Stochastic transitions and statistical features of one-dimensional chains

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Statistical consequences of the subdivision of the phase space of a classical nonlinear system (a Lennard-Jones chain) into regions of ordered and stochastic motions are investigated by numerical computations on two parameters, which are related to the average fluctuations and to the equipartition of the kinetic energy. While the former parameter behaves as if it were an ergodic function (i.e., its time average is correctly given by its canonical average), the time average of the latter cannot be so computed, and furthermore it exhibits a transition consistent with previous computations. Comparisons are made with a harmonic chain and with a Toda chain.

I. INTRODUCTION

Investigations on the statistical properties of classical nonlinear systems, which have recently undergone a great development,[1-11] have tackled three kinds of problems of increasing relevance to statistical physics. In the first place one has to establish the existence of qualitatively different types of motions, i.e., "ordered" and "disordered" or "stochastic" motions; secondly, to characterize the regions of the phase space associated with different types of motion. In particular, if at all possible, one has to find the connection between existence and extension of such regions and physical parameters, such as specific energy, strength of interaction, etc. In this context of utmost importance is, of course, the connection with the number of degrees of freedom, inasmuch as if in the thermodynamic limit such features disappear, they would be of no relevance in statistical physics. If, on the contrary, such features somehow are preserved, the assumptions on which the usual prescription for computing phase average is given are not satisfied. Consequently, in the third place, one has to reformulate this prescription.

The present paper is mainly devoted to the second type of problem. Moreover, it provides some evidence for the necessity of tackling the third kind. Along the same lines of Refs. 1, 7, and 8, we study a one-dimensional chain of particles interacting via a nearest-neighbor Lennard-Jones potential between fixed ends. By introducing two parameters connected with the fluctuations and with the equipartition of the kinetic energy of the individual particles, the time averages of these quantities are compared with the corresponding standard canonical averages. The time averages are computed by direct numerical integration of the equations of motion. One may remark that many of the early studies on stochastic transitions were performed by looking at quantities expressed in terms of collective coordinates (e. g., normal modes). One reason to study parameters expressed in terms of the coordinates of the individual particles is that they appear to be directly connected with important physical macroscopic observables. The analysis is carried out by considering the dependence of our parameters on different classes of initial conditions, on specific energy, and number of degrees of freedom.

Comparisons are also made with the corresponding behavior of the parameters for two typical integrable systems, such as a pure harmonic chain and a Toda chain. Details about the models we consider, and known results relevant to our studies are given in Sec. II. In Sec. III we introduce our parameters and discuss their numerical evaluation in connection with their canonical value. Results of the numerical experiments are given in Sec. IV while in Sec. V we give some final comments.

II. DESCRIPTION OF MODELS AND CONNECTION WITH PREVIOUS RESULTS

Most of our numerical experiments have been performed on a one-dimensional chain of $N+2$ particles of mass m, interacting via a nearest-neighbor Lennard-Jones potential

$$V_{LJ}(r) = 4\epsilon[(\sigma/r)^{12} - (\sigma/r)^{6}] \ . \tag{1}$$

The extreme particles are fixed at a distance $L = (N+1)d_0$, where $d_0 = \sigma(2)^{1/6}$ is the equilibrium distance. The values used for the parameters are $m = 1, \sigma = 1, \epsilon = 27.5$. A characteristic time τ may be defined as the limit for $N \to \infty$ of the shortest period of the corresponding harmonic system, and it turns out to be, in our units, $\tau = 0.079$. For comparison, an interaction potential of the following type (Toda potential)

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$$V_T(r) = \alpha e^{-\beta r} + \gamma r \qquad (2)$$

will be considered. The constants α, β, and γ are choosen in such a way that potentials (1) and (2) coincide up to second-order terms around the minimum: $\alpha = \lambda d_0^2 e^{-1}$; $\beta = -1/d_0$; $\gamma = -\lambda d_0$ where $\lambda = V''_{LJ}(d_0)$.

The equations of motion have been integrated using a standard third-order integration procedure. A typical time integration step was $2.5 \times 10^{-2}\tau$, and typical runs were of about 3×10^5 integration steps.[12,13] Before introducing our parameters, we briefly summarize here the relevant results concerning the dynamical properties of the considered models.

As is well known, both the Toda chain and the harmonic chain are integrable systems, i.e., there exist N independent integrals of motion which are in involution (the Poisson bracket of any two of them vanishes). With reference to the qualitatively different types of motion which can occur in classical dynamical systems mentioned in the Introduction, we recall that integrability allows only one such type, the so-called ordered one. In fact, if the system is integrable, the motion takes place on surfaces of lower dimensionality than that of the energy surface (invariant tori). There is, however, an important difference between the harmonic chain and the Toda chain, in that the latter is highly nonlinear, and this has as a consequence, for instance, that the frequencies depend on the initial conditions, whereas this is not the case for the former which is linear. From a geometrical point of view, integrable systems are characterized by a continuous foliation of the phase space, i.e., by the fact that the phase space is the union of invariant tori.

As regards the Lennard-Jones chain, which is not integrable, no simple geometrical picture of the structure of phase space can be given. It has been established, however, that their does still exist a region where the motion is "ordered." A plausible interpretation of this order consists in assuming that there are still invariant surfaces which, even if they do not constitute a continuous foliation of phase space, "fill it" in the sense that their measure μ_0 is positive and, denoting by μ the measure of such region, one has $\mu_0 \mu / \sim 1$. Furthermore, there exists another distinct region where the motion is "stochastic," that is to say, the representative point of the system moves erratically over practically the whole energy surface. This kind of motion exhibits all the features required by standard classical statistical mechanics: time averages of observables are independent of initial conditions, any correlation between nearby orbits is quickly lost, etc.

As before, one can interpret geometrically this state of affairs by saying that invariant surfaces (though still present) are statistically irrelevant inasmuch as their measure is close to zero.

For all the parameters considered to establish such results, the transition from order to stochasticity sets in with continuity. Therefore there exist a third region in phase space where the relative measure of invariant surfaces is neither close to 0 nor to 1 and where "solutions of different behavior exist side by side."[14] Even if a sharp picture of the boundaries between any two of these regions is still unknown, in practice it is possible to define two values of the specific energy, u_1 and u_2, such that "for energies lower than u_1, the overwhelming majority of initial conditions lead to ordered motion and, for energies higher than u_2, the overwhelming majority of initial conditions lead to stochastic motion."[15] One can therefore call "threshold energy" the value u_1. Such a threshold, as a function of the number of degrees of freedom, decreases quite rapidly increasing N from 2 to 10. For values of N around 20 one has $u_1 = 0.1$, $u_2 = 1.0$ in our units, and these values remain practically unchanged up to the maximum N considered ($N = 1000$). These numerical estimates are not sufficiently reliable to prevent the threshold falling to 0 when $N \to \infty$. All one can say is that they are not inconsistent with the possibility that such a fall actually does not occur.

III. PARAMETERS P_1 AND P_2

Let us define two parameters P_1 and P_2 in the following way: let $k_i(t) = m\dot{x}_i^2(t)/2$ be the kinetic energy of the ith particle, and $K(t) = (1/N)\sum_i k_i(t)$ be the average kinetic energy at time t. Define

$$S^2(t) = \frac{1}{N}\sum_{i=1}^{N} [k_i(t) - K(t)]^2$$

as the mean-square instantaneous deviation. Starting from fixed initial conditions $\{\vec{x}(0), \vec{\dot{x}}(0)\}$ one can follow the time evolution of $S^2(t)$ along the trajectory and perform the time average up to time T:

$$\overline{(S^2)}^T = \frac{1}{T}\int_0^T S^2(t)\,dt \ .$$

Denote by $\overline{S^2}$ the limit for $T \to \infty$ of $\overline{(S^2)}^T$. Analogously by $\overline{K}^T$ and $\overline{K}$ will be denoted the time average of $K(t)$ up to time T and the corresponding limit. Then, our parameter P_1 is

$$P_1 = \overline{S^2}/\overline{K^2} \ . \qquad (3)$$

P_1 is a dimensionless quantity which *a priori* depends on the initial conditions and thereby on physical parameters of the system, like energy, number of degrees of freedom, etc.

S^2 and K^2 are observables for which the phase-space canonical average can be easily computed. Define, for instance, as usual

$$S^2_{\text{can}} = \int_\Omega e^{-\beta H(\vec{p},\vec{x})} S^2(\vec{p})\, d\vec{p}\, d\vec{x} \Big/ \int_\Omega e^{-\beta H(\vec{p},\vec{x})} d\vec{p}\, d\vec{x},$$

where Ω is the phase space and $p_i = m\dot{x}_i$. Denoting by P_1^{can} the ratio $S^2_{\text{can}}/K^2_{\text{can}}$, one obtains then

$$P_1{}^{\text{can}} = 2(N-1)/N .$$

This value is independent, of course, of initial conditions and is also independent of the temperature. In the limit for $N \to \infty$ one has $P_1^{\text{can}} = 2$. Moreover this computation of $P_1{}^{\text{can}}$ does not depend on the potential, and therefore holds true in each of the considered models.

If the system were ergodic, one should have $\overline{S}^2 \to S^2_{\text{can}}$, $\overline{K}^2 \to K^2_{\text{can}}$ and therefore $P_1 \to P_1^{\text{can}}$ when $N \to \infty$. In practice one may compare P_1 and P_1^{can} also when N is finite and sufficiently large. Therefore $|P_1 - P_1^{\text{can}}|$ can be taken as a suitable measure of the deviation from the standard results of classical statistical mechanics.

Now let $\overline{K}_i^T$ and $\overline{K}^T$ be the time averages up to time T of the kinetic energy of the particles and of their average, respectively, and $\bar{k}_i, \overline{K}$ the corresponding limits when $T \to \infty$. We define then the second parameter P_2 as follows

$$P_2 = \frac{1}{\overline{K}^2} \sum_i (\bar{k}_i - \overline{K})^2/N . \tag{4}$$

This quantity is analogous to P_1, except for using the time averages of the kinetic energies instead of their instantaneous values to define the mean-square deviation. Clearly, if $\bar{k}_i$ had for every i, in time average, the average value $\overline{K}$ (i.e., if the kinetic energy were equipartitioned in time) one would obtain $P_2 = 0$, and this is what one expects according to standard statistical mechanics. Therefore we have that while P_1 give a measure of the average fluctuations of the kinetic energy, P_2 gives a measure of the deviation from equipartition. Both P_1 and P_2 are directly related to the kinetic energy of the particles and, from the standard point of view, to the temperature of the system. Therefore they can give information on possible discrepancies, due to the existence of ordered regions, with the expectations of classical statistical mechanics.

Since numerical computations to obtain P_1 and P_2 are performed following the trajectory of the system by numerical integration of the equations of motion, what is actually computed are parameters expressed in terms of $\overline{K}^T$, $\overline{S}^T$, etc., and obviously not with their limits when $T \to \infty$. In practice, however, with exceptions of special cases which will be pointed out, $\overline{P}_1^T$ stabilizes

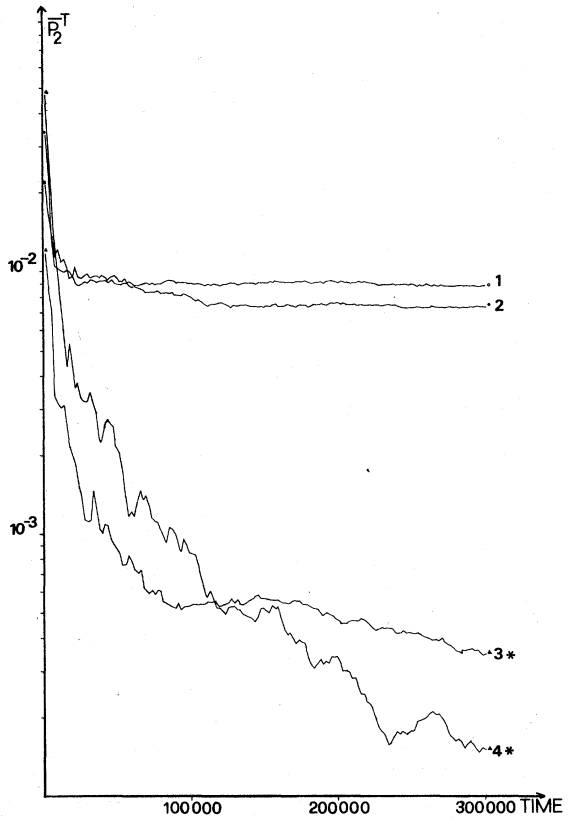

FIG. 1. $\overline{P}_2^T$ vs time (expressed in number of integration steps). Curves 1, 2, 3, and 4 refer, respectively, to specific energies $u = 0.01$, 0.1, 1.0, and 10.0. Curves 1 and 2 are considered as stabilized, curves 3 and 4 as decreasing to 0.

very well within the used computing time, and is therefore a good approximation to P_1. As for $\overline{P}_2^T$, two types of behavior, which are illustrated in Fig. 1, have been observed: in the first case, $\overline{P}_2^T$ reaches a well-stabilized value, and can be taken as a good approximation to P_2; in the second case, the value reached is not stabilized but definitively seems to approach the value 0. The latter behavior will be associated with final reaching of equipartition, i.e., $P_2 = 0$. This conclusion is arrived at by comparison of the order of magnitude of the considered quantity with the results of calculations carried out in a region of the phase space which is certainly stochastic. Such tendency to vanish will be denoted by a star in the tables.

IV. NUMERICAL RESULTS

Recalling that the phase space can be approximately subdivided into three regions (region I of ordered motion, region III of stochastic motion, and region II of transition) the behavior of P_1 and

P_2 has been analyzed in each of these regions separately, that is to say, at fixed N, by considering several values of specific energy u. Moreover, the behavior when the number of degrees of freedom increases at given fixed value of u has been naturally investigated.

The integration of the equations of motion requires a proper definition of the initial conditions, which turns out to play a rather important role in our analysis. Therefore, the actual choice of the initial conditions is presented here in some detail.

One type is the following:

$$x_i = A r_i s_i, \quad \dot{x}_i = B r_{i+N} s_{i+N}, \tag{5}$$

where x_i and $\dot{x}_i$ are the deviation of the i th particle from the equilibrium position and its speed, respectively, the r_i are random numbers generated by the subroutine RANF of the CDC 7600, the s_i are random signs, and A and B are two constants used to fix a given value of the total energy. This type of random initial conditions will be denoted by RC.

Another type, which will be called semiordered and denoted by SOC, consists in giving all the energy of the system to some modes of the corresponding harmonic chain. Most of the results reported here refer, for instance, to the following conditions

$$x_i = A(N+2+i)(-1)^i, \quad \dot{x}_i = B(N+2-i)(-1)^{i+1}, \tag{6}$$

which correspond to exciting practically only the high-frequency modes.

In Tables I and II the results for P_1 and P_2, respectively are summarized for several specific energies u at $N=50$. Both random and semiordered conditions are considered for the Lennard-Jones (LJ), the Toda (T) and the harmonic (H) chains.

From Table I one can see that, for RC, P_1 is practically canonical for the LJ chain at all energies. Moreover, the largest deviations from the canonical value occur in region III, and this fact makes more striking the canonical behavior of P_1 for small energies (i.e., in region I). While the T and the LJ chains give similar results, the behavior of the H chain is clearly noncanonical for all energies. Semiordered conditions influence these results for both the LJ and the T chains, besides the H chain increasing its noncanonical behavior. For $u<1$, the LJ chain deviates from the canonical value more than the T chain. Nevertheless, a transition is observable at high energies for the LJ chain: taking into account that the reported value of P_1 for $u=10$ is still increasing, it is possible to conclude that the canonical value is reached at this order of energy also for SOC.

TABLE I. Summary of results for P_1, $N=50$.

u	Type	P_1 with RC	P_1 with SOC
0.001	LJ	1.918 065	1.406 956
	T	1.905 519	1.410 108
	H	2.905 127	35.518 490
0.01	LJ	1.921 179	1.226 921
	T	1.913 658	1.337 401
	H	2.215 623	38.650 220
0.1	LJ	1.901 009	0.719 272
	T	1.882 233	1.211 761
	H	4.550 271	44.106 480
1.0	LJ	2.012 305	0.678 913
	T	1.894 914	1.386 542
	H	3.082 786	35.639 410
10.0	LJ	1.856 786	1.805 705 [a]
	T	1.923 274	1.138 668
	H	3.353 681	38.858 300

[a] Not stabilized increasing value.

Similar results are obtained also for P_2 with SOC, as one can see also from Table II: in particular, for the LJ chain the same transition already noted for P_1 may be observed for P_2, its value decreasing to 0.

But the most interesting difference between P_1 and P_2 refers to the random conditions. In region I we see that P_2 is well stabilized and differs from 0, both for the LJ and the T chains (for the H chain P_2 remains different from 0 independently of the energy). But, for the LJ chain, a transition toward equipartition occurs precisely on region II, and the result is confirmed in region III. In other words, P_2 behaves coherently with

TABLE II. Summary of results for P_2, $N=50$.

u	Type	P_2 with RC	P_2 with SOC
0.001	LJ	$1.297\,835\times10^{-2}$	$2.151\,463\times10^{-1}$
	T	$1.695\,121\times10^{-2}$	$2.161\,636\times10^{-1}$
	H	1.564 18	23.526 07
0.01	LJ	$8.907\,245\times10^{-3}$	$2.275\,891\times10^{-1}$
	T	$9.677\,600\times10^{-3}$	$2.393\,371\times10^{-1}$
	H	1.162 107	25.616 39
0.1	LJ	$7.392\,334\times10^{-3}$	$1.602\,374\times10^{-1}$
	T	$2.630\,341\times10^{-2}$	$2.754\,232\times10^{-1}$
	H	2.725 723	29.255 89
1.0	LJ	$3.505\,767\times10^{-3}$ [a]	$4.519\,564\times10^{-2}$
	T	$7.693\,890\times10^{-3}$	$2.172\,848\times10^{-1}$
	H	1.737 498	23.601 71
10.0	LJ	$1.649\,356\times10^{-4}$ [a]	$1.696\,595\times10^{-4}$ [a]
	T	$7.744\,648\times10^{-3}$	$2.164\,704\times10^{-1}$
	H	1.917 180	25.755 43

[a] Not stabilized decreasing value.

TABLE III. Summary of results for P_1 and P_2 vs N.

N	u	P_1	P_2
	0.01	1.921 179	$8.907\,245 \times 10^{-3}$
50	0.1	1.901 009	$7.392\,334 \times 10^{-3}$
	1.0	2.012 305	$3.505\,767 \times 10^{-4}$ [a]
	0.01	1.966 929	$3.652\,729 \times 10^{-3}$
100	0.1	1.947 240	$2.068\,129 \times 10^{-3}$
	1.0	1.860 479	$3.128\,203 \times 10^{-4}$ [a]
	0.01	1.987 725	$1.045\,973 \times 10^{-3}$
200	0.1	1.998 815	$6.378\,348 \times 10^{-4}$ [a]
	1.0	1.935 643	$2.336\,750 \times 10^{-4}$ [a]
	0.01	1.987 509	$9.160\,128 \times 10^{-4}$
300	0.1	1.995 760	$3.763\,121 \times 10^{-4}$ [a]
	1.0	1.963 771	$2.326\,956 \times 10^{-4}$ [a]
	0.01	1.984 974	$1.173\,471 \times 10^{-3}$
400	0.1	2.015 222	$3.516\,170 \times 10^{-4}$ [a]
	1.0	1.969 315	$2.496\,345 \times 10^{-4}$ [a]
	0.01	1.986 230	$1.323\,059 \times 10^{-3}$
500	0.1	2.011 861	$4.387\,798 \times 10^{-4}$ [a]
	1.0	1.957 522	$2.399\,355 \times 10^{-4}$ [a]

[a] Not stabilized decreasing value.

the other stochastic parameters used to establish the subdivision of the space into regions of stochastic and ordered motions.

Several test experiments, which will not be reported here, carried out at various values of N,

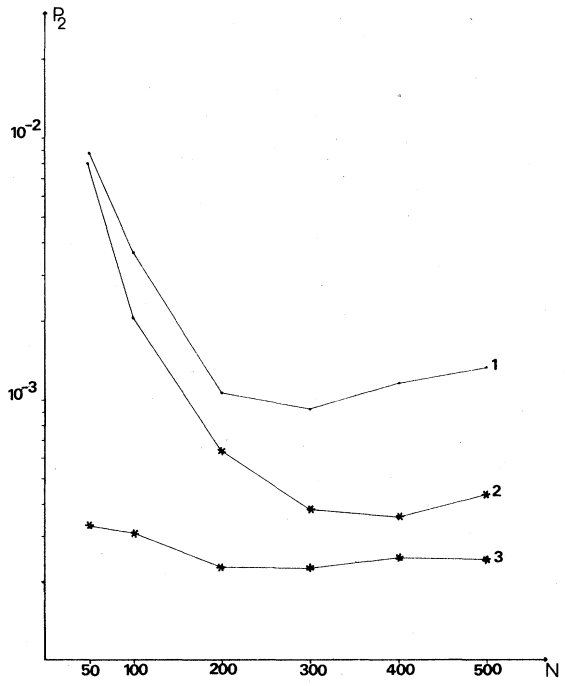

FIG. 2. Parameter P_2 vs N. Curves 1, 2, 3 refer, respectively, to specific energies $u = 0.01$, 0.1, and 1.0.

qualitatively confirm the general pattern of Tables I and II. Therefore, the following two points have been considered in greater detail: whether or not, by increasing N, (i) the canonical character of P_1 for the LJ chain with RC is confirmed and improved, and (ii) whether the stochastic transition of P_2 is still obtained.

As to the first point, from Table III one can indeed see that the above question can be answered in the affirmative. Also for the second point, the answer is affirmative in the sense that the stochastic transition for P_2 still occurs up to the highest value of N considered ($N = 500$), and the threshold specific energy u^c does not seem to decrease to 0, as is apparent from Fig. 2 where the curve corresponding to $u = 0.01$ shows a minimum around $N = 300$. Therefore, on the basis of our computations, we can only give a lower bound for the threshold energy: $u^c > 0.01$. This bound is slightly smaller than the one approximately indicated by previous computations with other parameters.

V. CONCLUSIONS

To clarify the analysis of our results, it is expedient to classify them in relation to the evidence they give in favor of or against the viewpoint which states that the existence of ordered motions is relevant for the foundations of statistical mechanics. The former will be noted by (a), the latter by (b).

(a1) Sensitivity to the initial conditions: the results are notably different for RC or SOC. To this typical nonergodic feature one could object that the special initial conditions fill a negligible part of the phase space, or, at least, a part which becomes negligible with increasing N. Further experiments are needed to confirm or to reject this plausible objection [see also (b1)].

(a2) The transition of P_2: for RC (the class of initial conditions which reasonably deserves a greater statistical consideration) the parameter P_2 exhibits a noticeable transition in the same region already indicated by previous stochastic parameters (this makes P_2, of course, a suitable alternative to those parameters, taking into account both precision and the computer time required).

(a3) Independence from N: the threshold of stochasticity, while smaller with respect to previous rough estimates, appears to be stabilized on a finite value when N increases.

On the other side are the following:

(b1) P_1 is practically canonical for RC even in region I for the LJ chain. One could suspect P_1 to be a function intrinsically ergodic; but if such

conjecture were true, P_1 should not depend on the initial conditions, as it does. As for the point (a1), there remains the possibility that the part of the phase space corresponding to special initial conditions vanishes in measure when $N \to \infty$.

(b2) Even at ver low energies, P_2 is considerably different for the LJ and the H chains. This fact may be regarded as an indication of the practical irrelevance of the conservation of the invariant surfaces.

(b3) In spite of the feature noted in (a3), the maximum value of N reached in the experiments might be not sufficiently large to give reliable information on the stability of the threshold.

To recover completely the standard point of view, both facts are therefore required: the vanishing of the measure of special conditions, and [against (a3)] the falling to 0 of the threshold in the thermodynamic limit. So, apart from the perspective of using P_2 as stochastic parameter, the necessity of a precise definition and estimate of the statistical weight of the different classes of initial conditions emerges from these experiments as the main direction for future work.[16]

At last, among the results which have not yet been classified against or in favor of any thesis, and which are nevertheless noteworthy, there is the fact that the nonlinearity seems to be a more characterizing feature than the nonintegrability, as shown by the substantial agreement at low energies between the LJ and the T chains.

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[14]Reference 5, p. 17.
[15]Reference 7, p. 205.
[16]These problems are probably related to those of Ref. 11.