

New phenomenon in the stochastic transition of coupled oscillators

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We have performed a detailed numerical investigation around the region of transition from quasiperiodic to stochastic motions for a chain of particles with Lennard-Jones interaction. We have found that the curve for the stochastic parameter (or maximal Lyapunov characteristic number) as a function of energy presents successive bifurcations in that region, a phenomenon not yet observed in this field. This phenomenon is interpreted as indicating that the so-called stochastic region is in general subdivided into disjoint invariant components, which merge into a unique stochastic region as energy increases.

I. INTRODUCTION

The investigation of the way in which the transition from quasiperiodic to stochastic motions takes place in a classical system of coupled oscillators appears to be of great interest in many fields of physics and mathematical physics and has recently received much attention.¹⁻³

In this connection a most useful technical tool from the point of view of numerical computations has proved to be the so-called stochastic parameter⁴⁻⁶ k , because it has been shown⁷ to give excellent estimates for a well-defined mathematical quantity, namely, the maximal Lyapunov characteristic number λ_{\max} . This, in turn, as a function of the point x of phase space, has the property of being positive or vanishing according to whether x belongs to the stochastic region or to the region of quasiperiodic motions (ordered region). Actually, this characteristic (i.e., λ_{\max} being positive or vanishing) can also be considered to be a consistent definition of the stochastic and the ordered regions themselves.

Having in mind to look for new information about the transition from quasiperiodic to stochastic motions, we performed detailed numerical investigations on a model⁸ which has been much studied: that of a set of $N+2$ points of equal mass m on a line, the two extreme ones being fixed a distance L_N apart, and interacting with nearest-neighbor Lennard-Jones potential

$$V(r) = 4\epsilon[(\sigma/r)^{12} - (\sigma/r)^6] + \epsilon,$$

where r is the distance between two neighboring particles, and ϵ and σ are positive parameters; moreover, $L_N = (N+1)2^{1/6}\sigma$.

The stochastic-parameter technique has been applied before to such a model,⁶ and curves for k as a function of the specific energy $u = E/N$, E be-

ing the total energy, have been given (see Fig. 2 of Ref. 6), both for $N=10$ and $N=50$. The two curves, which are very close to each other, give a rough indication of the specific energy ($u=1$, in the units defined below) around which the transition occurs, and this value is in agreement with previous estimates.^{8,9} However, a detailed study of the transition region is desirable.

In this paper we present the results of such a detailed study of the transition region, which has displayed a new phenomenon, namely, the occurrence of successive bifurcations of the curve $k(u)$ as the specific energy u approaches its minimum value.

Such detailed analysis has been performed for $N=5$. Indeed from previous works it is known that the relevant features of our model (such as the "specific energy of transition") for large N are already displayed even for $N=5$, while, on the other hand, the computation times are drastically reduced.

In Sec. II we present the results for the bifurcation of the curve $k(u)$ and interpret them as indicating the existence of disjoint invariant components on the energy surfaces in the stochastic region. In Sec. III we support this interpretation by an analysis of the densities of the probability distributions for the normal-mode energies, a technique which allows one to form a certain representation of the region of phase space invaded by a single trajectory, even in the case of more than two degrees of freedom.¹⁰ The conclusions follow.

Here we add now some details on the computation times and on the units employed by us. In order to introduce a natural time unit for our system, let us first recall what the normal modes are. Considering as canonical coordinates the displacements of the particles from their equilibrium positions and the corresponding momenta, the Hamiltonian can

be expanded around the equilibrium point in phase space, starting from terms of second order. By a linear transformation⁸ one can then introduce new canonical variables $(q, p) = (q_1, \dots, q_N, p_1, \dots, p_N)$ such that the contribution of second order to the Hamiltonian takes the form

$$H^0(q, p) = \sum_{k=1}^N H_k^0(q_k, p_k),$$

where $H_k^0(q_k, p_k) = \frac{1}{2}(p_k^2 + \omega_k^2 q_k^2)$ and $\omega_1, \dots, \omega_N$ are positive constants.

Moreover, if terms of higher order are neglected and one of the H_k^0 's, say H_1^0 , is different from zero while the other ones vanish, all particles execute periodic motions with the same angular frequency, say ω_1 . Thus the H_k^0 's are called the normal-mode energies. In our model one has⁸

$$\omega_k = 2^{1/3} 12m^{-1/2} \epsilon^{1/2} \sigma^{-1} \sin[k\pi/2(N+1)].$$

As a natural time unit for our system one could take the shortest period $T_N = 2\pi/\omega_N$ of the corresponding harmonic chain. It is more convenient to consider its limit when the number of particles goes to infinity (so that one has a unit which is independent of N), namely, $T = (2\pi/2^{1/3} 12)m^{1/2} \epsilon^{-1/2} \sigma$ (actually one has $T_N \approx T$ even for small N). However, for consistency with the previous works^{8,9} on our model, we also consider here units such that $m = \sigma = 1$, $\epsilon = 27.5$ and in such a way one has $T = 0.079$. Thus one has to multiply our times by $1/0.079 \approx 13$ in order to have times in natural units.

The numerical solutions of the equations of motion were computed on a CDC7600 by a method correct to third order. Typically, the solutions were computed up to times of $10^6 T$ by integration steps of $2.5 \times 10^{-2} T$. It turned out that the results of the computations were sometimes dependent on the integration step, and special care was put by us in checking that our results were actually stable with respect to it. This independence of the computed results from the integration step (at least for what concerns time averages and very probably also the stochastic parameter) has indeed theoretical support, when the stochastic region is concerned.¹¹

II. RESULTS ON THE BIFURCATIONS OF THE CURVE $k(u)$

The stochastic parameter $k(x)$, x being a point in phase space, is defined as the limit, as time $t \rightarrow \infty$, of a function $k_t(x)$; the latter is computed by following up to time $t > 0$ a trajectory starting from x at $t = 0$, and another nearby trajectory, which is initially a distance d away and is suitably readapted to the first trajectory at times $\tau, 2\tau, \dots, n\tau$, τ being a positive fixed number. For details we refer to Ref. 7, where $k_t(x)$ is more properly denoted by $k_n(\tau, x, d)$. We choose here the shorter notation

$k_t(x)$, t replacing the discrete time $n\tau$, in virtue of the independence from τ and d , at least for suitable ranges of such variables, as discussed in Ref. 7 and also checked again in our case. To that paper we also refer the reader for a discussion of how $k(x) = \lim_{t \rightarrow \infty} k_t(x)$ gives an excellent estimate for the maximal Lyapunov number $\lambda_{\max}(x)$ of the corresponding dynamical system, and also for a summary of the results of Oseledec and Millionschikov on the Lyapunov numbers themselves. As shown by those authors, $\lambda_{\max}(x)$ exists for almost every x . This function is measurable and by definition is obviously an integral (or constant of motion); thus λ_{\max} takes values which are equal for almost¹² all points x belonging to an ergodic component of the energy surface: if such a value is positive, the corresponding ergodic component will be called stochastic. Moreover, λ_{\max} vanishes in a domain covered by quasiperiodic motions.

We present first of all a series of results showing that $k(x)$, and thus very presumably $\lambda_{\max}(x)$, has several values when x ranges over an energy surface. In Fig. 1 six curves, labeled 1, 2, ..., 5, and Eq, respectively, are reported for k_t vs t , corresponding to six initial data on the same energy surface, namely, with $u = E/N = 4$. The six initial data are suitably described in terms of normal-mode energies. Indeed, for curve 1 one had at the initial time $p_1^2 = 40, p_2 = \dots = p_5 = 0, q_1 = \dots = q_5 = 0$; in other words $H_1^0 = 20, H_2^0 = \dots = H_5^0 = 0$, and $q_1 = 0$, i.e., only the first normal mode was excited, and purely with kinetic energy. Analogously for curves 2, ..., 5, while Eq refers to initial equipartition among the normal modes, $H_1^0 = \dots = H_5^0 = 4$, still purely with kinetic energy. Quite clearly, starting from values of the same order of magnitude, the curves appear to approach rather well-stabilized values, three of which are equal, while three are definitely different.

Five more initial data have also been considered, which have given curves not reported in the figure, and all tending to the common value of curves 1, 2, and Eq. These initial data were: (a) modes 1 and 2 only equally excited; (b) modes 3 and 4 only equally excited; (c) modes 4 and 5 only equally excited; (d) modes 4 and 5 only excited, with energies 19 and 1, respectively; (e) all modes excited with energies proportional to their respective harmonic frequencies.

At lower energies we could have drawn analogous figures with all the curves considered tending to different values. The figure reported here, however, is more indicative in our opinion, just because three curves tend to a common value; indeed in such a way we intend to show to which precision the limit values can be considered to be different. Moreover, as has already been said, the results

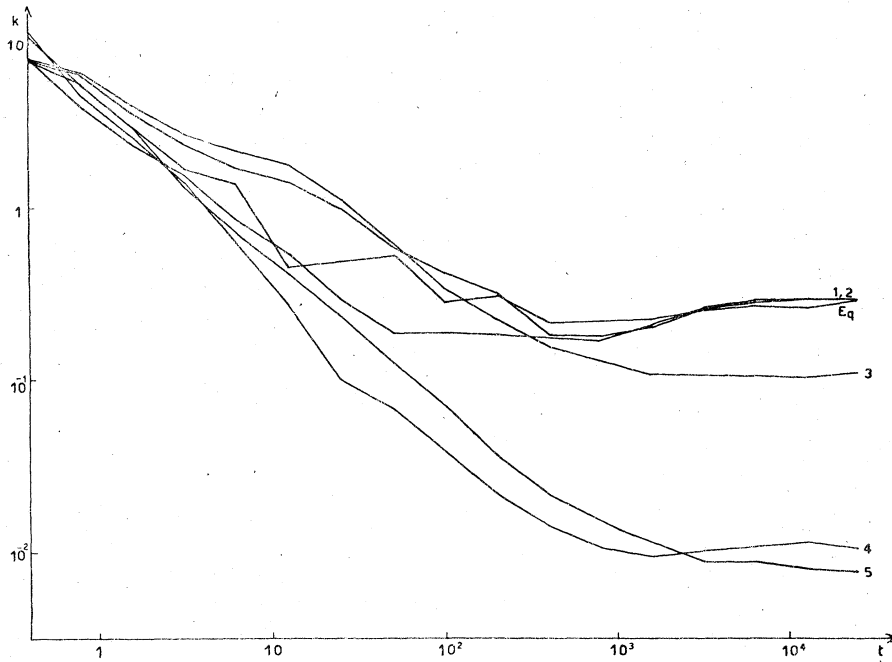


FIG. 1. Curves for k_t vs t , on a log-log scale, for six different initial conditions at specific energy $u = 4$.

were checked to be independent of the integration step.

In conclusion, if we denote by $k(u)$ the limit values of $k_t(x)$ when $t \rightarrow \infty$ and the initial point x belongs to the energy surface with specific energy $E/N = u$, it appears that there exist several

branches for the function $k(u)$.

In Fig. 2 some of the several branches observed by us are reported as functions of u in the interval $0.5 < u < 1000$; for graphical convenience just six branches, corresponding to the various curves of Fig. 1, have been reported. The criterion by which

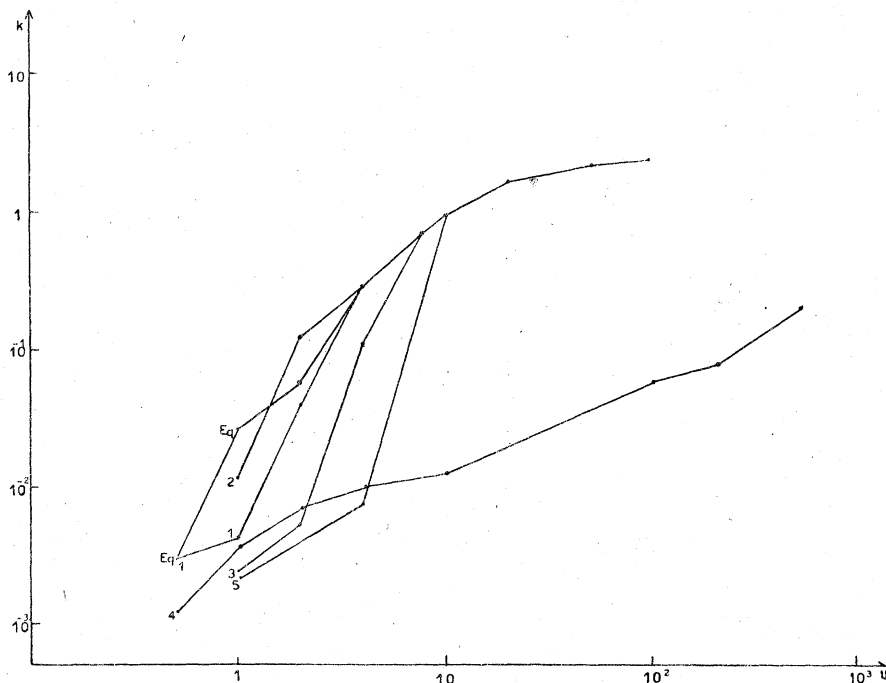


FIG. 2. Bifurcation curve for $k = \lim_{t \rightarrow \infty} k_t$ as a function of the specific energy u .

points have been ascribed to the same branch is that they pertain to analogous initial data, for example, data corresponding to the whole energy being initially purely kinetic and only on the first mode, and so on. In other words, all points of a same branch refer to initial points of phase space being on a certain half-line issuing from the origin, i.e., from the point with zero energy.

From the computations of Ref. 6 we know that at high enough energies all initial data there considered gave a unique branch for $k(u)$; this then means that all our branches have to merge into a common "main branch" at high enough energies. Actually, from Fig. 2 it appears that at $u=100$ branch 4 is already separated from the main one, while branch 5 separates at $u=10$, branch 3 at $u=8$, and all of the remaining ones separate around $u=4$. The same happened for the other already mentioned five branches not reported in the figure.

The results presented above clearly suggest the interpretation that the energy surfaces considered be actually separated into mutually disjoint components which tend to merge into an unique component; this in turn invades a greater part of the energy surface as energy increases. Generalizing an established use,¹³ we will call the stochastic regions "seas," and in particular the main stochastic component "big sea." Indeed, as already stated, k is an excellent estimate for λ_{\max} and this, as a measurable function, which is an integral, has values which are to be equal for almost all

points x belonging to an ergodic component of the energy surface. One can also have an idea of how "big" the various seas are. Indeed, considering again, for example, the energy surface with $u=4$, we have looked at what happens when the initial point is slightly displaced. Let us consider the initial point with the whole energy ($E=20$) on the fifth mode, which gives the value of branch 5. If the initial point is so displaced that mode 5 has energy 19.8 and mode 4 has energy 0.2, then we get for $k(x)$ already the same value of the main branch and so, presumably, we already are in the big sea. Now let us consider the point with the whole energy ($E=20$) on mode 4, which gives the value of branch 4. Then, if the initial point is so displaced that mode 4 has energy 19.9 and mode 5 has energy 0.1 we still have the same value for $k(x)$; if the initial energies are 19.5 and 0.5, respectively, the function k_t does not reach a stabilized value in the times considered by us, so that we can say nothing; instead, for initial energies 19 and 1, respectively, we get the value of the main branch. The same happens, as already stated, if the initial energies are both 10. So it appears that the stochastic seas which are separated from the big sea have indeed a small measure at high enough energies.

It is of interest to compare our Fig. 2 with Fig. 2 of Ref. 6 (note that our quantity k was denoted there by $k^{(N)}/t$, t being a fixed time, actually our τ , and not the current time). One thus sees that the values for $N=5$ are below those for $N=10$, in agree-

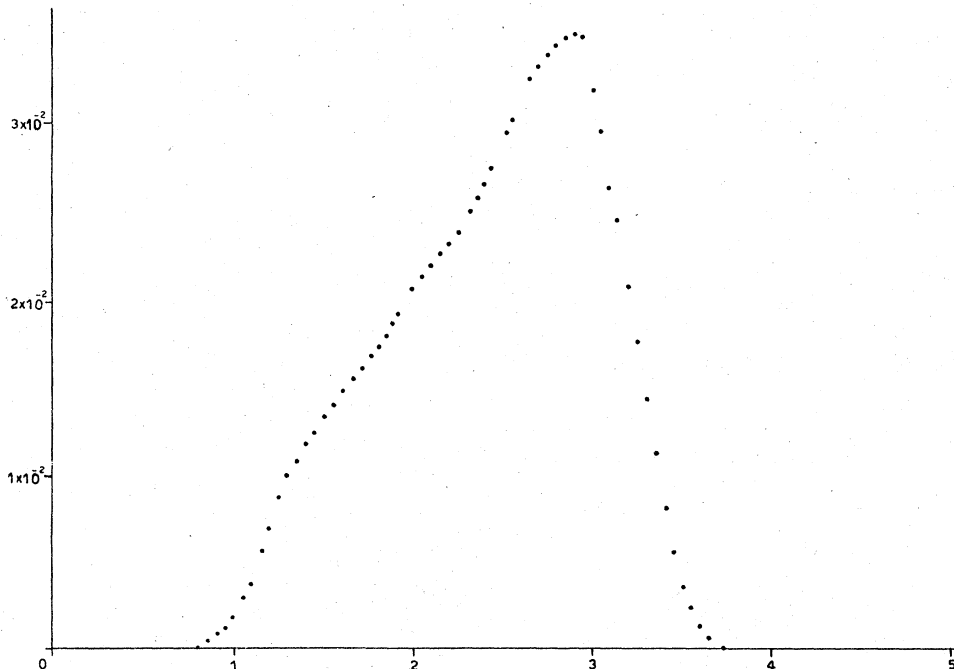


FIG. 3. Density ρ_3^* of the probability distribution for the energy of the third normal mode at $u=1$, with initially modes 3 and 4 only equally excited. Time elapsed, 6×10^3 .

ment with the general behavior of k as a function of N , illustrated by Fig. 3 there. For what concerns the main difference, namely that no bifurcation was observed there, the explanation is possibly that the analysis there performed was not sufficiently detailed, because we have found here that in general most of the initial data give values in the main branch; on the other hand, in Ref. 6 the attention was mainly concentrated on the dependence of k from N .

Finally, a point of great interest is to know the behavior of the various branches as energy decreases. As seen from Fig. 2, at $u=0.5$ we were able to give values of k with sufficient accuracy only for branches 1, 4, and Eq. For the other branches we found that $\log k_t$ vs $\log t$ gives curves which decrease almost linearly and this suggests that one could have $k = \lim_{t \rightarrow \infty} k_t = 0$. Actually, it is impossible to foresee what will happen with increasing time. Indeed, looking at Fig. 1 one can see that a reliable positive limit for k_t is reached after a certain stabilization time, and this time was found to increase as the limit value decreases. In addition, the results of the computations appear to become the more dependent from the integration step when one moves in the transition region towards more ordered regions. Thus it happens that in general the calculations are the more unreliable, and we were not able to produce sufficiently precise results at energies smaller than $u=0.5$.

We conclude the present section with a further remark. If initially only mode 2 or only mode 4 are excited, it is immediately proved by symmetry considerations that the odd modes cannot have energy at any time. Instead, in our computations at high enough energies we find the odd modes to have nonvanishing energies (see especially Fig. 6) and this is certainly due to numerical errors. The interpretation is that in such cases numerical errors bring the orbit into a stochastic region so that the value of k thus found refers to that stochastic region; and this is indeed an indication that a large stochastic region actually surrounds the exact orbit which corresponds to the considered initial data. Instead, at low enough energies we find that energy does not flow to the odd modes, and correspondingly the stochastic parameter vanishes. This then means that there is no appreciable stochastic region near enough to the exact orbit.

III. FURTHER RESULTS SUPPORTING THE EXISTENCE OF DISJOINT STOCHASTIC COMPONENTS ON THE SAME ENERGY SURFACE

The previous results on the bifurcations of the curve $k(u)$ thus clearly indicate that in the transition region every surface appears to be subdivided into disjoint stochastic components, each of them

corresponding to a branch of $k(u)$. For $N=2$, this picture is in agreement with the existence of two-dimensional invariant tori, as guaranteed by the Kolomogorov, Arnol'd, and Moser theorem. Indeed, in such a case it is well known that a "discontinuous set" of invariant tori divides the complementary region of the three-dimensional energy surface into disjoint invariant parts. On the other hand, such a separation of the stochastic region is not guaranteed by the existence of N -dimensional invariant tori for a Hamiltonian system with N degrees of freedom with $N>2$, and this fact gives rise to the possibility of the so-called Arnol'd diffusion. What happens for $N>2$ is thus a completely open problem to which our results gave a first contribution, with the indication of the existence of disjoint invariant components in the stochastic region.

Here we give a more detailed and possibly more direct evidence for such a fact. In the case $N=2$ this would be rather simple, as it would be enough to produce two-dimensional surfaces of section showing that different trajectories actually invade different parts of the allowed region. With $N>2$, two-dimensional surfaces of section become the more untreatable; thus, in order to display visual results, we have to rely on a different technique which certainly gives a little less impressive picture, but is, however, very simple even for rather a large number N of degrees of freedom. We refer to the technique of the densities of the probability distributions for the normal mode energies,¹⁰ which we now describe very briefly.

The definition of the normal mode energies H_1^0, \dots, H_N^0 has been recalled in the introduction. Clearly, in the limit case of the harmonic approximation, where terms of order higher than two in the Hamiltonian are neglected, the normal mode energies H_k^0 are integrals, so that their values do not vary with time. In presence of an anharmonicity, instead, they can take *a priori* any value in a certain interval $(0, a_k)$, where a_1, \dots, a_N are positive constants which depend on the total energy E ; moreover, for not too high energies, where the anharmonicity is not too large, one has $a_k \simeq E$ for any k . Thus, given an initial condition and the corresponding trajectory $q(t), p(t)$, one can define the probability distribution for the function H_k^0 in an obvious way. Indeed, if θ is the characteristic function of the interval $(-\infty, 0)$, the probability distribution $\sigma_k(s)$ ($0 \leq s \leq a_k$) for H_k^0 is defined by

$$\sigma_k(s) = \lim_{T \rightarrow \infty} \frac{1}{T} \int_0^T \theta [H_k^0(q(t), p(t)) - s] dt .$$

We will make reference to the corresponding density $\rho_k^*(s) = d\sigma_k(s)/ds$. Moreover, in order to have the possibility of easy comparisons at different en-

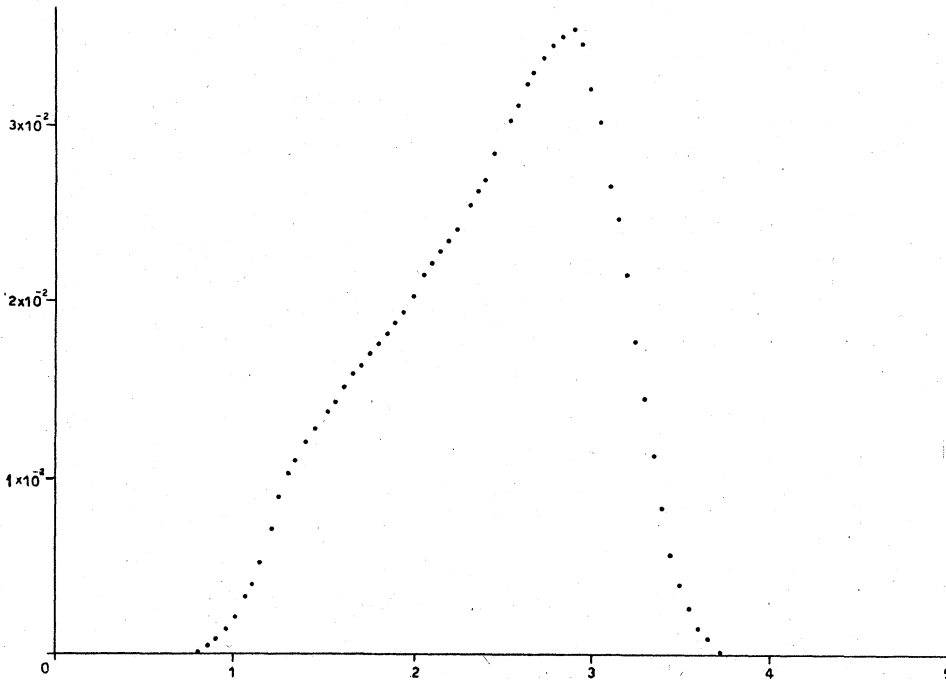


FIG. 4. Same as in Fig. 3, after time 1.4×10^4 .

ergies E , we reported as in a previous paper¹⁰ the densities of the probability distributions not for the functions H_k^0 themselves, but for the functions H_k^0/E . These densities will be denoted by $\rho_k(s)$, with $0 \leq s \leq a_k/E \approx 1$.

A limit case, opposite to the harmonic one, is that of an ergodic system, where the probability densities do not depend on the initial data on an energy surface. For example, if at an energy E our system is ergodic and the anharmonicity is still so small that it can in practice be neglected (apart from the circumstance of causing ergodicity), the densities are rather easily computed and they turn out to be all equal to the function $\rho^0(s) = (N+1)(1-s)^{N-2}$, independent of k (the "microcanonical density in the harmonic approximation").

In practice, by numerical computations of a trajectory, the densities $\rho_k(s)$ are easily evaluated as limits, with increasing time, of suitable frequency distributions, and such limits were in many cases reached in times shorter than those required for the function k_t . As an example, Figs. 3 and 4 show the function ρ_3^* at times 6×10^3 and 1.4×10^4 , respectively: the initial data were $u=1$ and modes 3 and 4 equally excited.

In order to display our results, we present the densities ρ_1, \dots, ρ_5 on a single strip from left to right. In addition, for graphic convenience, the curves $\rho_k(s)$ are represented by continuous lines. As an example, in Fig. 5 the first strip (from top) gives the densities for the same initial condition of

Figs. 3 and 4, so that the third density (from left) corresponds to that of Fig. 4.

The scales for the abscissas and the ordinates are the same throughout the figure, and the initial values for H_k^0 ($k=1, \dots, 5$) are marked by a cross on the corresponding axes of abscissas. For reference, the theoretical curve ρ^0 for the ergodic case (in the harmonic approximation) is reported (dotted line) in the upper strip (left).

Let us now describe the results of Fig. 5. The first strip has already been considered. The remaining strips refer to a different class of initial conditions, namely with all modes excited at energies proportional to the respective harmonic frequencies, i.e., $H_k^0 = \alpha \omega_k$ ($k=1, \dots, 5$), α being suitably chosen in order to have the desired energy. Precisely, the specific energies u were 0.05 for the second strip, 1 for the third strip, and 50 for the fourth one.

As one sees, at very low energies (second strip) the anharmonicity just produces a small perturbation with respect to the harmonic case: indeed the normal mode energies, although not constant, take values with probability densities very neatly peaked around the initial values. This situation presumably corresponds to a quasiperiodic motion, and indeed the corresponding curve for k_t vs t was found to decrease up to time considered. An intermediate situation appears in the third strip, for $u=1$, while the opposite situation is shown in the fourth strip ($u=50$), where all the densities are

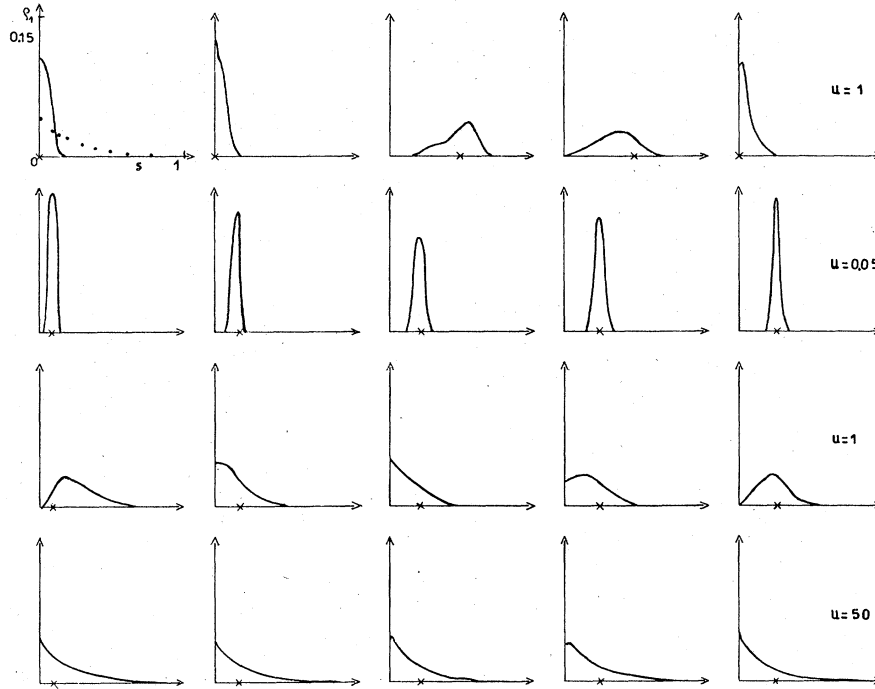


FIG. 5. Densities $\rho_k(s)$, $k=1, \dots, 5$ (from left) of the probability distributions of the energy of the normal modes divided by total energy. Each strip refers to a different initial condition at the specific energy u indicated to the right. The initial values of the energies (divided by total energy) are indicated for each mode by a cross. The data computed have been interpolated by smooth curves. For example, the third figure of the first strip (from top) corresponds to the curve of Fig. 4. The microcanonical curve (in the harmonic approximation) is dotted at top (left).

indistinguishable from ρ^0 , i.e., from ergodicity in the harmonic approximation.

The same "microcanonical distributions" were also obtained for other initial conditions at the same specific energy $u=10$, and even for all initial conditions at various high enough energies, corresponding to $k(u)$ in the main branch, even for $u=100$.

The most important point for our purposes, however, is to compare the first and the third strips, which correspond to different initial conditions at the same specific energy $u=1$. For reference, the corresponding values for the stochastic parameters were 7×10^{-3} and 10^{-2} , respectively, and from the difference of these two values we would have concluded that the motions take place in disjoint regions. This is very beautifully confirmed by our strips. Indeed, first of all, we note that the densities are different for the two cases, while, being time averages of suitable measurable functions, they should be equal if the initial points belonged to the same invariant component. In addition, however, our strips allow us to give a certain "description" of such invariant regions themselves. Thus, for example, for the initial condition cor-

responding to the first strip, the point in phase space passes through regions where the third mode has energies rather large, while, for the initial condition of the third strip, the point generally remains in regions where the third mode has small energies.

In Fig. 6 four strips are reported for a different class of initial conditions, i.e., only the second mode excited, at the specific energies $u=0.02, 0.5, 2, \text{ and } 10$, respectively (from top). The scales of the abscissas and ordinates are the same as in Fig. 5. In the first and the second strip, the odd modes 1, 3, and 5 did not receive any energy (we found values smaller than 10^{-18}) and energy is exchanged only among modes 2 and 4. At $u=0.02$ the average values of H_2^0 and H_4^0 were 9.924×10^{-2} and 6.4×10^{-4} , respectively, and the curves ρ_2 and ρ_4 in the first strip were a little bit enlarged for graphical convenience and truncated above 0.15. At $u=0.5$ (second strip) we were unable to draw clear conclusions concerning the stochastic parameter, while it stabilized to positive values in correspondence to strips 3 and 4.

As a conclusion to this section, it appears that the technique of the densities of the probability dis-

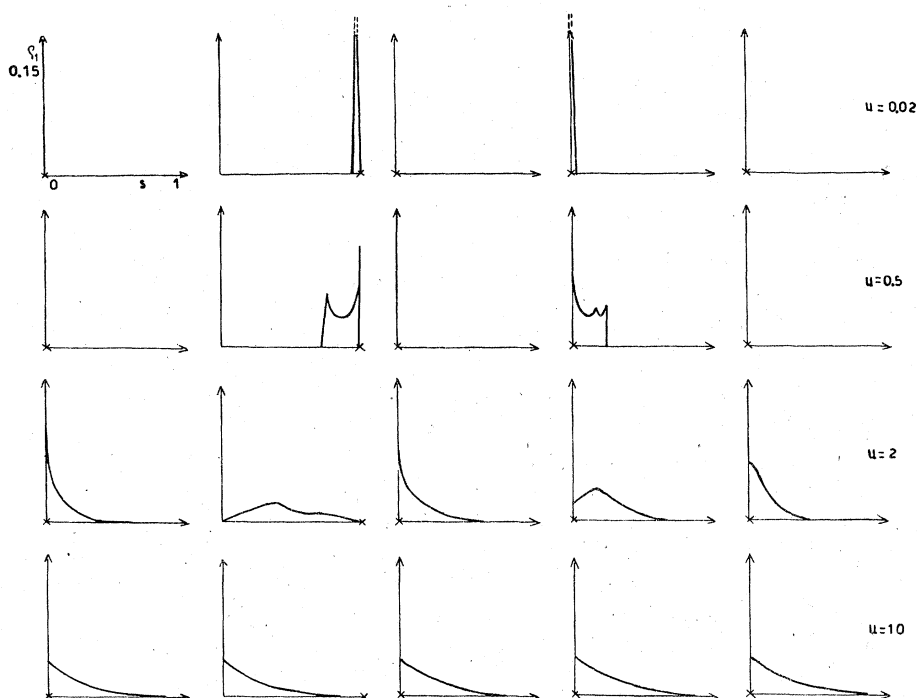


FIG. 6. Same as in Fig. 5 for a different set of initial conditions at various energies.

tributions for the normal mode energies strongly supports the existence of disjoint invariant components in the stochastic region.

IV. CONCLUSIONS

We have reported two kinds of results: the bifurcation curve for the stochastic parameter (or maximal Lyapunov number) and the curves for the densities of the probability distributions for the normal mode energies. These results appear to indicate that in general, in our model, on the same energy surface the stochastic region is subdivided into mutually disjoint invariant components. Let us now add some comments.

(i) *A posteriori* it may appear not so surprising that we found our bifurcation curve. Indeed, it seems to be a general feature that some kind of accumulation of bifurcations occurs in any transition to something like a turbulent state. On the other hand, a kind of bifurcation was already observed by Contopoulos¹⁴ for Hamiltonian systems with two degrees of freedom. Actually that author looked for periodic orbits. Let x be the abscissa of the point of intersection of a periodic orbit at energy E with a given surface of section; then one can consider the curve $x(E)$. Contopoulos found that such a curve bifurcates at the energies where the

orbit becomes unstable, because two new stable periodic orbits then appear. In such a way several accumulations of bifurcations were observed.

(ii) A confirmation of our results has been given, just after our observations, by Benettin and Strelcyn,¹⁵ in a study of the way in which a certain model for billiards passes from being integrable to being a K system as the border is continuously deformed. Indeed they found a bifurcation curve for the stochastic parameter, just analogous to ours reported in Fig. 2. In this connection it may be remarked that their results are particularly interesting because in their case of two degrees of freedom it is possible to provide figures by surfaces of section, so that a visual observation of the disjoint stochastic regions can be afforded. On the other hand, our case with $N > 2$ provides new information because, as we have already remarked, the existence of disjoint stochastic components is then no more guaranteed by the existence of invariant N -dimensional tori. Thus our results appear to indicate that there is a phenomenon which points out some general features and could be of interest in connection with the problem of the so-called Arnol'd diffusion.

(iii) The transition from quasiperiodic to stochastic motions has been repeatedly investigated by Froeschlé and Scheidecker.^{16,17} The main conclusion they draw is that their results "confirm the

conjecture that a dynamical system with N degrees of freedom has in general N or 1 isolating integrals." Actually, our results suggest that some kind of constraints exist even in the stochastic re-

gion, but it is not yet clear how and whether they can possibly be described in terms of formal integrals. This is an open problem to which we hope to come back in the future.¹⁸

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