Chaos, ergodic convergence, and fractal instability for a thermostated canonical harmonic oscillator

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The authors thermostat a qp harmonic oscillator using the two additional control variables ζ and ξ to simulate Gibbs' canonical distribution. In contrast to the motion of purely Hamiltonian systems, the thermostated oscillator motion is completely ergodic, covering the full four-dimensional $\{q,p,\zeta,\xi\}$ phase space. The local Lyapunov spectrum (instantaneous growth rates of a comoving corotating phase-space hypersphere) exhibits singularities like those found earlier for Hamiltonian chaos, reinforcing the notion that chaos requires kinetic—as opposed to statistical—study, both at and away from equilibrium. The exponent singularities appear to have a fractal character.

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I. INTRODUCTION

Nonequilibrium statistical mechanics is undergoing rapid change, driven by computer simulation, with *thermostated, time-reversible* simulation techniques and nonequilibrium boundary conditions suggesting novel theoretical analyses. The classic background [1], dating back to Poincaré and Lyapunov, is too closely tied to two-dimensional models and to Hamiltonian systems to provide an understanding of current nonequilibrium work. Nevertheless, notions from dynamical systems theory—in particular the study of the Lyapunov instability (exponential error growth $\propto e^{\lambda t}$) of the chaotic dynamics and the characterization of the fractal dimensionality of the resulting statistical distributions—have proved seminal in understanding the irreversibility of the second law of thermodynamics in terms of an underlying time-reversible, but non-Hamiltonian, dynamics [2].

There are two distinct approaches to solving thermomechanical problems involving irreversible processes: (i) trajectory analysis based on time averages and (ii) phase-space distribution function analysis. The dynamical trajectory methods have been employed ever since nonequilibrium methods were first developed, in the early 1970s. Dynamic methods are relatively simple to implement and to understand [2–4]. More recently, statistical methods have been applied to these same problems. The corresponding statistical tools (such as maps, Poincaré surfaces, periodic orbits, and equilibrium escape rates) entail more formal structure and have a mathematical, as opposed to physical, orientation [4–6].

We abandoned our initial plan to study the chaotic Hamiltonian Hookean pendulum problem [7] when dynamical tests, of the type described in the next section, revealed the existence of several Lyapunov-stable regions surrounding periodic orbits in addition to the unstable chaotic sea which comprises most of the phase-space probability density for the pendulum. The existence of the periodic orbits is strongly suggested by the Kolmogorov-Arnold-Moser theorem [1]. The complex structures of phase-space flows for conservative Hamiltonian systems, like the pendulum, have been explored in great depth for a century. Some non-Hamiltonian systems exhibit much simpler behavior which we believe to be typical of nonequilibrium systems. In the present work we study what we believe to be the simplest "ergodic"—meaning covering the entire phase space—dynamical system relevant to statistical mechanics, an harmonic oscillator. The oscillator is stabilized by *two* thermostat-control variables, a generalization of the simpler one-variable Nosé-Hoover control. An alternative method of thermostating an harmonic oscillator, with quartic feedback forces, has also been investigated recently [8,9].

The plan of the present paper is as follows: first, we introduce the doubly thermostated oscillator. Next, we study its *ergodicity* under the influence of simple quadratic feedback forces. We then characterize its chaotic character, through the mean values and fluctuations of the local Lyapunov exponents $\{\lambda\}$, and their associated offset vectors $\{\delta\}$. Finally, we list the conclusions to which we have come as a result of this work.

II. THERMOSTATED HARMONIC OSCILLATOR

Simulations of nonequilibrium systems require "thermostats" able to extract the heat generated by irreversible processes. Integral and differential feedback forces, usually of the form $\{\dot{p} \equiv -\zeta p\}$, have been developed to satisfy this

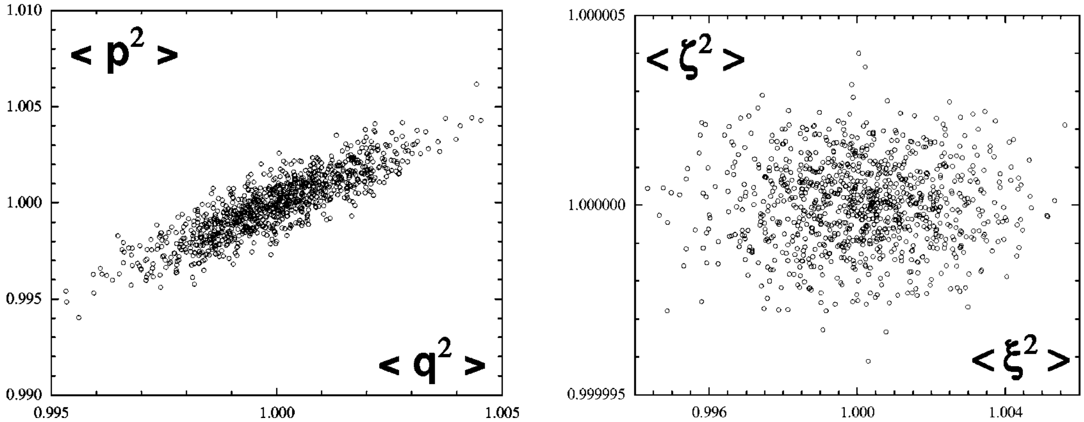

FIG. 1. Distribution of 1000 trajectory-averaged moments, $\langle q^2,p^2\rangle$ on the left-hand side, and $\langle \zeta^2,\xi^2\rangle$ on the right-hand side. Initial conditions were chosen randomly within the four-dimensional hypercube $-1<\{q,p,\zeta,\xi\}<+1$ with the trajectories followed for 10^8 time steps of length 0.01 each.

need [10]. In our work here, a conventional Hamiltonian qp oscillator interacts with a heat reservoir—represented by the two control variables, or ''thermostat variables,'' $\{\zeta,\xi\}$:

$$\dot{q}=p;\;\; \dot{p}=-q-\zeta p;\;\; \dot{\zeta}=p^2-1-\xi\zeta;\;\; \dot{\xi}=\zeta^2-1.$$

Notice that the friction coefficient ζ is itself controlled by a second thermostat variable, ξ. More-complex many-body versions of this thermostating scheme were first introduced by Martyna, Klein, and Tuckerman [11].

The time evolution of the trajectory motion can also be expressed as an equivalent phase-space-probability flow, in terms of the probability density $f(q,p,\zeta,\xi)$:

$$\dot{f}\equiv(\partial f/\partial t)+v\cdot\nabla_r f=-f(\nabla_r\cdot v)=f(\zeta+\xi),$$

$$r\equiv\{q,p,\zeta,\xi\};\;\; v\equiv\{\dot{q},\dot{p},\dot{\zeta},\dot{\xi}\}.$$

In the steady (equilibrium) state, where $(\partial f/\partial t)$ vanishes, the thermostated oscillator motion equations give the solution corresponding to Gibbs' canonical ensemble for an oscillator at unit temperature:

$$f_{\mathrm{equilibrium}}\propto e^{-(q^2+p^2+\zeta^2+\xi^2)/2}.$$

The form of this stationary distribution suggests an effective ''Hamiltonian'' $\mathcal{H}_e$:

$$\mathcal{H}_e\equiv(q^2+p^2+\zeta^2+\xi^2)/2.$$

The strong mixing properties induced by the quadratic forces in the equations of motion cause changes in the numerical value of $\mathcal{H}_e$ as time goes on, $\dot{\mathcal{H}}_e\equiv-\zeta-\xi$, so that all the ''energy shells'' of constant $\mathcal{H}_e$, with $0<\mathcal{H}_e<\infty$, are included in the resulting distribution.

It is remarkable that the entire canonical distribution eventually results from *any* smooth initial choice for *f*. In previous work this fact was inferred from a study of long-time Lyapunov exponents (average rate of divergence of two nearby phase-space trajectories). Here we have confirmed this finding by studying the convergence of the averages $\langle\{q^2,p^2,\zeta^2,\xi^2\}\rangle$ with time, using an ensemble of 1000 randomly chosen initial conditions. The entire ensemble of averages converges to the expected canonical average, unity for each of the quadratic forms, with deviations of order $t^{-1/2}$ for $\langle\{q^2,p^2,\xi^2\}\rangle$ and t^{-1} for $\langle\zeta^2\rangle$. Direct integration of the $\dot{q}$ and $\dot{\xi}$ equations, giving

$$\Delta q\equiv t\langle p\rangle,\quad \Delta\xi\equiv t[\langle\zeta^2\rangle-1],$$

establishes that the two averages, $\langle p\rangle$ and $\langle\zeta^2\rangle$, converge rapidly, with *linear* corrections in $1/t$ rather than the much larger ''statistical'' central-limit-theorem corrections of order $t^{-1/2}$. To see this rapid convergence it is only necessary that the sampling time t be long relative to the oscillator period of $\simeq 2\pi$. Figure 1 shows the ensemble averages at $t=10^6$, using 10^8 fourth-order Runge-Kutta time steps of 0.01 each. Any regions associated with periodic orbits, or partitions of the occupied phase space into disjoint parts, would be revealed by persistent clustering, away from the full canonical averages, in such ensemble plots.

III. LOCAL LYAPUNOV EXPONENTS

With the ergodicity of the oscillator motion confirmed, we next studied the dependence of the *local* Lyapunov exponents, and their associated directions, on phase-space location. These ''local,'' or ''instantaneous,'' exponents describe the linear deformation of a comoving corotating phase-space hypersphere *at* the location $\{q,p,\zeta,\xi\}$ where the exponents are evaluated [2,3]. In general, they depend upon the past history of the system, as opposed to the future. Hamiltonian systems behave in a much simpler way, as a consequence of their symplectic nature (with symmetric contributions from the past and future). The Hamiltonian exponents obey an instantaneous pairing rule, with each positive exponent $+\lambda$ ''paired'' with its opposite negative exponent, $-\lambda$ [1]. The thermostated oscillator displays a much richer variety of behavior, typical of nonequilibrium systems. The four local Lyapunov exponents $\{\lambda\}=\{\lambda_1,\lambda_2,\lambda_3,\lambda_4\}$, where the subscripts indicate the order (largest to smallest) based on long-time averages,

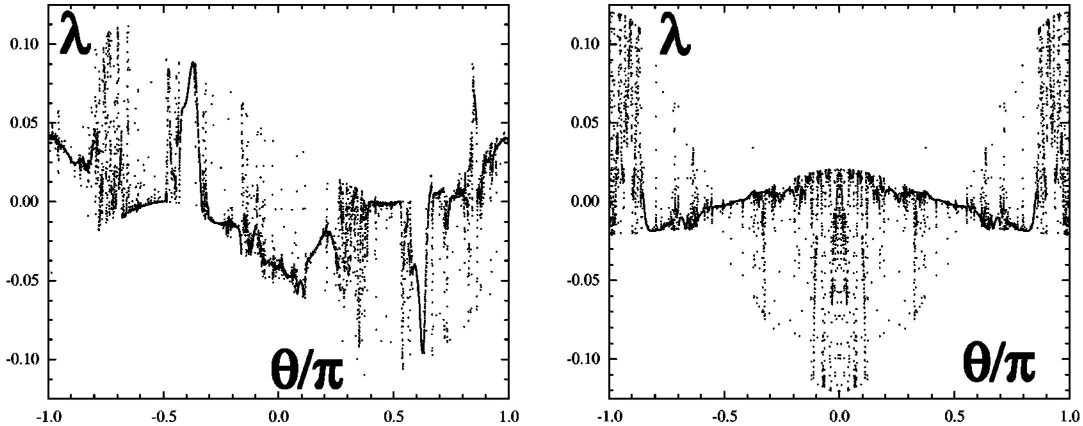

FIG. 2. Variation of the local (instantaneous) Lyapunov exponents $\lambda_1(\theta)$ along two circles in phase space. At the left both q and ζ are $0.1 \cos\theta$ while p and ξ are $0.1 \sin\theta$. At the right q and $-p$ are $-0.1 \sin\theta$ while ζ and $-\xi$ are $-0.1\cos\theta$. In both cases the phase-space location parameter θ varies from $-\pi$ to $+\pi$. Each of the 10^4 points represents a reversed trajectory of 10^6 time steps with $dt=0.001$.

$$\langle\lambda_1\rangle > \langle\lambda_2\rangle \geqslant \langle\lambda_3\rangle > \langle\lambda_4\rangle,$$

have instantaneous fluctuations an order of magnitude larger than the long-time-averaged exponent $\langle\lambda_1\rangle$. The *time-averaged* exponents *do* satisfy a pairing relation:

$$\langle +\lambda_1\rangle = 0.066 = \langle -\lambda_4\rangle, \quad \langle +\lambda_2\rangle = 0.000 = \langle -\lambda_3\rangle.$$

The *instantaneous* exponents only satisfy the identity

$$\lambda_1+\lambda_2+\lambda_3+\lambda_4 \equiv -\zeta-\xi,$$

which follows from the equations of motion. There is no simple identity linking the separate pairs (λ_1,λ_4) and (λ_2,λ_3). Because the fluctuations in these local instantaneous exponents are so large, accurate calculations of them require a somewhat shorter Runge-Kutta time step (0.001) than do the averages discussed in the last section.

We found that not only did the four local exponents exhibit all possible ($2^4=16$) sign combinations—of which a paired Hamiltonian system could have only four—the four exponents also could appear, locally, with all possible ($4! = 24$) orderings, while a Hamiltonian system could have only eight of these. The observed orderings of the thermostated oscillator's exponents include even the most extreme fluctuation, with the instantaneous exponents reversed:

$$\lambda_1<\lambda_2<\lambda_3<\lambda_4.$$

Likewise, locally, the exponents can *all* be positive or *all* be negative, for a short while. These features suggest that the dynamical view of fixed stable and unstable manifolds suggested by the study of two-dimensional hyperbolic maps [1,5,6], cannot be applied to the present relatively simple four-dimensional situation.

Figure 2 indicates that the spatial dependence of the Lyapunov exponents is wildly *singular*, just as was the case for the Hamiltonian systems studied earlier [7]. The figure was generated by (i) integrating *backward* in time from a set of 10 000 equally spaced initial conditions, saving the resulting four-dimensional ''reference'' trajectories; (ii) integrating each of the corresponding sets of four ''satellite'' trajectories *forward* in time, with the four vectors

$$\{\delta \equiv (q,p,\zeta,\xi)_{\text{satellite}} - (q,p,\zeta,\xi)_{\text{reference}}\}$$

constrained to remain orthogonal, with a fixed length of 0.000 01 or 0.000 001. The constraints were imposed by rescaling, as originally suggested by Benettin [12] following related work carried out by Stoddard and Ford [13]. The rate of rescaling of the vector lengths $\{\delta\}$, on reaching the initial conditions once more, gives the local Lyapunov spectrum. The directions of the vectors are those of a comoving corotating hyperellipsoid's principal axes, with the four-dimensional hyperellipsoid centered on the reference trajectory. The results of the local-exponent analysis, for two small phase-space circles centered on the origin, are shown in Figs. 2 and 3. The angle $-\pi<\theta<+\pi$ there parametrizes the circumference of the phase-space circles. Figure 2 suggests that the variation of the largest Lyapunov exponent is singular in the phase space. In the next section we investigate this singular variation in detail. The behavior of the other exponents

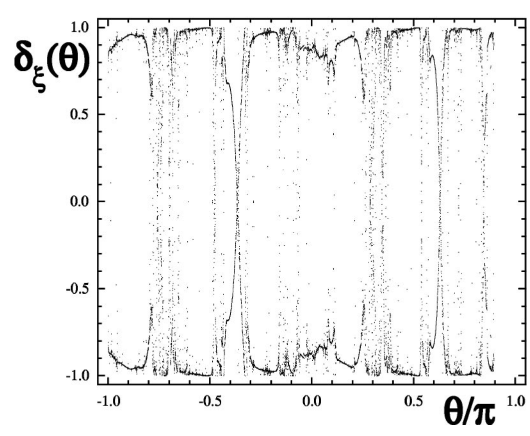

FIG. 3. Variation, in the ξ direction, of the projections of the eigenvector corresponding to the local Lyapunov exponents $\{\lambda_1(\theta)\}$ with $q=p=0.1\cos\theta$; $\zeta=\xi=0.1\sin\theta$. The parameter θ varies from $-\pi$ to $+\pi$. Because the *sign* of the projections is arbitrary, both the positive and negative choices are shown here.

is similar. Figure 3 shows that the projections of the principal-axis vectors are likewise singular. We used fourth-order Runge-Kutta integration throughout, choosing the timestep small enough that errors from the numerical integrator were dominated by those from the finite (double-precision) computer word length. Although generalized symplectic methods might appear to offer advantages for such studies we were unable to develop an approach subject to the instantaneous constraint which follows from Liouville's theorem,

$$\dot{f} \equiv -f(\nabla_r \cdot v) \equiv f(\zeta + \xi).$$

IV. SPATIAL FLUCTUATIONS OF THE LYAPUNOV EXPONENTS

The look of the wildly fluctuating local Lyapunov exponents is reminiscent of ''fractal'' curves (curves of ''unbounded variation''). To check the validity of this idea we have studied the dependence of the summed-up vertical jumps of the curve,

$$\Delta(\lambda) \equiv \langle |\lambda_{\theta+(\delta\theta/2)} - \lambda_{\theta-(\delta\theta/2)}| \rangle,$$

as a function of the coarsening interval $\delta\theta$ separating adjacent phase-space sampling points. It is necessary to use double-precision (14-digit) arithmetic, because two separate differencing operations are required: (i) analyzing the offset, of order 10^{-5} or 10^{-6}, between the reference and satellite trajectories and (ii) analyzing the dependence of these small differences on similarly small changes in the initial conditions. We were able to study samples of 80 000 initial conditions, all of equal Gibbs' measure, lying on a circle in the four-dimensional phase space. The results show that over a 1024-fold change in interval length,

$$(2\pi)/80\,000 \leqslant \delta\theta \leqslant (2^{11}\pi)/80\,000,$$

the jumps $\{\Delta\}$ in the local values of λ_1 vary roughly as a fractional power of the interval length $\delta\theta$. The data shown in Fig. 4 indicate a ''fractal dimension'' near 1.7, suggesting an underlying simplicity in the chaotic structure. It is interesting to find traces of fractal character, usually associated with dissipative systems, at equilibrium. This is reminiscent of the equilibrium fractals found in the ''escape-rate'' theory of transport developed by Dorfman, Gaspard, and Nicolis [6].

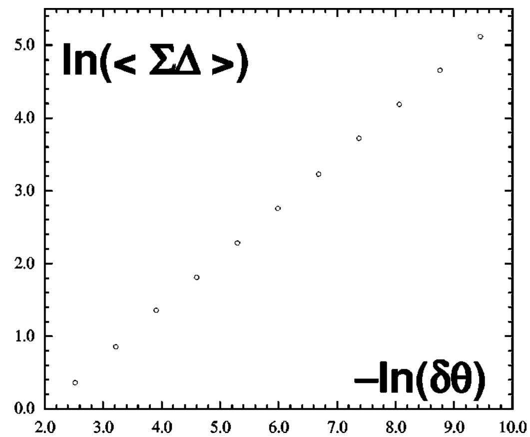

FIG. 4. Interval dependence of the summed-up vertical jumps (analogous to the ''length'' of the fractal line) as a function of the interval between successive points $\delta\theta$, using up to 80 000 points on the phase-space circle with q and ζ equal to $0.1\cos\theta$ while p and ξ are $0.1\sin\theta$. The slope of this double logarithmic plot, 0.69, indicates that the ''line'' corresponding to the data shown at the left in Fig. 2 has an effective ''fractal dimension'' of 1.69, rather than 1.0.

V. CONCLUSIONS

The thermostated oscillator, despite the simple analytic, though nonlinear, nature of its quadratic forces, exhibits dynamical variety far beyond the capability of analytical methods, with rapidly changing directions for the $\{\delta\}$ and rapidly changing magnitudes of the local growth rates $\{\lambda\}$. The numerical data considered here suggest that the spatial dependence of the local Lyapunov exponents is fractal, with a characteristic exponent near 1.7 in the case detailed in Fig. 4:

$$\Delta(\lambda) \propto |\delta\theta|^{1.7}.$$

Nevertheless, the dynamics faithfully generates the simple smooth Gibbs' distribution characteristic of the canonical ensemble. This oscillator model, and its properties, suggest that the smooth *time* development of trajectories, rather than the irregular *spatial* structure of distributions, is the more fruitful route toward theoretical understanding of chaotic systems.

Whether or not a generalization of the symplectic integrators, satisfying the local constraint, $\dot{f} \equiv f(\zeta+\xi)$, can be found for this simplest of ergodic chaotic models, remains an interesting open problem. The present work suggests a variety of investigations designed to classify possible forms of the phase-space dependence of local Lyapunov spectra. The extension of these results to nonequilibrium systems is complicated by the lack of a useful Gibbs' measure away from equilibrium. For nonequilibrium systems it is tantalizing [14] to try to express phase-space measures in terms of local Lyapunov spectra. Corresponding approaches can be readily tested with the present model. In the equilibrium case, with $kT \equiv 1$, there is an exact relationship [2,3]:

$$d \ln f/dt \equiv \sum -\lambda \equiv \zeta + \xi \rightarrow f(t)/f(0) \equiv e^{+t\langle \zeta+\xi \rangle}$$
$$\equiv e^{\mathcal{H}_e(0) - \mathcal{H}_e(t)},$$

where $\langle \zeta + \xi \rangle$ gives the dissipation *time-averaged* over the time interval from 0 to t. The *nonequilibrium* case could be explored by making the imposed mean kinetic temperature $\langle T \rangle \equiv \langle p^2/mk \rangle$ an explicit function of the coordinate q [2,9]. Off hand, it appears that the fractal character of the spectrum's spatial dependence will present insuperable difficulties for these formal phase-space-measure approaches.

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[1] M. Tabor, *Chaos and Integrability in Nonlinear Dynamics* (Wiley, New York, 1989).

[2] Wm.G. Hoover, *Time Reversibility, Computer Simulation, and Chaos* (World Scientific, Singapore, 1999).

[3] Wm.G. Hoover, *Computational Statistical Mechanics* (Elsevier, New York, 1991).

[4] D.J. Evans and G.P. Morriss, *Statistical Mechanics of Nonequilibrium Liquids* (Academic, New York, 1990).

[5] J.R. Dorfman, *An Introduction to Chaos in Nonequilibrium Statistical Mechanics* (Cambridge University Press, Cambridge, 1999).

[6] P. Gaspard, *Chaos, Scattering, and Statistical Mechanics* (Cambridge University Press, Cambridge, 1998).

[7] Ch. Dellago and Wm. G. Hoover, Phys. Lett. A **268**, 330 (2000).

[8] Wm.G. Hoover and B.L. Holian, Phys. Lett. A **211**, 251 (1996).

[9] H.A. Posch and Wm. G. Hoover, Phys. Rev. E **55**, 6803 (1997).

[10] D. Kusnezov, A. Bulgac, and W. Bauer, Ann. Phys. (N.Y.) **204**, 155 (1990).

[11] G.J. Martyna, M.L. Klein, and M.E. Tuckerman, J. Chem. Phys. **97**, 2635 (1992).

[12] G. Benettin, L. Galgani, and J.M. Strelcyn, Phys. Rev. A **14**, 2338 (1976).

[13] S.D. Stoddard and J. Ford, Phys. Rev. A **8**, 1504 (1973).

[14] D.J. Evans, E.G.D. Cohen, and G.P. Morriss, Phys. Rev. Lett. **71**, 2401 (1993).