Numerical computations on a stochastic parameter related to the Kolmogorov entropy

M. Casartelli
Istituto di Fisica dell'Università, Parma, Italy

E. Diana
CCR Euratom Ispra, Varese, Italy

L. Galgani
Istituto di Fisica and Istituto di Matematica dell'Università, Milano, Italy

A. Scotti
Istituto di Fisica dell'Università, Parma, Italy
and CCR Euratom Ispra, Varese, Italy

(Received 10 November 1975)

A stochastic parameter which appears to be related to the Kolmogorov entropy is computed for a system of N particles in a line with the nearest-neighbor Lennard-Jones interaction. It is found that the parameter depends on the initial conditions, and is equal to zero or to a positive value which depends on the specific energy u. A limit seems to exist for the parameter at fixed u when $N \to \infty$, as shown by computations from $N = 10$ to 200.

I. INTRODUCTION

For many systems of coupled oscillators to which the Kolmogorov-Arnol'd-Moser theorem applies, it turns out that there is a region of phase space practically filled by invariant tori.[1] The problem of a quantitative estimate of the extension of such a region is usually investigated by means of numerical computations.

Since the very first works of Contopoulos, Hénon, and Heiles[2] and of Barbanis,[2] the following criterion has been considered to characterize the region with tori (ordered region) with respect to the complementary one (disordered region): One computes as a function of time the distance between orbits starting from nearby points in phase space, and linear growth is associated to ordered motions, exponential growth to disordered motions. Analogous computations have since been undertaken in several connections,[3] including one by the present authors for a system of 1000 particles in a line.

It is also of interest to provide a parameter which gives an estimate of the degree of stochasticity in the disordered region.[4] If the distance $d(t)$ between the two orbits grew in an exponential way, $d(t) = d(0)e^{\beta t}$, β being a constant, β would be such a natural parameter. Actually, the function $d(t)$ turns out to be rather irregular and, moreover, does not increase after a saturation time which depends on the initial conditions; thus a more suitable procedure has to be worked out.

Consider the quantity defined by $(1/t)\ln[d(t)/d(0)]$ after a fixed time t and evaluate its time average, the stochastic parameter. In particular, the fixed time t can be taken very small, so that the problem of the saturation time disappears, and, moreover, it turns out that the dependence of the results on t is totally controllable. The quantity so defined is not only a computational tool, but is deeply related to the Kolmogorov entropy, a fundamental concept of probability theory.

Our computations deal with a model of N particles in a line coupled by a nearest-neighbor Lennard-Jones interaction, and are addressed particularly to the investigation of the dependence of the stochastic parameter both on the specific energy and on N.

In Sec. II we define the stochastic parameter, in Sec. III we describe the model and report the numerical results, and in Sec. IV we discuss the connections with the Kolmogorov entropy.

II. STOCHASTIC PARAMETER

Let us consider a Hamiltonian system with N degrees of freedom in a phase space M with a given Hamiltonian H_N. A flow $\{T_t\}$, $t \in R$ (t real), is then defined, i.e., $T_t x(0) = x(t)$, where $\{x(t)\}$ is a solution of the Hamiltonian equations of motion. Given a fixed time t, we shall simply designate T_t by T; in such a way an automorphism T is defined on M.

For any initial point x_0 an orbit $x_i = Tx_{i-1}$ ($i = 1, 2, 3, \ldots$) is defined. Consider then another initial point $y_0 = x_0 + d_0$; this point will be eventually taken sufficiently close to x_0; i.e., $|d_0|$ will be sufficiently small, if $|\cdots|$ denotes the norm (for ex-

ample, the Euclidean one). We then consider the quantity $|d_1|/|d_0| = |Ty_0 - Tx_0|/|y_0 - x_0|$, which can be defined after the first step; a new orbit is now started near x_1 at $y_1 = x_1 + [d_1/|d_1|]|d_0|$, and so the quantity $|d_2|/|d_0| = |Ty_1 - Tx_1|/|y_1 - x_1|$ is defined after the second step, and so on. In such a way we can compute the time average of $\ln[|d_i|/|d_0|]$.

Precisely, one defines recursively the quantities x_0, y_0, $d_0 = y_0 - x_0$, $x_i = Tx_{i-1}$, $d_i = Ty_{i-1} - Tx_{i-1}$, $y_i = x_i + [d_i/|d_i|]|d_0|$ $(i = 1, 2, 3, \ldots)$, and the time average after n steps:

$$k_n^{(N)}(t, x_0, d_0) = \frac{1}{n}\sum_{i=1}^{n} \ln\left(\frac{|d_i|}{|d_0|}\right).$$

One is obviously interested in the limit, if it exists, of $k_n^{(N)}$ as $n \to \infty$.

III. MODEL AND NUMERICAL RESULTS

We consider a system of $N+2$ points of mass m in a line, the two extreme points being a distance L apart, with nearest-neighbor Lennard-Jones interaction potential $V(r) = 4\epsilon[(\sigma/r)^{12} - (\sigma/r)^6]$, where r is the distance between two neighboring particles and ϵ and σ are positive parameters. Their meaning is given by $V(\sigma) = 0$, $\inf_r V(r) = V(2^{1/6}\sigma) = -\epsilon$. In our model, $L = (N+1)2^{1/6}\sigma$. Being specially interested in the range of energies just above the minimum, we shifted the zero of energy at the bottom of the potential well, so that our potential was $\tilde{V}(r) = V(r) + \epsilon$. In our computations the values of the parameters were $m = 1$, $\sigma = 1$, $\epsilon = 27.5$. We recall that for such a system a characteristic time, which we call τ, is the limit as $N \to \infty$ of the shortest period of the corresponding harmonic system; in our units, $\tau = 0.079$.

In the numerical computations the integration step was typically $2.5 \times 10^{-2}\tau$, and the longest runs took 4×10^6 steps, which corresponds to a time of $10^5\tau$. Most parts of the computations were performed with $N = 10$ and $N = 50$, and the specific energy $u = E/N$ ranged from 0.01 to 40, i.e., from $3.6 \times 10^{-4}\epsilon$ to 1.45ϵ.

We report now the dependence of $k_n^{(N)}(t, x_0, d_0)$ on the various parameters.

i. Dependence on n. The limit $k^{(N)}$ of $k_n^{(N)}$ as $n \to \infty$ seems to exist in all cases, with two possibilities, i.e., it tends to a finite positive limit or monotonically decrease towards zero. For example, for $t = 0.75\tau$, $N = 50$, and two pairs of x_0, d_0 we have the diagrams of Fig. 1. In the upper curve, all the values after the first one are equal within 0.6%. The monotonic decrease was confirmed also by longer computations; for example, with $N = 40$ and t as above, we worked with values up to $n = 130\,000$,

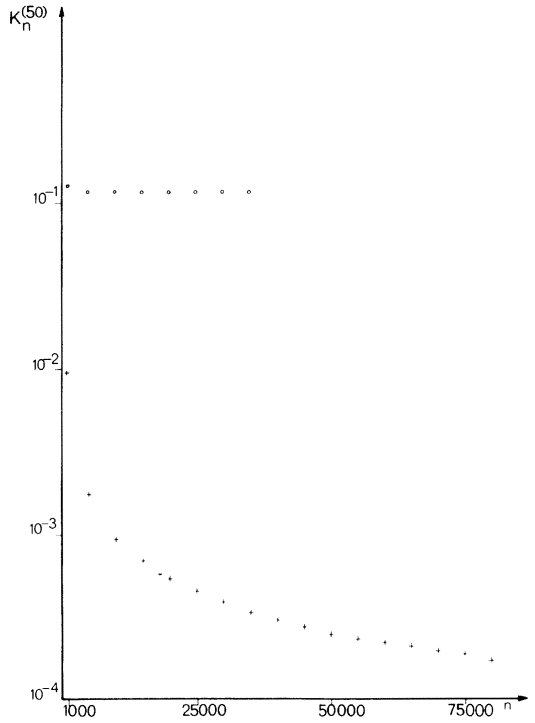

FIG. 1. $k_n^{(50)}$ vs n, for $u = E/N = 0.05$ and 8.

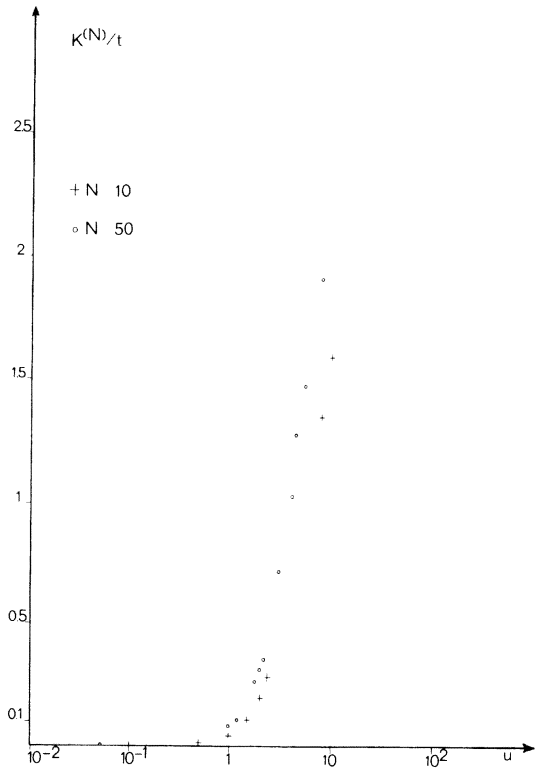

FIG. 2. $k_n^{(N)}/t$ vs $u = E/N$, for $N = 10$ and 50.

which corresponds to a time of $97\,500\tau$.

ii. Dependence on t. For $N=50$ and fixed values of x_0 and d_0 we found that with very good accuracy the relation $k^{(N)}(jt,x_0,d_0)=jk^{(N)}(t,x_0,d_0)$ was satisfied with j keeping five values between 1 and 20. Indeed, for example, in two computations with $t_2=8t_1=\tau$ this relation was satisfied within 1% after a time of $1.5\times10^4\tau$. Analogous results were found for $N=10$. These results are in agreement with the relation $k^{(N)}(t,x_0,d_0)=tk^{(N)}(1,x_0,d_0)$ for any t. As a consequence, in order to make the various results comparable, from now on we report the values of $k^{(N)}(t,x_0,d_0)/t$, i.e., presumably of $k^{(N)}(1,x_0,d_0)$.

iii. Dependence on d_0. The results are largely independent of both the direction and the length of d_0. For example, the initial point of the second orbit was defined by shifting both the positions and the velocities of all the particles of the first orbit in the positive direction, the positions by $10^{-6}\sigma$ and the velocities by $10^{-5}\sigma/\tau$. In other cases the displacements were changed by a factor of 10^2 without any appreciable difference in the results. The same result happened with other kinds of displacements.

iv. Dependence on x_0. In Fig. 1, the case of a finite limit (upper curve) corresponds to an energy $E=H(x_0)=400$, and the case of limit zero to an energy $E=2.5$. In general it turns out that the limit $k^{(N)}(t,x_0,d_0)$ is equal to zero or to a positive value which depends on the corresponding energy $E=H_N(x_0)$. For example, for $E/N=8$, ten different initial conditions have been considered, but a systematic survey of the energy surface has not been performed.

v. Dependence on the specific energy u. For $N=10$ and $N=50$ we found the diagrams of $k^{(N)}/t$ as functions of $u=E/N$, as given in Fig. 2. Note that for $u\leq0.1$ the values reported as zero are meant in the sense of the discussion of point (i), while for $u>0.5$ the positive values were rather well stabilized. In the intermediate region the relaxation times seem to be much longer,[5] and it is presently difficult to assign definite values to the limits, which are expected to exist. It may be of interest to remark that for $u>2$ one has approximately $k^{(N)}=\alpha^{(N)}\ln u$.

vi. Dependence on N. For fixed specific energy $u=8$ we obtained the diagram of Fig. 3. Analogous results were obtained for $u=1$ and N between 10 and 50. This strongly indicates that a limit exists when $N\to\infty$, for all values of u.

Thus we have summarized our results concerning the Lennard-Jones chain. In addition, analogous computations were performed for systems of 10 and of 50 harmonic oscillators for many cases of initial conditions at various energies; we always found $k^{(N)}=0$, in the asymptotic sense of (*i*).

In conclusion, these results suggest the existence of the quantity

$$k(u)=\lim_{\substack{d_0\to0\\ n\to\infty\\ N\to\infty}}k_n^{(N)}(1,x_0,d_0),\quad u=H_N(x_0)/N.$$

IV. CONNECTIONS WITH KOLMOGOROV ENTROPY

In this section we first recall briefly some well-known facts about the Kolmogorov entropy[6] and then come to heuristic considerations on the possible connections with the stochastic parameter.

We take a differentiable manifold M and a flow $\{T_t\}$, $t\in R$, on it, we denote by $\mathsf{M}(M)$ the set of all Borel measures μ invariant under the flow, as described in the Krylov-Bogoliubov theory. For each $\mu\in\mathsf{M}(M)$ the Kolmogorov entropy $h_\mu(\{T_t\})$ of the flow is defined by $h_\mu(\{T_t\})=\sup_{t>0}[h_\mu(T_t)/t]$, where $h_\mu(T_t)$ denotes the Kolmogorov entropy of the automorphism T_t. It has been proven by Abramov that $h_\mu(T_t)=|t|h_\mu(T_1)$, so that one has $h_\mu(\{T_t\})=h_\mu(T_1)$.

In some examples[7] it has been shown that the Kolmogorov entropy is related to the dilation coefficients of a dynamical system. These examples refer to C systems, for which the expanding and the contracting manifolds, and correspondingly the coefficients of expansion and of contraction, can be defined.

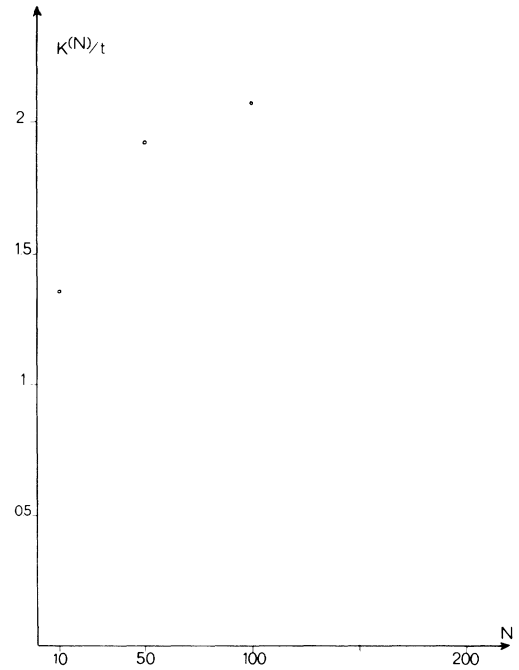

FIG. 3. $k^{(N)}/t$ vs N.

General statements on the connections between entropy and expansion coefficients can be found in a paper by Sinai,[8] where, for example, it is said: "It already seems clear that positiveness of the entropy and the presence of mixing are related to extreme instability of the motion of the system: trajectories emanating from nearby points must, generally speaking, diverge with exponential velocity,.... Thus entropy is characterized here as the speed of approach of the asymptotic trajectories or, what is the same thing, the speed of their divergence." More precisely, the entropy $h_\mu(\{T_t\})$ turns out to be proportional to the average (with respect to μ) of the expansion coefficient.

We come now to the connections with our calculations. It may be remarked that the exact expression for the entropy quoted above makes reference to expanding manifolds, which are rather hard to handle within a computer program; moreover, the expansion coefficient is defined as the logarithm of the relative increase, under the flow, of a volume element (in the expanding manifold), while we consider relative increases of distances along orbits, which is an approximation for the relative increase of vectors in the tangent space.

However, we may note first that although the vectors d_0 that we consider can have a component in the contracting manifold, such a component will tend to vanish during the time evolution, so that this should not be a difficulty if t is not too small. In addition, if l is the dimension of the expanding manifold, the relative increase of distances can be expected in the mean to be approximately the lth root of the relative increase of volumes, so that our quantity $k^{(N)}$, being the (time average of the) logarithm of the relative increase of distances, should be proportional to $h^{(N)}/l$. Assuming then, as seems reasonable, that the dimension l is proportional to N, one finally determines $k^{(N)}$ to be proportional to $h^{(N)}/N$. In conclusion, $k^{(N)}$ should be an intensive quantity (i.e., independent of N) if $h^{(N)}$ is expected to be extensive (i.e., proportional to N). This last conjecture seems to be in agreement with a general inequality given by Katok and Stepin,[9] according to which one has for an automorphism T on a manifold M

$$h_\mu(T) \leq \tfrac{1}{2}\dim M \times \max\left(\int_M \ln \|dT\|_x \, d\mu(x),\ \int_M \ln \|dT^{-1}\|_x \, d\mu(x) \right),$$

where x is a point of M, dT is the differential of the mapping T, and $\|\cdots\|$ denotes the norm of a linear operator.

Finally, another class of problems is related to the fact, already mentioned, that the Kolmogorov entropy can be shown to be proportional to the average of the expansion coefficient with respect to an invariant measure μ (in fact, in the papers of Sinai, the Lebesgue measure), while we consider time averages. Owing to the Birkhoff theorem, these two quantities are the same almost everywhere with respect to μ if the flow $\{T_t\}$ is μ ergodic, but this fact leaves open the problem of the choice of the invariant measure in $\mathfrak{M}(M)$.

In connection with our computations, however, we remark that our quantity $k^{(N)}$ turns out to be intensive for sufficiently large N as shown by Fig. 3, and moreover to satisfy the relation $k^{(N)}(t) = tk^{(N)}(1)$, $t>0$, which is exactly proved for the Kolmogorov entropy.[10]

V. CONCLUSIONS

For a system of N particles our numerical calculations suggest the existence of a function $k^{(N)}(u)$, u being the specific energy, which can be considered to be a stochastic parameter in the sense discussed in Sec. I; moreover, the limit

$$k(u) = \lim_{N\to\infty} k^{(N)}(u)$$

seems to exist and, in our model, to be practically reached for $N=200$. The parameter $k^{(N)}(u)$ might be related to the Kolmogorov entropy of the same system.

Concerning the shape of the curve $k(u)$, we may say that there seems to be agreement with previous calculations, according to which for $N>10$ the transition between ordered and disordered motions takes place around $u=1$; indeed we have $k^{(50)}(u)=0$ for $u<0.1$ and $k^{(50)}(u)>0$ for $u>1$. Moreover, the method presented here has the advantage of affording the possibility, at least in principle, of a precise definition of a critical specific energy $\bar{u}$ as the intercept of the curve $k(u)$ with the axis of the abscissa. However, further calculations are required in order to determine the precise value of $\bar{u}$. In addition, the curve $k(u)$ is clearly increasing with u and is certainly concave at least for $u>2$, while the convexity properties below $u=2$ require further investigation.

Finally, we remark that it would be interesting to study possible connections between $k(u)$ and the specific thermodynamic entropy.

ACKNOWLEDGMENTS

We thank V. I. Arnol'd for useful suggestions and J. M. Strelcyn for discussions on the Kolmogorov entropy. We hope in the future to discuss the connections of our results with those reported by Izrailev, Khisamutdinov, and Chirikov[4] and by Chirikov, Izrailev, and Tayurrski[4] and obtained by very similar methods.

[1]See, for example, L. Galgani and A. Scotti, Riv. Nuovo Cimento 2, 189 (1972); L. Galgani, Scientia (to be published).

[2]G. Contopoulos, Astron. J. 68, 3 (1963); Bull. Astron. 2, 223 (1967); M. Hénon and C. Heiles, Astron. J. 69, 73 (1964); B. Barbanis, *ibid.* 71, 415 (1966).

[3]B. V. Chirikov, CERN Translation No. 71-40 (CERN, Geneva, 1971); J. Ford, in *Lectures in Statistical Physics*, edited by W. C. Schieve (New York, 1972); S. D. Stoddard and J. Ford, Phys. Rev. A 8, 1504 (1973); G. Casati and J. Ford (unpublished); H. Hirooka and N. Saito, J. Phys. Soc. Jpn. 27, 815 (1969); G. Ciccotti and G. Jacucci (unpublished); M. Casartelli, G. Casati, E. Diana, L. Galgani, and A. Scotti (unpublished).

[4]F. M. Izarailev, A. I. Khisamutdinov, and B. V. Chirikov, LASL Report No. LA-4440TR (1970); B. V. Chirikov, F. M. Izrailev, and V. A. Tayurrski, Comput. Phys. Commun. 5, 11 (1973); C. Froeschle, Astron. Astrophys. 16, 172 (1972); C. Froeschle and J. Scheidecker, *ibid.* 22, 431 (1973); J. Comput. Phys. 11, 423 (1973).

[5]This is in agreement with results of M. Carotta, C. Ferrario, L. Galgani, and G. Lo Vecchio (unpublished).

[6]A. N. Kolmogorov, Dokl. Akad. Nauk SSSR 119, 861 (1958); 124, 754 (1959); R. Adler, A. Konheim, and M. H. McAndrew, Trans. Am. Math. Soc. 114, 309 (1965); V. I. Arnol'd and A. Avez, *Problèmes Ergodiques de la Mêcanique Classique* (Gauthier-Villars, Paris, 1967); Ja. G. Sinai, *Theory of Dynamical Systems, Part I, Ergodic Theory*, notes by J. M. Strelcyn (Aarhus, 1970); V. A. Rokhlin, Russ. Math. Surv. 22, 5 (1967); J.-M. Strelcyn, *Leçons sur quelques notions élémentaires de la thêorie ergodique* (University of Parma, Parma, 1975).

[7]Ja. G. Sinai, Izv. Akad. Nauk SSSR Ser. Mat 30, 15 (1966); G. A. Margulis, Funct. Anal. Appl. (to be published).

[8]Ja. G. Sinai, Am. Math. Soc. Transl. 31, 62 (1963), see page 72.

[9]A. B. Katok and A. M. Stepin, Russ. Math. Surv. 22, 77 (1967).

[10]After the completion of this work, J.-M. Strelcyn informed us that new results of Yu. B. Piesin (unpublished), together with the known work by V. I. Oseledec [Trans. Moscow Math. Soc. 19, 197 (1968)], substantially clarify the problem considered in this section. In particular, it turns out that the stochastic parameter k does not coincide, in general, with the Kolmogorov entropy, although it is nevertheless strictly related to it.