Numerical test of the Liouville equation

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Dynamic ensemble theory is tested numerically for an ensemble of 1000 classical one-dimensional oscillators obeying canonical "Nosé-Hoover" dynamics. This dynamics couples each oscillator to a canonical heat bath characterized by a temperature and a relaxation time. Some initial oscillator conditions correspond to regular phase-space orbits of the Kolmogorov-Arnol'd-Moser torus type while others generate wider-ranging chaotic trajectories. Among the regular oscillator orbits is a set of trajectories resembling "double bedsprings," with "quantized" values of the oscillator energy and mean-square displacement. The number which indexes these orbits corresponds to the number of coils between turning points. Despite the existence of this relatively complex mixture of regular and chaotic trajectories, the Liouville equation correctly describes phase-space flows, in both the steady equilibrium canonical-ensemble case as well as in the nonsteady cases which evolve from strongly nonequilibrium initial conditions. The source of apparent irreversibility seen in the nonsteady evolution of the oscillator ensemble is identified as a "second-law" attractor, usually characteristic of large thermodynamic systems. The attractor is that relatively small but highly probable portion of phase space for which observation times exceed recurrence times.

I. INTRODUCTION

The Liouville equation, which describes the flow of probability density in phase space, is the dynamical basis of classical statistical mechanics, both at and away from equilibrium. The existence of highly irregular structures in phase space—strange attractors—which are neither smooth nor continuous, calls into question the usefulness of smooth probability densities which obey continuity equations such as Liouville's. Although these structures are typically associated with dissipative sets of equations, such as those developed by Lorenz,[1] there is no reason to rule out the existence of similar structures in systems described by Hamiltonian dynamics.[2,3] The complex and irregular structure of such attractors, present even on the smallest length scales, suggested that Liouville's theorem might be invalid for dealing with the dynamics of chaotic systems.[1] We report here the results of the first numerical test of ensemble theory for an ensemble of dynamical systems.

The test addressed three fundamental questions. Is the Liouville equation valid as it stands for chaotic systems? Does the Liouville equation properly describe the irreversible behavior typified by the Boltzmann equation and the second law of thermodynamics, or must it be supplemented with stochastic terms, or by coarse graining? Is it necessary that a system behave in a chaotic way in order for ensemble theory to be applied correctly?

We begin by reviewing the basic concepts of ensemble theory.[4,5] The goal of this theory is to describe the result of a measurement on a dynamical system of particles which interact with specified interparticle and boundary forces. It is assumed that such measurements are sufficiently reproducible and insensitive to the initial conditions, even if the underlying dynamics are Lyapunov unstable ("sensitive" or "chaotic"). The ensemble approach is introduced with the hope of simplifying the averaging process, making it unnecessary to follow the detailed dynamics of the many degrees of freedom present in a macroscopic thermodynamic system.

To simulate the ensemble approach with molecular dynamics we follow the motion of each of the N systems in the ensemble. Each system is allowed to evolve under the influence of identical equations of motion with equilibrium or nonequilibrium boundary conditions until equilibrium or a nonequilibrium steady state is attained. Usually the ensemble viewpoint is macroscopic, with the goal of describing results of measurements on thermodynamic systems with many degrees of freedom. Computer storage and speed impose strict limits on computer simulation. Because only a few many-body systems can be followed, the many-body few-system results would require extrapolation in order to compare them to theoretical infinite-system predictions.

Here we will not be concerned with this interesting large system limit, but rather the opposite extreme, a one-body system, the one-dimensional Nosé-Hoover oscillator.[6–10] By choosing such a simple system it is possible to consider a relatively large ensemble. We use up to 1000 members, all with slightly different initial conditions, but all evolving under the same equations of motion and with the same boundary conditions.

As the number of systems N in the ensemble approaches infinity we can imagine describing the time

development of the trajectories by a continuous probability density or ensemble distribution function $f(\Gamma,t)$ in the phase space (Γ space contains the coordinates and momenta of the particles as well as the time-dependent friction coefficient z described in Sec. II). A smooth density function $f(\Gamma,t)$ must satisfy the continuity equation known as the Liouville equation:

$$\partial f/\partial t+(\partial/\partial\Gamma)\cdot(f\dot{\Gamma})=0\ . \tag{1}$$

Provided that the equations of motion, which give $\dot{\Gamma}$ as a function of Γ and t, are reversible in the time, then Liouville's equation is likewise time reversible.

The Langevin and Boltzmann equations, as well as the hydrodynamic equations incorporating diffusion, viscosity, and conductivity, are all irreversible. The solutions of these approximate equations approach equilibrium only in the direction of increasing time, in agreement with our observations of the real world. One of the main tasks of our numerical work is to reconcile the apparent paradox, emphasized by Boltzmann, that irreversible behavior can be described by reversible dynamics without invoking numerical or external causes for the irreversibility. Some systems, such as those composed of hard disks or spheres, are inherently unstable, without even a finite neighborhood of stability in the vicinity of reentrant phase-space trajectories.[11] To avoid such an unstable model we choose a relatively stable system, the harmonic oscillator, which does have finite KAM-like tori (Kolmogorov-Arnol'd-Moser), regions of stability in phase space which enclose reentrant periodic trajectories.[10]

A second task is to understand the usefulness of the Liouville equation at equilibrium. If we start with an ensemble of systems distributed according to the equilibrium distribution function $f(\Gamma,t=0)=f_0(\Gamma)$, is this distribution stationary? This can be tested by studying the time dependence of any observable $B(\Gamma)$ which depends on the phase variables Γ. At equilibrium the ensemble average $\langle B\rangle$ should be a constant of the motion. Away from equilibrium $\langle B\rangle$ varies with time:

$$\begin{aligned}\langle B(t)\rangle &= \int d\Gamma\, f(\Gamma,t)B(\Gamma)\\ &= \int d\Gamma\, f(\Gamma,0)B[\Gamma(t)]\\ &\cong \frac{1}{N}\sum_{i=1}^{N} B(\Gamma_i(t))\ .\end{aligned} \tag{2}$$

The first line of Eq. (2) expresses the Schrödinger or Eulerian picture, where the probability flows into fixed cells in phase space, while the second line expresses the Heisenberg or Lagrangian equivalence, where trajectories of ensemble members are followed through phase space;[9] the last line is the finite ensemble approximation, having chosen elements with initial weights $f(\Gamma_i,0)d\Gamma_i=1/N$. We will study the time development of the potential and kinetic energies as well as two functions which reduce, at equilibrium, to the thermodynamic entropy.

Finally, we wish to understand the relationship between ensemble averages and time averages along individual trajectories. With $B_i=B(\Gamma_i(t))$, we define the latter to be

$$\overline{B}_i=\lim_{t\to\infty}\left[\frac{1}{t}\int_0^t ds\, B_i(s)\right]\ . \tag{3}$$

Must $\langle B\rangle$ and $\overline{B}_i$ be equivalent for ensemble theory to hold? If the dynamical system of particles is quasiergodic, then each trajectory $(1,2,\ldots,N)$ covers the relevant part of phase space and $\overline{B}_i=\langle B\rangle$, except for a possible subset of trajectories of measure zero.

We emphasize that quasiergodicity is not required in order for the Liouville equation to hold. Quasiergodicity is often assumed to be essential, so that only a single time average is required, but in fact ensemble theory can be used as a method for insuring that averages do not depend on initial conditions. Thus here we investigate a system which is patently nonergodic. This Nosé-Hoover oscillator system is described in Sec. II. The nonergodicity is demonstrated in Sec. III. In Sec. IV we then study the question "Does the Liouville equation, and ensemble theory, describe the nonequilibrium time development of such a system?" The characteristic feature responsible for the irreversible behavior of the Nosé-Hoover oscillator is a "second-law attractor." This feature of the phase-space is described in Sec. V.

II. NOSÉ-HOOVER OSCILLATOR (REFS. 6–10)

Consider first a single oscillator maintained at constant temperature by an integral control (feedback) mechanism. The control mechanism is characterized by a relaxation time τ. The oscillator coordinate is x. The oscillator temperature is proportional to the time-averaged mean-squared momentum y^2. The control variable, or "friction coefficient" is z. For convenience we choose the oscillator mass and force constant, as well as Boltzmann's constant, equal to unity. Thus the fundamental frequency is unity and the period is 2π.

The time development of such an oscillator takes place in three-dimensional phase-space $\Gamma=(x,y,z)$ and is governed by three first-order ordinary differential equations:

$$\begin{aligned}\dot{x}&=y\ ,\\ \dot{y}&=-x-zy/\tau\ ,\\ \dot{z}&=(y^2-1)/\tau\ .\end{aligned} \tag{4}$$

From the standpoint of dynamical systems theory the set of equations (4) has no fixed point. Because the divergence of the phase-space velocity,

$$\Omega=(\partial/\partial\Gamma)\cdot\dot{\Gamma}=\partial\dot{x}/\partial x+\partial\dot{y}/\partial y+\partial\dot{z}/\partial z=-z/\tau\ , \tag{5}$$

is nonzero, the probability density varies along any system trajectory: The Liouville equation (1) can be written in the Lagrangian form $-d\ln f/dt=\Omega$, where $d/dt=\partial/\partial t+\dot{\Gamma}\cdot(\partial/\partial\Gamma)$.

The integral feedback thermostat works as follows. If the time-averaged kinetic energy exceeds the equilibrium value $\frac{1}{2}$, the friction coefficient z increases, tending to reduce the momentum y. If the time-averaged kinetic energy is too low, less than $\frac{1}{2}$, then $\dot{z}$ decreases, so that the friction coefficient z can become negative, leading to an increase in the magnitude of y.

An alternative control mechanism, differential control,

results if Gauss's principle of least constraint[12] is applied to keep the kinetic energy constant. This form of differential control is not useful for a single degree of freedom. The resulting oscillator, with constant kinetic energy, can have no turning point. Proportional control[13] is ruled out on different grounds. If the momentum response is proportional to the deviation from the mean kinetic energy, as in the Rayleigh and van der Pol equations, the resulting equations of motion are not time reversible.

The internal energy of the oscillator, kinetic plus potential, is

$$H_0=(x^2+y^2)/2 \ . \tag{6}$$

It is useful to define the total energy, including a contribution from the feedback thermostat, to be

$$H=(x^2+y^2+z^2)/2 \ , \tag{7}$$

and we note from (4) that its rate of change is

$$\dot{H}=\dot{\Gamma}\cdot\partial H/\partial\Gamma=x\dot{x}+y\dot{y}+z\dot{z}=-z/\tau \ . \tag{8}$$

(We shall reserve the symbol $E=\langle H\rangle$ for the ensemble average of the total energy.) The equations of motion (4) are not Hamiltonian; that is, they can not be derived from the energy function H. Indeed, comparing (5) and (8) we see that $\dot{H}=\Omega$ is not identically zero, as it must be for Hamiltonian dynamics.

The equations of motion (4) can be derived from the requirement that the canonical distribution function

$$f_0=(2\pi)^{-3/2}\exp(-\beta H) \tag{9}$$

be a stationary solution of the Liouville equation (1) ($\beta=1/kT=1$). This can be checked by inserting (9) into (1) with the equations of motion (4). The original Nosé approach, as discussed in Refs. 6–8, is more complicated and will not be explained in detail here. Suffice it to say that Nosé dynamics is derived from a Hamiltonian in a four-dimensional phase space which includes a time-scaling "coordinate" s and its conjugate momentum. In the Nosé-Hoover dynamics (three-dimensional phase space) the constant of the motion becomes $H+\int_0^t ds\, z(s)/\tau$.

From the equilibrium distribution function we can see that the linear and quadratic moments of the phase variables are

$$\begin{aligned}&\langle x\rangle_0=\langle y\rangle_0=\langle z\rangle_0=0 \ ,\\ &\langle x^2\rangle_0=\langle y^2\rangle_0=\langle z^2\rangle_0=1 \ .\end{aligned} \tag{10}$$

Throughout this paper we use the angular brackets to indicate an average over an ensemble of systems, a finite ensemble in the case of our numerical work. The theoretical infinite ensemble at equilibrium is indicated by a subscript zero.

The equations of motion provide less information. The stationarity of the time averages $\overline{dx_i/dt}=\overline{dy_i/dt}=\overline{dz_i/dt}=0$, gives $\overline{y}_i=0$, $\overline{y_i^2}=1$, and $\overline{x}_i=-\overline{z_i y_i}/\tau$ for every system in the ensemble. It is therefore possible to detect nonergodicity of a trajectory if $\overline{x}_i\neq\langle x\rangle_0=0$.

III. EQUILIBRIUM RESULTS

We choose 1000 initial conditions from a Gaussian distribution in x, y, and z by using the Box-Muller transformation.[14] A pair of random numbers ξ,η distributed uniformly on the unit interval generates a pair of Gaussian distributed numbers X and Y:

$$\begin{aligned}X&=(-2\ln\xi)^{1/2}\cos(2\pi\eta) \ ,\\ Y&=(-2\ln\xi)^{1/2}\sin(2\pi\eta) \ .\end{aligned} \tag{11}$$

It is straightforward to show that in the infinite-ensemble-size limit the odd moments of X and Y vanish and that the even moments correspond exactly to those from a Gaussian distribution, with $\langle X^{2k}\rangle_0=(1)(3)(5)\cdots(2k-1)$. Choosing 1500 uniformly distributed $\xi\eta$ pairs leads to 1000 x-y-z triples with a Gaussian distribution. In our numerical work, we replace the equations of motion with a centered difference approximation, where the error is of order Δt^4:

$$\begin{aligned}&(x_+-2x_0+x_-)/(\Delta t)^2=-x_0-z_0(x_+-x_-)/(2\tau\Delta t) \ ,\\ &(z_+-z_0)/\Delta t=\{[(x_+-x_0)/\Delta t]^2-1\}/\tau \ ,\end{aligned} \tag{12}$$

where the time step Δt is very small relative to unity (typically 0.01 or less). We have checked the moments of the x-y-z distribution dynamically, from the first through the eighth. The calculation was carried out for a time for 10 000 corresponding to nearly 1600 oscillator periods. This was done for three values of the thermostat's relaxation time: $\tau=0.1$, 1, and 10. Apart from the expected fluctuations the ensemble moments remain Gaussian, as shown in Fig. 1, where the first four moments are displayed in the case $\tau=1$. The fluctuations increase with

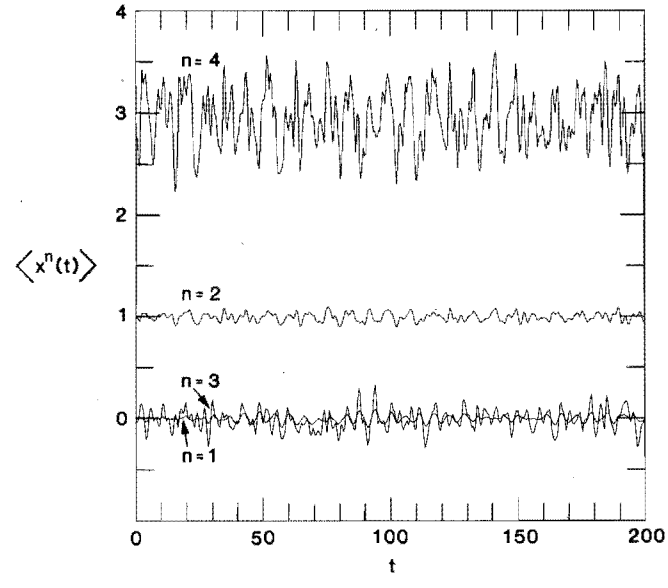
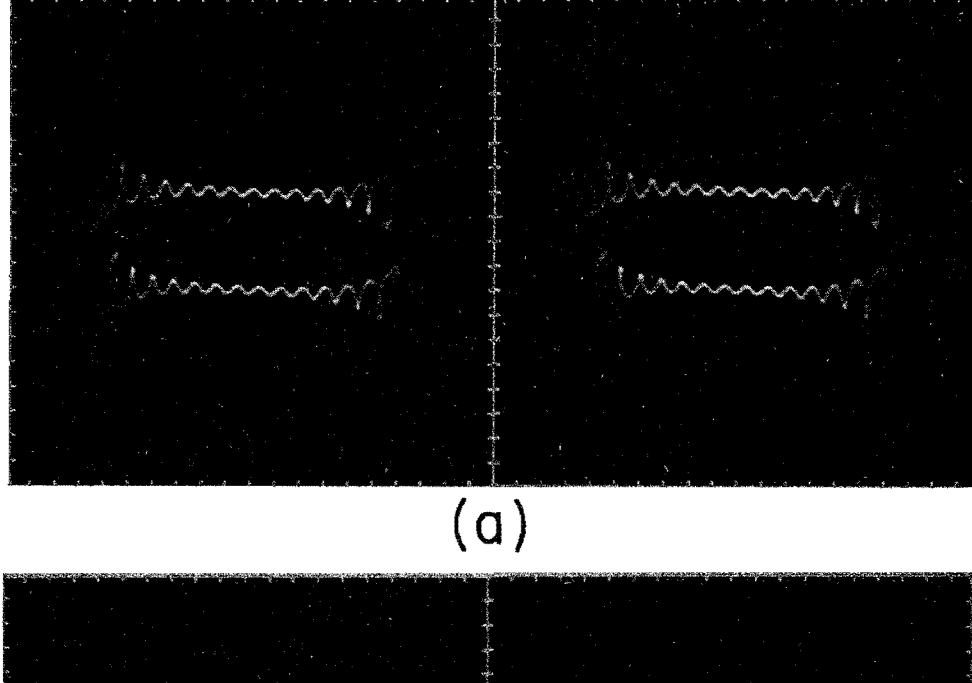
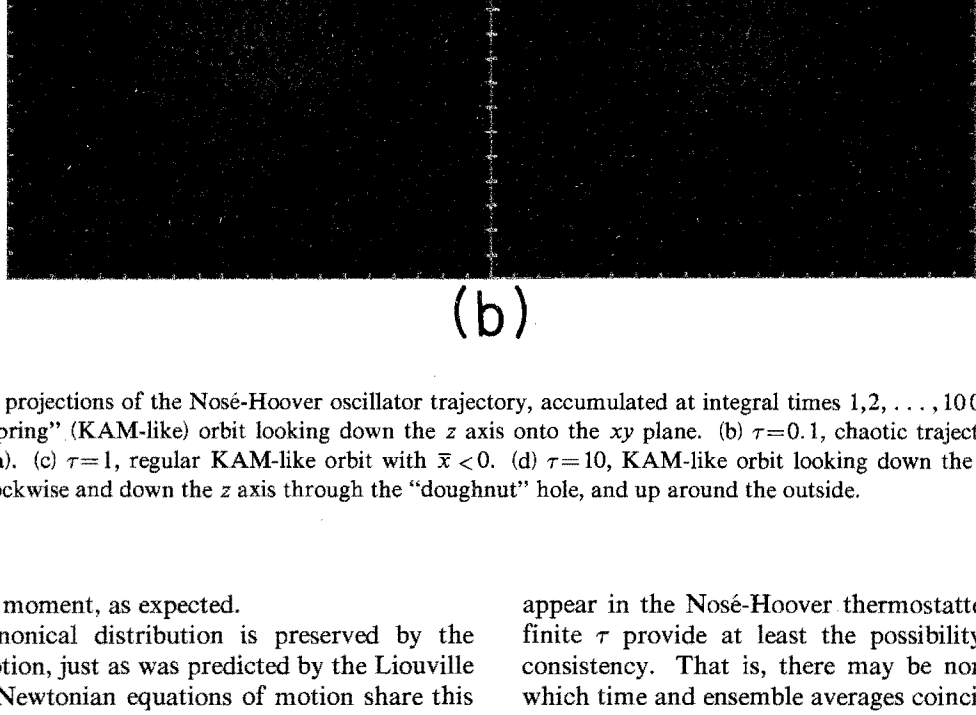


FIG. 1. Ensemble-averaged Nosé-Hoover oscillator coordinate moments $\langle x^n\rangle$ for a 1000-member ensemble. The equilibrium values are 0, 1, 0, and 3 for $n=1$, 2, 3, and 4. Note the increasing fluctuation size with n: $(1/N)^{1/2}$, $(2/N)^{1/2}$, $(15/N)^{1/2}$, and $(96/N)^{1/2}$. In our time units, the Newtonian period is 2π.



(a)



(b)

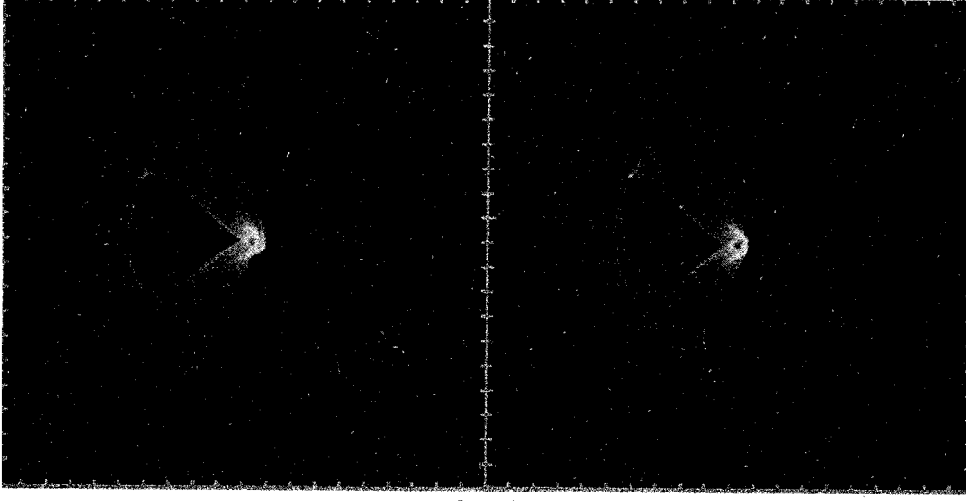
FIG. 2. Stereo projections of the Nosé-Hoover oscillator trajectory, accumulated at integral times 1,2, . . . ,10(coil "double-bedspring" (KAM-like) orbit looking down the z axis onto the xy plane. (b) $\tau=0.1$, chaotic traject viewpoint as in (a). (c) $\tau=1$, regular KAM-like orbit with $\bar{x}<0$. (d) $\tau=10$, KAM-like orbit looking down the plane. Flow is clockwise and down the z axis through the "doughnut" hole, and up around the outside.

the order of the moment, as expected.

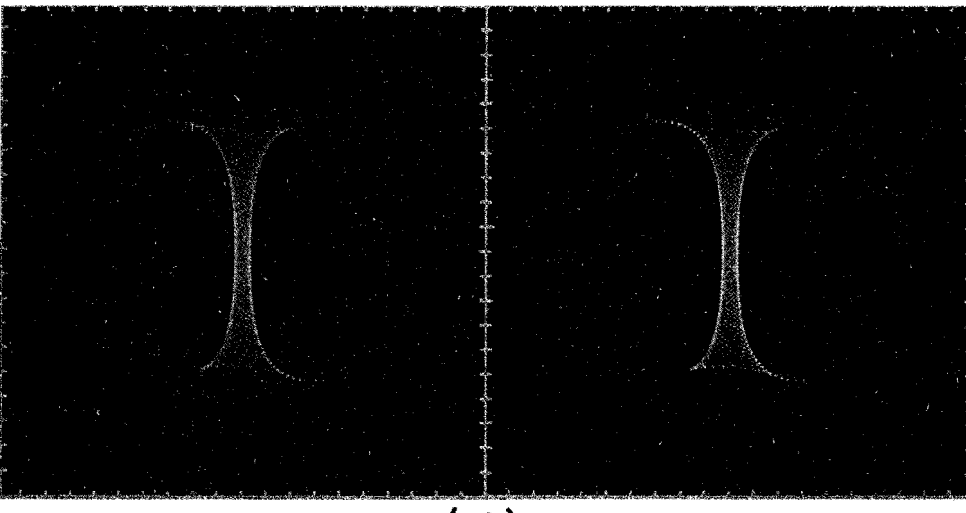
Thus the canonical distribution is preserved by the equations of motion, just as was predicted by the Liouville equation. The Newtonian equations of motion share this property. But in the Newtonian case the motion of the swarm of points resembles that of a rigid body circling the origin at a constant state-independent frequency, with all of the moments repeating at integral multiples of the oscillator period 2π. It is easy to show that in the Newtonian case the second moments fluctuate as $\sin(2t)$ with an average amplitude of order $1/N$.

The Newtonian dynamics, although it preserves the distribution, would likewise preserve *any* distribution which was a function of energy and in a completely nonergodic manner, never deviating from the original circular orbits in x,y space. On the other hand, the nonlinearities which appear in the Nosé-Hoover thermostatt finite τ provide at least the possibilit consistency. That is, there may be no which time and ensemble averages coinci

To address the questions of ergodicity sider a swarm (phase-space cloud) of en These might coalesce into inhomogeneo still preserving the canonical moments. suggested by the many incredible KAM type shown in Fig. 2(a), a 15-coil "doubl ular orbit. Figure 2(b) shows an irregu [A computer movie of this particular t strates that the nature of the chaos is re very long times, such as the accumulat 2(b). On a smaller time scale, such as th ing points, the chaotic trajectory is indist



(c)



(d)

FIG. 2. (*Continued*).

ple-bedspring" orbit, typified by Fig. 2(a). aracterized by gradual transitions in the between turning points.] But computer ption of a swarm of a thousand ensemble tendency for localization or segregation rding to their regular or chaotic nature.

ebraic way to distinguish between ordered s? One might expect that the time aver- nergy $\overline{H}_i$, would help. However, $\overline{H}_i$ has ution with a somewhat greater density e average value of $\frac{3}{2}$, so that this func- for characterizing the nature of a partic- ut the mean square displacement $\overline{x_i^2}$ or gy of the oscillator $(1+\overline{x_i^2})/2$ does pro- ngly useful discriminant (remember Provided that the thermostatting response ly small, less than about π, the ensemble sorted into discrete quantized levels, im- inuum background composed of chaotic trajectories, as shown in Fig. 3. It appe averages for the chaotic trajectories even an ergodic fashion to a common value than unity, in a time much greater than

The "quantum number" n associated corresponds to the number of coils arou between the turning points in x. T Poisson-like with a peak just below the as shown in Fig. 4(b). As τ is increase levels is reduced, and, for τ greater than be only KAM-like tori, as shown in Fig. we see [Fig. 2(c)] a dramatic demonstrat godicity of the oscillator: there are tor not zero. There tori exist in pairs, one and one with negative, both immerse chaotic sea.

In spite of these tremendous inh nonergodicities in the individual trajecto to see that Liouville's equation accurat equilibrium dynamics of this dynamica

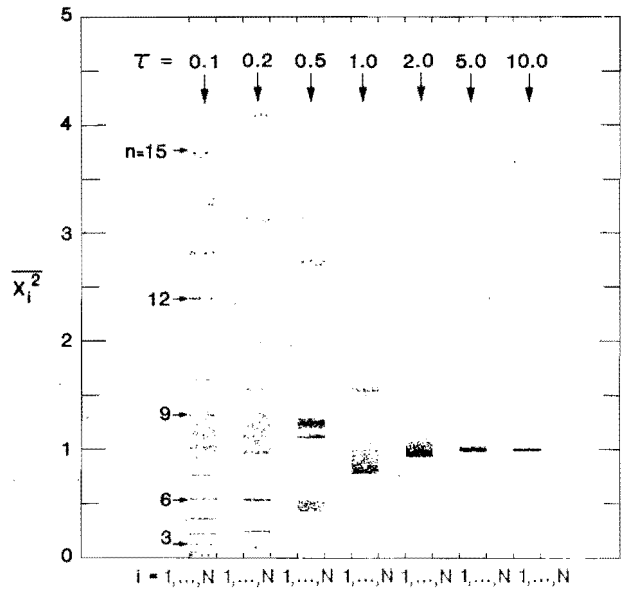


FIG. 3. Distribution of mean-squared displacements $\overline{x_i^2}$ time-averaged over a time of 10 000 for the classical thermostatted oscillator ensemble. The individual trajectory values are plotted as 1000 dots for each value of τ: 0.1, 0.2, 0.5, 1, 2, 5, and 10. Note that the "quantum" nature of the coalescence into ordered levels occurs as the coupling to the thermostat becomes stronger, as the relaxation time decreases. The quantized level numbers, corresponding to coils in the "double bedsprings" [see Fig. 2(a)], are indicated for $\tau=0.1$. For τ less than about π there is also a continuous spectrum, at least for early times, due to chaotic trajectories. In all cases the ensemble average $\langle x^2\rangle$, is 1, as shown in Fig. 1.

for ordinary observables like the energy. The moments retain their Gaussian values and the Gaussian appearance of the distribution remains unchanged.

IV. NONEQUILIBRIUM RESULTS

The most demanding test of the Liouville equation is its ability to describe far-from-equilibrium dynamics and the approach to equilibrium. We have accordingly studied experiments with initial temperatures $T_0 \gg 1$ and experiments with $T_0 \ll 1$, beginning with Gaussian distributions which are spherically symmetric in xyz space: $f(0)\sim f_0^{1/T_0}$. Qualitatively these two kinds of experiments correspond to rapid cooling (contraction of phase space, or the "Big Shrink") and heating (phase-space expansion, or "Big Bang"). To relate the time dependence to the predictions of Liouville's equations we consider the development of the information-theory entropy:[15,16]

$$S_{\text{info}} = -\int d\Gamma f \ln f = -\langle \ln f \rangle \ , \tag{13}$$

for which the Liouville equation predicts

$$\dot{S}_{\text{info}} = -\langle d \ln f/dt \rangle = \langle \Omega \rangle = -\langle z \rangle/\tau \ , \tag{14}$$

where integration by parts is used to convert derivatives of f into integrals weighted by f and where it has been assumed that f vanishes as the phase variables approach infinity.[5,9] The information-theory entropy production (14) has little to do with the true nonequilibrium entropy as

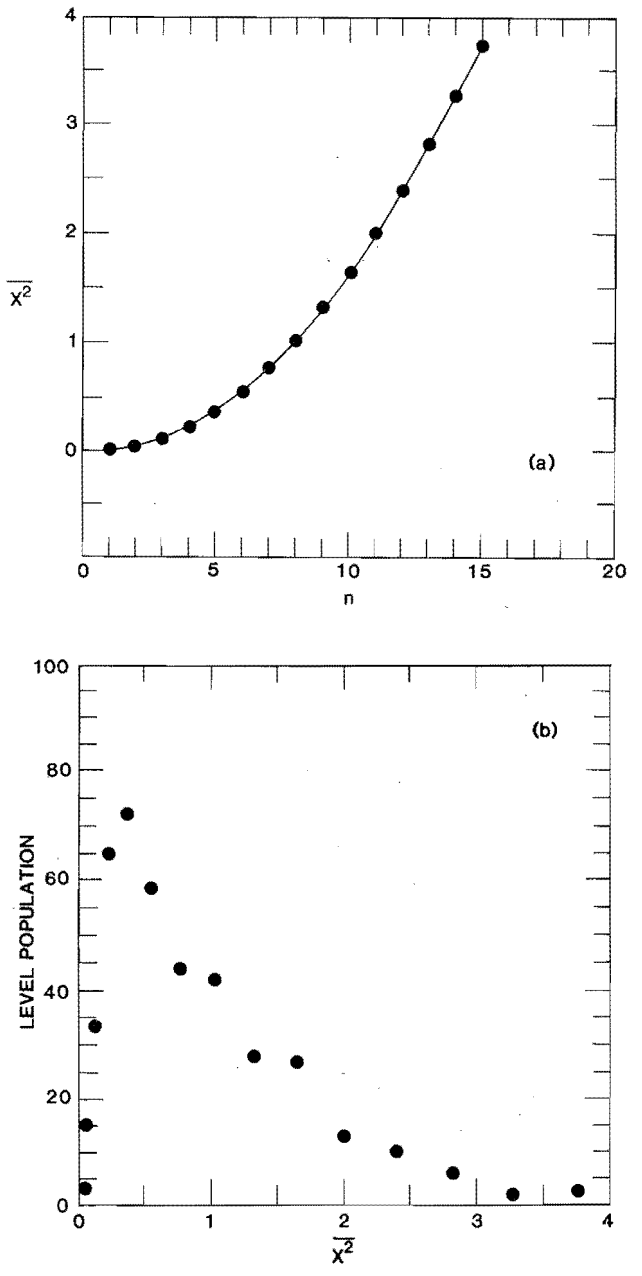


FIG. 4. "Quantization" of the $\overline{x_i^2}$ for the classical thermostatted oscillator with $\tau=0.1$. (a) $\overline{x^2}$ vs level number (coils in the bedspring between turning points). An analysis of the motion for $\tau \ll 1$ with $y=1+\delta\cos(\omega t)$, where δ is small, gives $\omega=2^{1/2}/\tau$, so that $\overline{x^2}$ approaches $(n\pi\tau)^2/6$ for large n. (b) Population of levels at equilibrium for $\tau=0.1$. There are 422 ordered trajectories out of 1000 chosen from the equilibrium Gaussian distribution.

has been noted previously.[4,5]

Zubarev suggested an alternative definition of entropy, based on the equilibrium distribution function[17]

$$S_{\text{Zub}} = -\langle \ln f_0 \rangle \ . \tag{15}$$

This definition produces exactly the same "entropy" for the Nosé-Hoover oscillator, as the more-usual

information-theory definition. From the equilibrium distribution Zubarev's entropy gives

$$\dot{S}_{\rm Zub} = \langle \dot{H} \rangle = \dot{E} = -\langle z \rangle / \tau \,, \tag{16}$$

which is consistent with a constant value of the free energy. In the general case $S_{\rm Zub}$ cannot be correct. In an isokinetic (constant kinetic energy) system of two hard spheres undergoing shear flow,[18] for instance, $S_{\rm Zub}$ has the same value far from equilibrium as in the equilibrium case.

The time dependence of the energy for the Nosé-Hoover oscillator can be developed in a Taylor series:

$$E = \tfrac{3}{2} T_0 - \tfrac{1}{2}(T_0 - 1)(t/\tau)^2 + \tfrac{1}{12} T_0 (T_0 - 1)(t/\tau)^4 + \cdots \,. \tag{17}$$

With $T_0 = 100$ and $\tau = 1$ the series $1 - 0.33t^2 + 5.5t^4$ describes the time development of the "Big Shrink" within 0.1% up to $t = 0.1$, as expected (see Table I). After that the decay toward equilibrium appears to be approximately exponential, with a decay time of roughly ten times τ, as shown in Fig. 5. Similar results were found for $\tau = 0.3$, 0.6, and 5. From (15) and (16) we see that $S_{\rm info}$ and $S_{\rm Zub}$ both decay from a large initial value toward a smaller equilibrium value, contrary to our expectations of the behavior of the entropy. The resolution of this apparent paradox is likely to be found in the assumption that a given Lagrangian phase-space trajectory can be followed indefinitely in time, without worrying about the difficulties associated with distortions of the volume element and phase-space mixing.

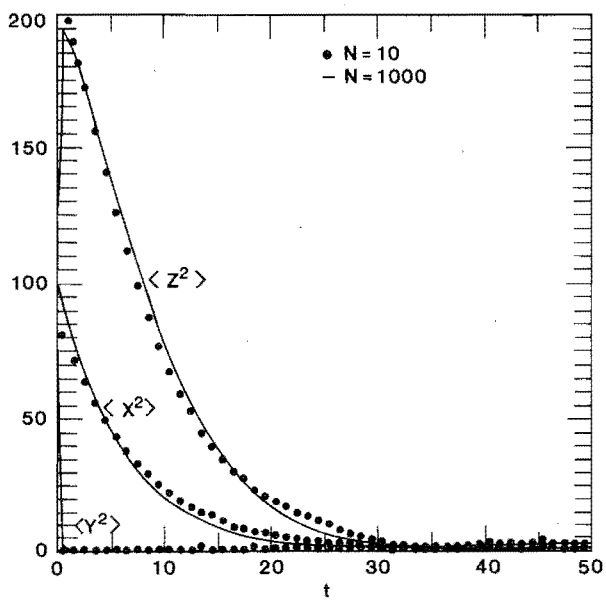


FIG. 5. Time dependence of the ensemble-averaged second moments for the "Big Shrink" initial condition, $T_0 = 100$ ($N = 1000$, $T = 1$, $\tau = 1$). The momentum y converges in a time of order 1, the thermostatting coefficient z expands and then both x and z decay toward equilibrium on a characteristic time scale of $\sim 10\tau$. The continuous curves for an ensemble of 1000 members can be distinguished from the discrete symbols which describe the case $N = 10$.

TABLE I. Early-time behavior of the energy of the Nosé-Hoover oscillator ensemble ($N = 1000$, $\tau = 1$, $T = 1$) for the "Big Shrink" experiment and with an initially spherically symmetric Gaussian distribution in the phase space, corresponding to $T_0 = 100$. The calculated value is the Taylor series (17) of the text.

t	E (calculated)	E (observed)
0.00	150.0000	150.0000
0.01	149.9951	149.9950
0.02	149.9803	149.9803
0.05	149.8814	149.8811
0.10	149.5875	149.5687

The dynamical approach to the equilibrium distribution is imperfect. Although x^2 and y^2 approach 1, z^2 converges to a larger value because y^4 greatly exceeds the equilibrium value of 3. This is because the initial distribution greatly emphasizes the chaotic trajectories relative to the regular ones. On the other hand, when τ is very large, z^2 is enhanced by the overabundance of large-radius tori.

Similar disparities result from "Big Bang" simulations. The final dynamical phase-space distribution is not homogeneous and isotropic. These nonequilibrium distributions are not failures of the Liouville equation but rather stem from the nonergodicity of the Nosé-Hoover oscillator. Apart from these discrepancies the approach to equilibrium is apparently irreversible, at least on the time-scale reasonably accessible to computer simulation.

The large-relaxation-time limit, with $\tau \gg 1$, leads to interesting behavior for the large-scale tori, such as is shown in Fig. 2(d). There are extremely short periods of large-amplitude oscillations in the oscillator variables x and y, followed by periods of quiescence with x and y executing very small spirals as z progresses at speed $1/\tau$ down its axis. This "flushing" process, from large z to negative z, takes a characteristic time $2x_0\tau$ where $x_0 \gg 1$ is the amplitude of the torus. It is easy to show that $\overline{x^2} = \overline{y^2} = \overline{3z^2} = 1$.

V. IRREVERSIBILITY

How is it that irreversibility comes from these reversible equations? This can be understood by considering the relative probability of volume elements in the phase-space $dx\,dy\,dz$. If we use the abbreviation r for the distance from the origin in this space, then the relative probability at equilibrium is proportional to $\exp(-r^2/2)$. Equivalently the recurrence time for such a state is of order $\exp(+r^2/2)$, exceeding the age of the universe if the simulation is carried out on the Cray, with 10^9 states per second, for $r > 11$.

We suggest calling the phase-space object traced out by a dynamical trajectory in a finite amount of computer time a second-law attractor. Such an attractor has four characteristics:

(1) The equations of motion are deterministic and reversible.

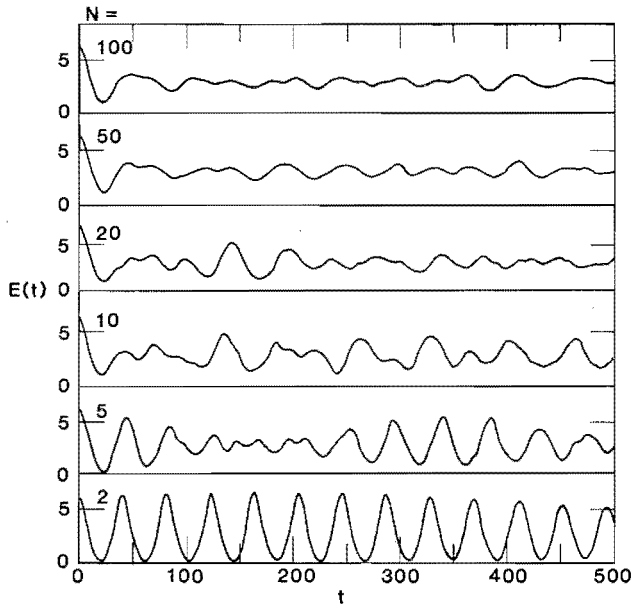


FIG. 6. Approximate Poincaré recurrence of the energy E for the Nosé-Hoover oscillator ensembles with $T=1$, $\tau=5$, and $T_0=4$. For N greater than ten members the energy appears to approach a steady value near 3 rather than the canonical value of $\frac{3}{2}$. With five members in the ensemble an approximate recurrence appears at time $t=350$. A two-member ensemble has an approximate recurrence time of 40.

(2) The phase space occupied by the attractor is infinite in extent.

(3) The probability distribution converges rapidly.

(4) $\langle \ln f \rangle$ is finite.

It differs from the usual strange attractors of dynamical systems[19,20] in the first two properties. This is a direct consequence of the logarithmic form of Nosé's thermostatting potential, which makes it possible for the other variables to range over an infinite portion of the phase space.

It seems possible that the irreversible behavior stems from the presence of chaotic trajectories. To test this idea we examined the case with $\tau=5$, too large for chaotic trajectories to appear. In Fig. 6 we display the number dependence of the time history of the energy for ensembles of 2, 5, 10, 20, 50, and 100 members. The recurrence phenomenon appears for the smaller ensembles of 2, 5, and 10 members, but takes too long to be seen for the large ones. This means that the cycle times are relatively incommensurate for the various tori, making it highly improbable for the elements of the ensemble to regroup as they were at the initial time. For smaller values of τ the cycle time is increased. This view of cycle time and Poincaré recurrence in its relation to ensemble size is analogous to the dependence predicted for one-dimensional harmonic chains as the number of masses increases. Because the elements of an ensemble are strictly noninteracting the analysis is simplified. The approach to equilibrium is only apparent, not mathematically rigorous. Nevertheless, it appears very probable that as N becomes infinite the recurrence time rapidly diverges too. For the Nosé-Hoover ensemble, the final state is not the equilibrium state. This is an artifact of the nonergodicity of the system.

VI. CONCLUSIONS

A numerical test of ensemble theory for the patently nonergodic Nosé-Hoover oscillator shows that the Liouville equation describes the equilibrium distribution, as characterized by its moments and its shape. The Liouville equation also describes the relaxation of mechanical observables from a nonequilibrium initial state, but gives paradoxical results for the entropy.[21] The nature of the irreversibility found in this finite and relatively stable oscillator ensemble stems from the incommensurability of cycle times. The latter greatly exceed the Newtonian value as the thermostat time becomes smaller than π.

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