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The statistical thermodynamics of steady states

Wm.G. Hoover [1]

Department of Applied Science, University of California at Davis / Livermore, Livermore, CA 94551-7808, USA

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Abstract

The suggestion that steady-state phase-space distributions might be smooth, rather than fractal, is investigated from the standpoint of stochastically-thermostatted systems. Let a pervasive, cool, rapidly-thermostatted ideal gas serve as a heat reservoir for macroscopic degrees of freedom. Flows of mass, momentum, and energy, thermostatted in this way, exhibit clear fractal distributions, just as do their counterparts with deterministic thermostats. © 1999 Published by Elsevier Science B.V. All rights reserved.

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1. Phase-space distributions: smooth, or fractal?

Tzeng and Chen [1] supported the notion that steady-state phase-space distributions are smooth, rather than fractal, despite a preponderance of evidence for fractals from simulations with deterministic thermostats [2]; despite compelling topological arguments relating the Second Law of Thermodynamics to fractals [3]; and despite rigorous efforts to furnish a mathematical basis for the results *inferred from simulations* [4]. The topological nature of the distributions, smooth versus fractal, had been discussed earlier [5], but the appearance of Ref. [1] shows that the question is unresolved [6–9].

There are two main obstacles to attaining a resolution. First, a steady state requires a thermostat, or heat reservoir, of some kind. Should such a thermostat be deterministic or stochastic? Perhaps this choice is crucial [10,11]? Second, numerical difficulties preclude the direct examination of phase-space probability densities $f(q,p)$, except for systems with only three or four phase-space variables. The evidence for or against fractals for larger systems is necessarily indirect. The Lyapunov spectrum $\{\lambda:\lambda_1 \geq \lambda_2 \geq \lambda_3 \ldots\}$ provides a powerful tool for quantifying fractal character. The maximum number of exponents whose interpolated sum, $\{\lambda_1+\lambda_2+\lambda_3+\ldots\}$ is positive, the generally-nonintegral ‘‘Kaplan–Yorke dimension’’, gives a reliable estimate for the fractal’s ‘‘information dimension’’ [12,13].

I consider here an idealized stochastic heat reservoir, simple enough to facilitate analyses, and com-

[1] E-mail: hoover@bonampak.llnl.gov

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plex enough to be able to generate nonequilibrium ''gedanken experiments'' or computer simulations – steady flows of mass, momentum, and energy responding to reservoir properties. In what follows, I show that this stochastic approach is fully consistent with the results found earlier with deterministic thermostats: steady-state phase-space distributions are typically fractals.

2. Stochastic reservoir model

Because nonequilibrium steady states generate heat, it is evident that any steady-state simulation must include a thermostatting mechanism for removing the heat as it is produced. In simulations, as in the laboratory, the means of thermostatting is not unique. But a variety of theoretical approaches [2,14] all lead to motion equations including deterministic time-reversible ''friction coefficients'' ζ:

$$\{\dot{q}=p/m;\ \dot{p}=F(q,p,t)-\zeta(q,p)p\}.$$

The force F is the usual summed-up Newtonian or Hamiltonian force applied to the degree of freedom q, and is possibly time-dependent. The force F includes not only interparticle interactions but also any contributions from external fields, while the friction coefficient ζ imposes an additional thermal or energetic constraint equivalent to the effect of a deterministic heat bath [2,14]. The time reversibility results in an attractor-repellor pair structure in the phase space with an overall flow which is often ergodic. There are also ''stochastic'' thermostats. The usual stochastic approach is to choose new velocities, from a Maxwell–Boltzmann distribution, whenever particles reach a stochastically-thermostatted boundary. Such a stochastic approach is not at all deterministic. Unlike their deterministic relatives, stochastic thermostats fail to impose the ''bath'' temperature on the ''system'', except at equilibrium. The usual stochastic implementations also complicate analysis [4,5,11], because the very useful time-reversibility property is lost.

Consider a stochastic approach to many-body dynamics based on the Langevin equation [15]:

$$\{\dot{q}=p/m;\ \dot{p}=F-(p/\tau)+\text{``noise''}\}.$$

At equilibrium the random accelerations representing ''noise'' can have an amplitude ensuring that the system and the heat bath share a common temperature, $T=T_{\text{bath}}=T_{\text{system}}$, with $\langle p^2/m\rangle = kT$. But far from equilibrium it is desirable to picture this motion equation as resulting from interactions with a pervasive, unchanging stochastically-thermostatted equilibrium heat bath made up of many noninteracting infinitesimal particles, with their own Maxwell–Boltzmann velocity distribution, characteristic of the bath temperature, not the system temperature, and with a perpetually uniform spatial distribution. Provided that the bath temperature is sufficiently low, relative to that of the accelerating macroscopic degrees of freedom which interact with the bath, the macroscopic equations of motion for the system particles become simpler:

$$T_{\text{bath}} \ll T_{\text{system}} \to \{\dot{q}=p/m;\ \dot{p}=F(q,p,t)-p/\tau\}.$$

Although these motion equations no longer contain the bath temperature T_{bath}, there is an implicit relationship linking the collision rate of the bath particles to the relaxation time τ. I will call these simple equations of motion the ''stochastic thermostat model''. The model is intrinsically irreversible. Brad Holian, commenting on a preliminary draft of this manuscript, pointed out that the failure of this stochastic bath to impose its own temperature on the system is shared by several other thermostat models [16–18].

The simplest computational model for a nonequilibrium steady state based on this stochastic thermostat model is ''color conductivity'', in which $N/2$ black particles are accelerated to the right, while $N/2$ white ones are accelerated to the left, by a constant field [13,19]. The drag forces $\{-p/\tau\}$ can stabilize a nonequilibrium current for which the fixed acceleration from the field just offsets the deceleration from the drag. The situation is inherently a stable one because an increasing current leads to increased drag. Evidently the Lyapunov spectrum for this simplest of nonequilibrium steady-state situations should obey the ''conjugate pairing rule'' [20]. That is, because the momentum contribution to each (q,p) pair is the negative constant $-1/\tau$, the spectrum of Lyapunov exponents $\{\lambda\}$, is shifted toward more negative values, with the shift per pair also equal to $-1/\tau$. This particular case has been investigated exhaustively for the Galton Board $(N=2)$ [21–23] and there is no difficulty in applying it to larger numbers of particles. We should expect a multifractal phase-space distribution for any such problem.

To verify this idea I carried out an analysis of the Lyapunov spectrum and color conductivity for 36 soft disks [13] – with a pair potential $\phi(r<1) = 100(1-r^2)^4$ – using arbitrary values of the accelerating field E and drag coefficient, $1/\tau$. In this case a simple time average makes it possible to estimate the actual system temperature:

$$\langle \sum (p/m) \times (\dot{p} - F) \rangle$$
$$= \langle \sum (p/m) \times (-p/\tau) \rangle$$
$$\equiv -2NkT_{\text{system}}/\tau .$$

Only the force from the field makes a nonvanishing contribution to the leftmost expression. We can express the color conductivity κ in terms of the current and field:

$$\kappa \equiv \langle \pm v_E \rangle / \pm E .$$

Here v_E is the mean drift velocity induced by the field (plus signs for black particles and minus signs for white). This yields the prediction,

$$kT_{\text{system}} = \kappa E^2 \tau/2 ,$$

quite different from the stochastic ‘‘bath temperature’’,

$$kT_{\text{bath}} \equiv 0 .$$

The system temperature prediction is nicely consistent with the computer simulations reported here.

Two typical spectra are shown in Fig. 1. In both cases, the summed Lyapunov spectra have the correct value,

$$-\sum \lambda = 2N/\tau = \langle \dot{S}_{\text{external}}/k = 2N\zeta \rangle ,$$

where $\dot{S}$ is the entropy production rate and k is Boltzmann’s constant. Partial sums of the spectra indicate Kaplan–Yorke phase-space dimensionality

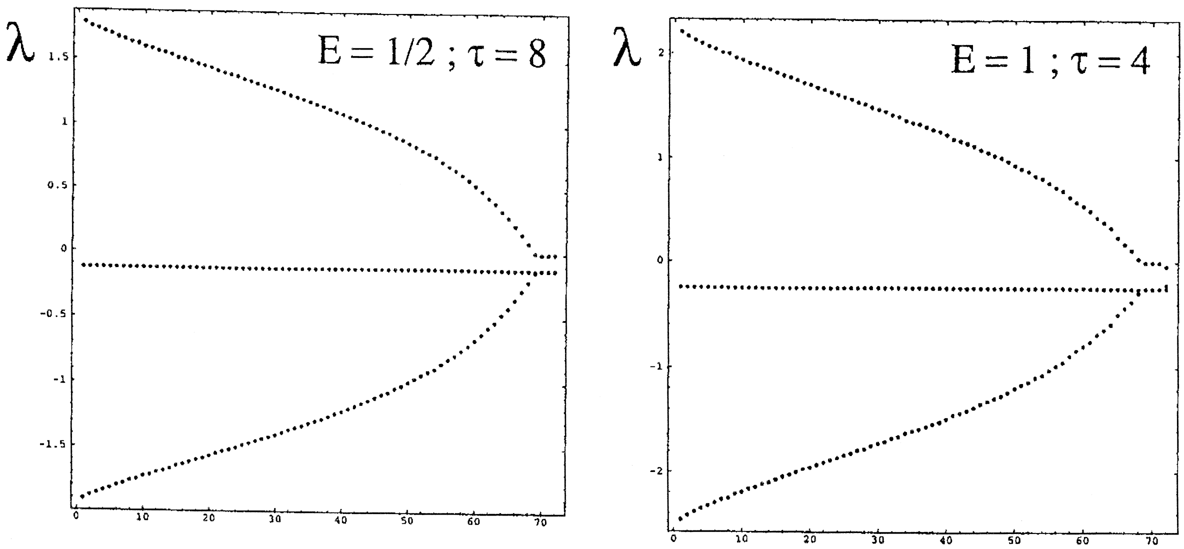

Fig. 1. Lyapunov Spectra for 36 soft disks of unit mass at unit density, accelerated by an external field E and thermostatted by a low-temperature stochastic heat bath with a relaxation time τ. The spectra correspond to $\{E,\tau,\langle\Phi/N\rangle,\langle K/N\rangle,\kappa\} = \{1/2,8,0.07,0.18,0.18\},\{1,4,0.15,0.35,0.18\}$, where Φ and K are the potential and kinetic energies of the system particles and κ is the color conductivity. The respective phase-space dimensionality losses are 4.8 and 7.7. These losses indicate the multifractal nature of the nonequilibrium steady-state distributions. The sums of the individual pairs of Lyapunov exponents are also plotted. The three vanishing exponents (at the extreme right of the spectra) correspond to the fixed center-of-mass coordinates and to the direction of phase-space trajectory motion, as described in Ref. [13].

losses of 4.8 for $[E=1/2;\tau=8]$ and 7.7 for $[E=1;\tau=4]$. The spectra differ only slightly in appearance from those found in isoenergetic color conductivity and viscosity simulations [13]. The similarity indicates that fluctuations in the deterministic friction coefficients [13] are relatively small, disappearing in the large-system limit. The three vanishing Lyapunov exponents, which can likewise be ignored in that limit, correspond to the fixed center-of-mass coordinates and to the direction of the many-body trajectory motion in phase space. The two exponents associated with the momentum of the center of mass are both equal to $-1/\tau$.

Could momentum and energy flows be treated in this way? Simulations based on the ''fluid walls'' introduced and studied by Ashurst [24] suggest that momentum reservoirs could be constructed by using the same stochastic-thermostat equations of motion as before, adjusting the drag force to damp relative velocities, $v-v_{\mathrm{wall}}$, obtaining the desired wall velocities, and adjusting the accelerating fields within the walls to provide the desired temperature. Particles within either of the momentum reservoirs would be separated from bulk fluid by an elastic wall, but interactions across the walls would provide sufficient coupling for accurate dense-fluid viscosity simulations. Just as with deterministic thermostats, the simple analytic nature of the motion equations establishes a connection between the friction coefficients and the overall macroscopic dissipation: the rate of shrinkage of the comoving phase volume $\dot{\otimes}$ is related to the rate of divergence of the phase-space distribution function f with time, $\dot{f}=df/dt$. The time-averaged values of $\dot{\otimes}$ and $\dot{f}$ can be described in terms of the drag coefficients or the Lyapunov exponents [2–4,13]:

$$\langle \dot{f}/f \equiv -\dot{\otimes}/\otimes \rangle = \sum \zeta = \sum 1/\tau = -\sum \lambda .$$

Because the friction coefficient ζ is constant, the fine-grained Gibbs' f diverges (exactly) $\propto e^{2Nt/\tau}$ while the comoving phase volume $\otimes$ approaches zero, $\propto e^{-2Nt/\tau}$. The friction-coefficient sum includes all $2N$ thermostatted degrees of freedom and the Lyapunov-exponent sum – with at least three zeros – includes all $4N$ Lyapunov exponents.

Energy flows could be treated in a similar way by considering heat reservoirs containing several opposed currents (there are just two in the color conductivity problem), artificially partitioning the thermostatted particles into groups with individual field directions. Evidently the overall loss of phase-space dimension in either momentum flows or heat flows, bounded by stochastically-thermostatted fluid-wall regions, depends on the size of the drag relative to the Lyapunov exponents. The heat-flow case involves additional complexity due to the extra dissipation caused by velocity disparities *within* the heat reservoirs.

3. Conclusion

By generalizing the Langevin picture to include two very different temperatures, with the system temperature T_{system} much greater than the thermal bath temperature T_{bath}, thought experiments and computer simulations demonstrating the fractal character of nonequilibrium steady states can be constructed. Although the irreversible stochastic heat bath seems qualitatively different to the deterministic Gauss or Nosé–Hoover thermostats [2,14], it is evident that all these approaches must agree in the large-system limit. The repellor structure present in the time-reversible phase-space distribution simply disappears in this limit. These conclusions reinforce those I reached in 1986 [3,21]. Nonequilibrium states are relatively rare; they occupy negligible zero-measure fractal regions within the equilibrium phase space; these fractals have a topological structure able to foil most analytic series-expansion techniques. The present work relates the stochastic and deterministic thermostats, showing that the two provide like results in the large-system limit.

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