to Chirikov.[5],[5] For the mixed case there appears to be appreciable overlap among the resonance layers

[5] Energy sharing in the presence of resonances was also discussed by Ford.[16]

(the resonances refer to the unperturbed system), and the system appears to be stochastic due to diffusion along these layers. The time scale for diffusion is extremely long. For the symmetric and nonsymmetric cases, stochastic behavior (and equipartition) is clearly achieved among all the modes except the two lowest modes. Using the Chirikov overlap criterion, one would conclude that the distance between the resonant modes is great enough such that no overlap occurs. This also suggests that there could exist isolating integrals (besides the energy) involving the low-frequency modes.

In order to test the above interpretation, we computed the ergodic measures for the symmetric case for the total energy $E = 50.0$. We found that there appears to be equipartitioning of the energy among all the modes except the lowest one. The calculated ergodic measures exhibit the characteristic scaling behavior if the contribution from the first mode is neglected. Thus, in the symmetric (as well as the antisymmetric) case the distance between the lowest resonance is great enough to avoid any mixing.

4. CONCLUSION

The central purpose of this paper was to show that the measures of ergodic behavior introduced recently can be used to study the approach to equilibrium in large nonlinear Hamiltonian systems. The main conclusions of the paper are as follows.

1. The measures involving the time-averaged values of the mode energies or the amplitudes exhibit a scaling behavior for times longer than a system-dependent characteristic time. The diffusion constant appearing in the scaling form can be used to obtain the approximate time scales for equipartition to be obtained. For the β-FPU model we have shown that equipartition is expected to be obtained only for certain initial modes of excitation. Even in this case, namely the mixed case, the time scales needed are very long, and therefore the approach to equilibrium is very slow.[4] When the energy is distributed among only the symmetric or antisymmetric cases, the system does not attain equipartition, and this is reflected in the dynamic behavior of the ergodic measures.

2. The time dependence of the spectral entropy also obeys a scaling form similar to that of the ergodic measures. Thus, the rate of growth of entropy also is a useful indicator of the stochasticity threshold. However, the scaling behavior for $d(t)$ is useful in assessing the time scales needed to approach equilibrium.

3. The structure of the constant-energy phase space for these systems is quite complicated. It is because of this that the mixing of various modes

occur only for certain initial conditions. In a sense this simple system appears to have the features seen in complex systems such as structural glasses and spin glasses.[17] For example, the lack of mixing seen in the asymmetric and the antisymmetric cases could be because the system is essentially in a metastable state with very long (much longer than the numerical time scale) relaxation times. If this were the case, the detailed examination of the phase space structure using the methods used here can give us insight into the nature of aperiodic states in complex systems.

ACKNOWLEDGMENTS

This work was supported in part by a grant from the National Science Foundation under grant CHE-86-57396.

REFERENCES

1. E. Diana, L. Galgani, M. Casartelli, G. Casati, and A. Scotti, *Theor. Math. Phys.* **29**:1022 (1976).
2. P. Bocchieri, A. Scotti, B. Bearzi, and A. Loinger, *Phys. Rev. A* **2**:2013 (1970).
3. G. Bennetin, G. Lo Vecchio, and A. Tenenbaum, *Phys. Rev. A* **22**:1709 (1980).
4. R. Livi, M. Petini, S. Ruffo, M. Sparpaglione, and A. Vulpiani, *Phys. Rev. A* **31**:1039, 2740 (1985).
5. A. J. Lichtenberg and M. A. Lieberman, *Regular and Stochastic Motion* (Springer-Verlag, New York, 1983).
6. M. Pettini and A. Vulpiani, *Phys. Lett.* **106A**:207 (1980).
7. P. Ehrenfest and T. Ehrenfest, *The Conceptual Foundations in Mechanics* (Cornell University Press, Ithaca, New York, 1959).
8. A. Houghton, S. Jain, and A. P. Young, *Phys. Rev. B* **28**:2630 (1983); D. Thirumalai and T. R. Kirkpatrick, *Phys. Rev. B* **38**:4881 (1988).
9. F. M. Izrailev and B. V. Chirikov, *Sov. Phys. Dokl.* **11**:30 (1966).
10. B. Callegari, M. Carotta, C. Ferrario, G. Lo Vecchio, and L. Galgani, *Nuovo Cimento B* **54**:463 (1979); L. Galgani and G. Lo Vecchio, *Nuovo Cimento B* **52**:1 (1979).
11. G. Bennetin and A. Tenenbaum, *Phys. Rev. A* **28**:3020 (1983).
12. D. Thirumalai, R. D. Mountain, and T. R. Kirkpatrick, *Phys. Rev. A* **39**:3563 (1989).
13. R. D. Mountain and D. Thirumalai, *J. Phys. Chem.* **93**:6975 (1989).
14. E. Fermi, J. Pasta, and S. Ulam, Los Alamos Science Laboratory Report No. LA-1940 (1955) (unpublished); also in *Collected works of Enrico Fermi*, Vol. 2 (University of Chicago Press, Chicago, 1965), p. 978.
15. B. I. Henry and J. Grindlay, *Phys. Rev. A* **38**:2594 (1988).
16. J. Ford, *J. Math. Phys.* **2**:387 (1961); J. Ford and J. Waters, *J. Math. Phys.* **4**:1293 (1963).
17. T. R. Kirkpatrick and D. Thirumalai, *J. Phys. A* **22**:L149 (1989).