Second-law irreversibility and phase-space dimensionality loss from time-reversible nonequilibrium steady-state Lyapunov spectra

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We consider steady-state nonequilibrium many-body flows of mass and momentum. For several such diffusive and viscous flows we estimate the phase-space strange-attractor Lyapunov dimensions from the complete spectrum of Lyapunov exponents. We vary the number of particles and the number of thermostated degrees of freedom, as well as the deviation from equilibrium. The resulting Lyapunov spectra provide numerical evidence that the fractal dimensionality loss in such systems remains extensive in a properly defined nonequilibrium analog of the equilibrium large-system thermodynamic limit. The data also suggest a variational principle in the vicinity of nonequilibrium steady states.

I. INTRODUCTION

Since 1972, control variables, "thermostats, barostats, ergostats, etc.," have been used in simulations to maintain atomistic systems in nonequilibrium steady states [1]. The theories developed to analyze these steady states [2] led to paradoxical results. Typically, theoretical "Kawasaki" expressions [2] for the steady-state phase-space distribution functions diverge, $f(q,p,t \to \infty) \to \infty$. The explanation was discovered in 1987. The nonequilibrium phase-space structures of steady states are multifractal *strange attractors* [3]. This topological finding explained the puzzling divergence of the phase-space probability density, away from equilibrium, and led to a simple geometric understanding of the second law of thermodynamics [4]. The steady-state phase-space probability density flows out of, and away from, zero-volume unstable repellors toward, and into, geometrically similar zero-volume attractors, upon which the second law of thermodynamics is satisfied. Thus the repellors and attractors correspond to sources and sinks, respectively, for steady-state phase-space flows. This geometric explanation of the second law incorporates concepts which were developed earlier in order to explain the chaotic properties of nonlinear dynamical systems.

In the past 15 years, several particle-based strange attractors, all characterizing time-reversible and deterministic nonequilibrium steady, or time-periodic, states, have been analyzed [5–9]. The underlying system sizes considered have ranged upward, from one or two particles, to the computational limit, now about one hundred particles. (Depending upon the method selected, the required computer time varies as N^2, N^3, or N^4 for N particles). In every case studied, the attractors turned out to be multifractal objects. Their information or Lyapunov dimensions were always strictly less than the dimensionality of the phase space within which these objects were embedded. The information dimension of attractors in three- or four-dimensional spaces could be estimated directly, by phase-space box-counting methods [8]. The Lyapunov dimensions of higher-dimensional attractors could only be estimated by evaluating the Lyapunov spectra of the underlying dynamical systems.

The second law of thermodynamics declares that the global entropy production is positive. Thus the entropy production external to any nonequilibrium steady state must be positive, $\dot{S} > 0$. In the prototypical situation of steady-state hot-to-cold heat flow, with energy provided, at rate $\dot{Q} > 0$, to a system's hot end, and extracted, at the same rate, from the cold end, the *external* entropy change rate is

$$\dot{S} = \dot{Q}[(T - \Delta T/2)^{-1} - (T + \Delta T/2)^{-2}] \approx \dot{Q}\Delta T/T^2 .$$

In *continuum* mechanics the corresponding negative change of the steady-state *system* entropy $-\dot{Q}\Delta T/T^2$ is exactly offset by a phenomenological internal entropy production. In *statistical* mechanics there is no such phenomenological mechanism for offsetting the drop in system entropy. The Gibbs system entropy for such a steady heat flow diverges to $-\infty$. For a study of the time dependence of this Gibbs entropy drop see Ref. [9].

With a nonequilibrium stationary state maintained by deterministic time-reversible equations of motion (using Gauss's or Nosé-Hoover thermostats, for instance) the second law corresponds to the collapse of the phase-space probability density onto a strange attractor. This result was clearly and precisely established, numerically, for a variety of small systems. Whether or not the topological proof of the second law found in these small systems could be extended to large systems hinged on two questions.

The first question is the following. Is the shift in the Lyapunov exponents confined primarily to a few exponents, or is the shift spread over the entire spectrum?

If the distribution of shifts *is* distributed over the entire spectrum, then the loss of Lyapunov (Kaplan-Yorke) dimension ΔD can be accurately estimated, for very small gradients, from a Taylor series in the deviation from equilibrium. Including just the first close-to-equilibrium term gives the loss in terms of the largest exponent λ_1:

$$\Delta D = \dot{S}/k\lambda_1 ,$$

where $\dot{S}$ is the total external entropy-production rate and k is Boltzmann's constant.

The second question is the following. Can these small-system arguments be extended to a large-system limit? How can the behavior of large-system attractors be judged on the basis of small-system evidence?

A breakthrough in the theoretical understanding of both these questions, at least for *some* spatially homogeneous nonequilibrium systems, was made by Sarman, Evans, and Morriss. They considered the spectrum of Lyapunov exponents. These exponents characterize all the time-averaged orthogonal growth and decay rates in a complete set of comoving and corotating phase-space directions. Sarman, Evans, and Morriss showed [10] that the sums of individual "Smale pairs" of Lyapunov exponents show *identical shifts*, away from equilibrium. That is, for the ordered spectrum of Lyapunov exponents $\{\lambda_1 > \lambda_2 > \cdots > \lambda_\Omega\}$, all of the possible summed pairs of exponents $\{\lambda_j + \lambda_{\Omega+1-j}\}$, for $j = 1, 2, \ldots, \Omega/2$, have the *same* value $-2\dot{S}/k\Omega$. Note that we are using Ω as a pure number, equal to the total number of independent directions in phase space. Provided that the Lyapunov exponents are bounded (which seems obvious on physical grounds), this result establishes the qualitative validity of the dimensionality reduction formula given above.

This proof holds for arbitrarily large deviations from equilibrium and for arbitrarily large systems, at least for systems which are "homogeneous" and which satisfy a relatively weak restriction on their time evolution [10]. By homogeneous we mean that all particles are treated equally. The result of Sarman, Evans, and Morriss is therefore a convenient starting point for discussing *inhomogeneous* systems, in which some particles are singled out for special treatment.

Steady flows of mass, momentum, and energy, as well as more complicated cyclic hysteretic thermodynamic processes, all exhibit losses of phase-space dimensionality in their phase-space attractors. The coexistence of microscopic time reversibility with macroscopic thermodynamic irreversible behavior seems paradoxical, but it can be understood in terms of the *Lyapunov instability* of the time-reversed motion. In the reversed motion the positive Lyapunov exponents exceed those on the normal trajectory, so that the reversed motion is less stable. In fact, the reversible character of the differential equations for the Lyapunov exponents [7] establishes directly that the entire Lyapunov spectrum $\{\lambda\}$ changes sign in the time-reversed motion $\{+\lambda\} \rightarrow \{-\lambda\}$. This property has been verified numerically, both for the most negative Lyapunov exponent [11] and, in our unpublished work, for the complete spectrum.

The generic nonequilibrium situation is as follows: In the *forward* direction of time the summed Lyapunov spectrum (from a single long trajectory) is negative, $\sum \lambda < 0$, though nearly half the Lyapunov exponents are positive. In the backward (reversed) time direction the summed spectrum changes sign and becomes positive, so that the underlying trajectory is accordingly less stable, though still nearly half its Lyapunov exponents are negative. This difference in global stability leads to time-symmetry breaking and an *overwhelming favoring* of those multifractal attractor states which obey the second law of thermodynamics [4].

The phase-space attractors and repellors for these problems typically display the equilibrium value of the Hausdorff dimension together with a substantially reduced, relative to equilibrium, information or Lyapunov dimension, so that the probability of selecting an unstable repellor state, violating the second law of thermodynamics, is exactly zero.

Through the efforts of mathematicians [12,13], this simple topological interpretation of thermodynamic irreversibility is being put on a rigorous basis, at least for some simple one- and two-body systems. Intuitive arguments suggest that, because (i) dissipation is extensive, $\dot{S} \equiv \eta \dot{\varepsilon}^2 V/T$, for a small-strain-rate shear flow with strain rate $\dot{\varepsilon} \equiv du_x/dy$ and shear viscosity η, for instance, and because (ii) loss of dimension can be roughly estimated by dividing the dissipation rate by the maximum Lyapunov exponent (which is intensive, corresponding to a microscopic collision rate), the loss of dimension persists for large macroscopic systems. A numerical estimate suggests, for instance, that the phase-space dimensionality loss in water is negligible at strain rates of order 1 Hz, but becomes of the same order as the *total* dimensionality at typical shockwave strain rates of order 10^{12} Hz.

At the simplest intuitive level, a loss of occupied phase-space dimensionality ΔD is quite sensible. *Any* effective constraint on the time development of a dynamical system reduces the dimensionality of phase-space states available to the system. All solutions of Hamilton's equations of motion lie on phase-space surfaces of constant energy. Constraining the kinetic temperature, rather than the energy, of a selected set of ν degrees of freedom, $C \equiv \nu kT - \sum p^2/m \equiv 0$, likewise restricts the phase-space states, permitting only states on the momentum hypersphere given by the constraint condition. A second constraint, $dC/dt \equiv 0$, were it independent of the first, would further increase the dimensionality loss ΔD from 1 to 2. The second derivative d^2C/dt^2 could lead to a further reduction. Thus it is quite plausible that the *steady-state requirement*, that C, as well as all its time derivatives, be zero, could lead to an extensive loss of dimensionality $\Delta D \approx D$. In a nonequilibrium driven system, for which the energy could vary with time, the set of constraints $\{d^n E/dt^n \equiv 0\}$ could likewise lead to an extensive loss of phase-space dimension, relative to the equilibrium distribution.

The twofold geometric explanation of irreversibility, as being due first to the zero probability of multifractal states and second to the relative mechanical instability of nearby time-reversed states, is appealing in its simplicity. But it contradicts a second appealing notion: the existence of a nonequilibrium analog of Gibbs's equilibrium

entropy, $S_{\text{Gibbs}} \equiv -k \langle \ln f \rangle$. Because such a nonequilibrium entropy would be a casualty of a singular phase-space distribution function $f(q,p,\ldots) \approx \infty$, there is some reluctance to accept the simple multifractal geometric picture of second-law irreversibility. In discussing these ideas, a test was formulated.

The test begins with a homogeneously thermostated nonequilibrium steady state, for which the very interesting exact sum rule of Sarman, Evans, and Morriss must hold. In the homogeneous case, the dissipation rate $\dot{S}$ and the dimensionality loss ΔD must both be extensive. Then, as the thermostat is made progressively less intrusive, by reducing the number of directly affected degrees of freedom, and as the system size is increased, changes in the phase-space dimensionality loss can be monitored. If ΔD becomes smaller under these conditions this could mean that the drop in dimension is not extensive. On the other hand, a steady, or increasing, dimensionality drop ΔD would strongly suggest that the simple picture of reduced dimensionality persists for macroscopic systems. We take up this test, in the present work, for two types of nonequilibrium systems.

There are conceptual difficulties in considering *large* nonequilibrium systems. These are best known in two dimensions, where there is a relatively widespread opinion that "transport coefficients diverge." Because this divergence is thought to be logarithmic in the system size, there are severe conceptual difficulties in defining the nonequilibrium analog of the *large*-system "thermodynamic limit" in two dimensions. Even in three dimensions, any fixed and finite velocity gradient leads, for large enough systems, to divergent boundary velocities, as well as to turbulence, rather than to nonequilibrium steady states.

Both these twin difficulties, divergence and turbulence, can be avoided by using homogeneous thermostats. In both the two- and the three-dimensional cases, deterministic time-reversible thermostats, developed in order to carry out nonequilibrium computer simulations, provide a natural *definition* of a large-system nonequilibrium limit analogous to the large-system equilibrium "thermodynamic limit." We elaborate on this idea in the following section, and then devote the remainder of the paper to numerical tests of the extensive nature of ΔD for two types of relatively simple two-dimensional nonequilibrium systems.

II. LARGE-SYSTEM LIMIT FOR NONEQUILIBRIUM SYSTEMS

The "extensive" natures of the energy and free energies of thermodynamic systems, with "extensive" meaning proportional to system size, are familiar consequences (neglecting gravity) of sufficiently repulsive short-ranged forces along with the overwhelming tendency for gradients to dissipate. Once reached, thermodynamic equilibrium, for a large number of bodies N, exhibits negligible fluctuations of order $N^{1/2}$ about the mean values, of order N, of the extensive energies. The mathematical approach to statistical mechanics incorporates an idealized thermodynamic limit in which system properties are tru-

ly extensive and in which surface effects and fluctuations can be ignored.

At equilibrium time is unimportant. Nothing interesting happens. Negligibly small fluctuations, of order $N^{1/2}$, come and go. Away from equilibrium *time* must be considered. In a system with sidelength L, gradients dissipate in a diffusion time proportional to L^2. Thus, in general, nonequilibrium properties involve the past history of the system, for a time of order L^2/D, where D is a diffusive transport coefficient. For macroscopic systems these times are so large that the concept of equilibration is more mathematical than physical. An "isolated" cubic meter of water would only reach mechanical "equilibrium," through the diffusion of momentum and energy, in a time on the order of years.

Long equilibration times are not the only undesirable feature of large systems. Boundary values for large systems with fixed gradients diverge. Even small gradients can lead to unpredictable chaotic behavior. At a modest strain rate, say 1 Hz for liquid water, the flow becomes turbulent once the system size exceeds a few centimeters. The idealizations of the linear flow relations—Fick's law for diffusion, Newtonian viscosity, and Fourier's law for heat conduction—can only be realized in small systems.

Nonequilibrium steady states, with stationary boundary conditions involving only composition and temperature, can become independent of their initial conditions once the necessary diffusion times have passed. But because these times are unphysically large, for macroscopic systems, and reach no useful large-system limit, a simpler limit concept is welcome. The main problem is describing the boundaries themselves. Steady-state boundaries cannot obey Hamiltonian mechanics (because dissipated heat has to be extracted at the boundaries). Occam's razor (of fewest assumptions), combined with Gauss's principle (of least constraint), suggests that the *simplest* means of thermostating is a global homogeneous one, in which each degree of freedom in the system has an additional constraint force $\delta \dot{p} = -\zeta p$ designed to maintain the temperature or the internal energy [2]. Temperature is a more appealing independent variable than is energy because temperature is a directly measurable quantity. The mechanical definition of temperature, based on an ideal-gas thermometer enclosed in a semipermeable membrane, has recently been discussed [14]. But, for technical reasons, an energy-sensitive ergostat turns out to be more useful than a temperature-sensitive thermostat. This is because the ergostat, unlike a thermostat, need do nothing in the equilibrium situation. Thus near-equilibrium states require relatively small thermostat activity.

At equilibrium it is known that an isokinetic Gaussian constraint force on the momenta provides Gibbs's canonical distribution for the coordinates [15]. For a local-equilibrium description of a nonequilibrium shear state, characterized by temperature, density, and strain rate, for instance, the same thermostat idea seems to be a natural choice. But eliminating temperature fluctuations, by constraining the kinetic energy, results in an undesirable artificial stiffness, *even in the equilibrium case*. This stiffness in the equilibrium dynamics can be avoided by using an ergostat, which plays no role whatsoever in the

equilibrium case, and remains relatively small in non-equilibrium states sufficiently close to equilibrium.

Simple homogeneous thermostats or ergostats can be readily relaxed, modified, or amplified whenever more local information is available concerning local properties of the globally restricted nonequilibrium system. It is straightforward to include space- and time-dependent constraints fixing components of the stress tensor, the magnitude of the heat flux, or the rate of heating, for instance. In nonequilibrium systems the addition of such constraints plays the same role as does the acquisition and implementation of "information" in Jaynes's approach [16] to statistical mechanics.

In the *equilibrium* case the occupied phase *volume* can be reduced by decreasing the volume accessible to the particles or by decreasing their total energy. In the *nonequilibrium* case it appears that, rather than reducing the occupied phase volume, the *dimensionality* of the occupied phase space is itself reduced. Thus the nonequilibrium driving and constraints associated with the nonequilibrium independent variables such as strain rate and field strength are more far-reaching constraints than are the equilibrium state variables.

It seems intuitively evident that a *global* homogeneous thermostat or ergostat, applied equally to all degrees of freedom, is less intrusive than a *local* one applied to only a few. It is plausible that, "other things being equal," an *inhomogeneous* thermostat results in a larger *dimensionality* loss ΔD than the limiting homogeneous thermostat. At equilibrium, for instance, a single thermostated variable in an N-body system would need to undergo very large constraint forces, of order $N^{1/2}$, while the alternative, global constraint forces, applied to all degrees of freedom, in such a system, would have a negligible amplitude, of order $N^{-1/2}$.

Thus a *hydrodynamic* limit analogous to the equilibrium *thermodynamic* limit *can* be defined for systems in near-equilibrium steady nonequilibrium states. The prototypical limiting case is based on *global* (as opposed to local-boundary) thermostats (or barostats or ergostats). The corresponding control variables were first introduced in molecular-dynamics simulations in order to speed the equilibration of atypical initial conditions [17]. Later, we will discuss specific formulations of these control variables developed based on ensemble theory. The Nosé-Hoover thermostat (of which Gauss's simpler version, used much earlier, is a special case) allows temperature to be specified, for a selected set of degrees of freedom, in a way which is exactly consistent with Gibbs's equilibrium ensembles.

Such thermostats can also be applied to nonequilibrium systems either homogeneously or in specified local boundary regions. From the logical standpoint a nonequilibrium steady state stabilized by a global thermostat, applied to degrees of freedom throughout the system, has much to recommend it. It is exactly consistent with the Green-Kubo equilibrium fluctuation theory of transport. It provides well-defined nonlinear transport coefficients. It stabilizes systems against the long-wavelength fluctuations which generate turbulence. It can be easily incorporated into the Boltzmann equation so that the Chapman-Enskog procedure can be applied to the analysis of far-from-equilibrium states of dilute gases, the only class of nonequilibrium problem so far accessible to exact theoretical treatment at the atomistic level. For all these reasons we believe that *globally controlled homogeneous nonequilibrium steady states are a uniquely well-suited basis for nonequilibrium statistical mechanics.* We investigate these states, in the present work, for a simple model force law, chosen to minimize computational difficulties, and described in the following section.

III. MODEL SYSTEMS

The simplest homogeneous nonequilibrium steady state is obtained when two species are accelerated by an external field in opposite directions, but at constant temperature or at constant internal energy. Provided that the field is not too strong and the density is not too low, a homogeneous nonequilibrium steady state, fully consistent with the Green-Kubo theory of conduction, results [18]. Despite the more measurable nature of temperature, it is better, computationally, to constrain the internal energy, for this minimizes the task of the corresponding control variable (the "friction coefficient" ζ).

In the present work we investigate two-dimensional systems with up to 100 particles. Similar investigations, for 8-particle systems, were recently carried out by Sarman, Evans, and Morriss [10]. All these system sizes are small enough that the complete Lyapunov spectrum can be generated. Here we use a smooth (three continuous derivatives) pair potential with a finite range σ,

$$\phi(r) = 100\varepsilon[1-(r/\sigma)^2]^4 , \quad r/\sigma < 1$$

solving the equations of motion with fourth-order Runge-Kutta integration, in order to reduce computational errors. In reporting our results we choose the potential parameters σ and ε, as well as the particle mass m, all equal to unity. A careful study of the size dependence of the largest Lyapunov exponent for equilibrium systems (with $N=4^2, 6^2, 8^2, \ldots, 16^2$) at an internal energy $E=N$ indicated a limiting value of the largest exponent $\lambda_1 = 3.0$.

We evaluated the entire *nonequilibrium* coefficient spectrum for two different system sizes $N=6^2$ and 10^2 with a few additional simulations at $N=4^2$. The different system sizes allowed us to gauge the dependence of the dimensionality reduction ΔD on the total number of particles N as well as the number of ergostated particles N_e. We followed the (36- or 100-) particle motion in the full (144- or 400-) dimensional phase space, solving the (144×145 or 400×401) ordinary differential equations required to characterize the time-averaged growth and decay rates in that space—the set of (144 or 400) Lyapunov exponents. We varied the total number of ergostated particles in the system while keeping the total integral energy of the system fixed. Thus the equations of motion for the diffusive model (choosing an atomic mass m of unity, a field strength F_{ext}, and unity for the two potential parameters ε and σ) are

$$dx/dt = p_x \ , \quad dy/dt = p_y \ ,$$

$$dp_x/dt = F_x \pm F_{ext} - \zeta p_x \ , \quad dp_y/dt = F_y - \zeta p_y \ ,$$

where the Gaussian friction coefficient ζ, which keeps the internal energy fixed, is given by the expression

$$\zeta \equiv F_{ext} \sum [\pm p_x] \Big/ {\sum}' [p_x^2 + p_y^2] \ .$$

The current sum, in the numerator, includes *all* the particles (half with plus signs and half with minus signs) and the primed sum, in the denominator, includes only those which make up the ergostat. This form for the control parameter ζ makes explicit the number dependence of the constraint forces through the number of degrees of freedom participating in the constraint. An alternative procedure, which we have not followed here, would thermostat the kinetic energy or internal energy of only a selected group of particles. This seems to us less interesting because such a choice would include phase-space states lying off the equilibrium internal energy surface of the total system. In such a case both the numerator and denominator sums would include only contributions from that group. Our diffusive flow results appear in Table I. In addition to the dissipative current, $\sum \pm P_x$, we display the largest Lyapunov exponent, the smallest Lyapunov exponent, the loss in phase-space dimensionality ΔD, and the sum of all the Lyapunov exponents, equal to $-k$ times the overal dissipation rate dS/dt a series of 36- and 100-particle simulations.

For a homogeneous periodic shear, with strain rate $\dot{\varepsilon} \equiv du_x/dy$, it is usual to define the peculiar momenta $\{p_x, p_y\}$, relative overall shear flow $(u_x, u_y) \equiv (\dot{\varepsilon}y, 0)$. The "Sllod" motion equations (so named because of their relationship to the Doll's tensor algorithm) then become

TABLE I. Results for N-particle two-dimensional color-conductivity simulations. N_e particles are ergostated. The successive columns list field strength, summed velocity contributions to the dissipative current, maximum and minimum Lyapunov exponents, the sum of all exponents, and the phase-space dimensionality loss. The 36- and 100-particle results are averages over at least 2000 and 200 time units. The statistical uncertainty for ΔD is about 2%.

N	N_e	F_{ext}	$\sum (\pm p_x)_x$	λ_1	λ_Ω	$\sum \lambda$	ΔD
36		0.00	0.00	3.08	−3.08	0.00	0.00
36	36	0.25	1.16	3.07	−3.08	−0.41	0.13
36	36	0.50	2.32	3.06	−3.09	−1.65	0.45
36	36	1.00	4.79	3.02	−3.11	−6.79	2.20
36	24	0.25	1.16	3.07	−3.08	−0.41	0.13
36	24	0.50	2.39	3.06	−3.08	−1.72	0.56
36	24	1.00	4.84	3.01	−3.12	−7.03	2.28
36	12	0.25	1.04	3.06	−3.06	−0.40	0.13
36	12	0.50	2.41	3.06	−3.09	−1.80	0.58
36	12	1.00	4.59	3.02	−3.12	−7.32	2.38
100	100	0.25	4.3	3.07	−3.08	−1.5	0.50
100	100	0.50	7.9	3.05	−3.07	−5.6	1.84
100	100	1.00	18.2	2.97	−3.10	−25.4	8.38

$$dx/dt = p_x + \dot{\varepsilon}y \ , \quad dy/dt = p_y \ ,$$

$$dp_x/dt = F_x - \dot{\varepsilon}p_y - \zeta p_x \ , \quad dp_y/dt = F_y - \zeta p_y \ ,$$

where the Gaussian ergostating variable ζ is given by the relation

$$\zeta \equiv -\dot{\varepsilon} \sum [yF_x + p_x p_y] \Big/ {\sum}' [p_x^2 + p_y^2] \ .$$

With periodic boundaries the yF_x contributions to the single-particle sum can be combined in pairs to give terms of the form $y_{ij}F_{ij}^x$. Thus the sum in the numerator is just $P_{xy}V$, proportional to the shear stress.

With periodic boundaries the center of mass can drift, even if *all* the particles are ergostated. But the x and y momentum sums, as well as the kinetic energy, are all constant, so that the N-particle motion takes place in a

TABLE II. Results for N-particle two-dimensional shear-flow simulations. N_e particles are ergostated. The successive columns list strain rate $\dot{\varepsilon}$, the xy component of the shear stress $-P_{xy}$, the maximum and minimum Lyapunov exponents, the sum of all exponents, and the phase-space dimensionality loss. For the lowest shear rate $\dot{\varepsilon}=0.25$ the length of the simulation runs varies between 20000 time units (4 million time steps) for $N=16$, and 1200 time units (240000 time steps) for $N=100$. The ensuing statistical uncertainty for ΔD is better than 2%. For higher shear rates the length of the simulation runs was only half as long, resulting in uncertainties for ΔD of about 3%.

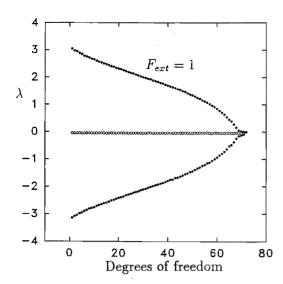| N	N_e	$\dot{\varepsilon}$	$-P_{xy}$	λ_1	λ_Ω	$\sum \lambda$	ΔD
16		0.00	0.00	3.06	−3.06	0.0	0.00
16	16	0.25	0.30	3.05	−3.11	−1.77	0.57
16	16	0.50	0.59	3.02	−3.25	−7.0	2.21
16	16	1.00	1.09	2.94	−3.80	−27.9	8.17
16	12	0.25	0.30	3.05	−3.11	−1.82	0.59
16	12	0.50	0.58	3.01	−3.23	−7.3	2.30
16	6	0.25	0.30	3.03	−3.10	−2.03	0.66
25	25	0.25	0.31	3.06	−3.12	−2.85	0.91
25	17	0.25	0.31	3.05	−3.11	−2.86	0.93
25	9	0.25	0.31	3.05	−3.11	−3.13	1.01
36		0.00	0.00	3.08	−3.08	0.00	0.00
36	36	0.25	0.31	3.06	−3.11	−4.11	1.33
36	36	0.50	0.62	3.03	−3.26	−16.4	5.20
36	36	1.00	1.14	2.95	−3.83	−63.7	19.0
36	24	0.25	0.31	3.05	−3.11	−4.16	1.35
36	24	0.50	0.61	3.03	−3.27	−17.0	5.37
36	24	1.00	1.13	2.99	−4.02	−75.3	22.0
36	12	0.25	0.31	3.05	−3.11	−4.43	1.43
36	12	0.50	0.61	3.06	−3.32	−20.4	6.43
64	64	0.25	0.32	3.08	−3.13	−7.37	2.37
64	42	0.25	0.32	3.07	−3.13	−7.53	2.42
64	22	0.25	0.31	3.07	−3.13	−7.62	2.46
100	100	0.25	0.32	3.07	−3.14	−11.43	3.68
100	100	1.00	1.16	3.00	−3.90	−176.7	53.1
100	66	0.25	0.32	3.09	−3.15	−11.60	3.73
100	66	1.00	1.14	3.07	−4.03	−203.0	60.4
100	34	0.25	0.31	3.08	−3.14	−11.84	3.81

FIG. 1. Complete spectrum of 143 Lyapunov exponents for a two-dimensional color-conductivity simulation with field strength equal to 1.0. All 36 particles are ergostated and the phase-space energy surface has 143 dimensions. Three exponents vanish. The arithmetic means of the Smale pairs of the exponents are indicated by open circles.

$(4N-3)$-dimensional subspace of phase space. In the locally ergostated case, both the center of mass and the momentum associated with it drift, so that the subspace is $(4N-1)$ dimensional. It is desirable to remove, from time to time, components of the offset vectors perpendicular to the constant-internal-energy surface [19]. Because this step is inexpensive, we have carried it out at every time step.

Results for the shear-flow Lyapunov exponents and dimensionality reduction appear in Table II. Typical complete Lyapunov spectra characteristic of both system
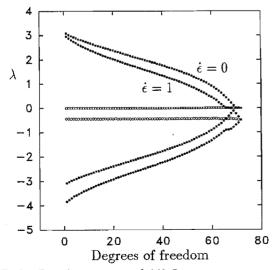

FIG. 2. Complete spectra of 143 Lyapunov exponents for two-dimensional shear-flow simulations with strain rates $\dot{\epsilon} \equiv du_x/dy$ equal to 0.0 (equilibrium) and 1.0. All 36 particles are ergostated and the phase-space internal energy surface has 143 dimensions. Three exponents vanish. The arithmetic means of the Smale pairs of the exponents are indicated by open symbols.

types, diffusive and shear, appear in Figs. 1 and 2. Our conclusions regarding the loss of phase-space dimensionality, based on the results tabulated here, are described in the following two sections.

IV. RESULTS

Tables I and II include long-term averages for the dissipation, the corresponding loss of phase-space dimension ΔD, and the overall dissipation rate $\sum \lambda \equiv -\dot{S}/k$ at fixed energy, for a varying number of ergostated particles. The fraction of these particles can be varied considerably without changing the topological laminar nature of the flow.

We have chosen to concentrate on moderate field strengths and strain rates in our numerical work. These choices provide a non-negligible dimensionality reduction ΔD in the corresponding diffusive and viscous phase-space strange attractors. All these results lie sufficiently close to the regime of linear irreversible thermodynamics to make that theory meaningful in analyzing them.

The differential equations have been integrated with the classic fourth-order Runge-Kutta method. The Lyapunov spectra were generated using methods based on Benettin's ideas, which have been thoroughly and repeatedly discussed in the recent literature [6,7].

The numerical data presented here are fully in accord with the theoretically based expectation that the dissipation is approximately quadratic in the departure from equilibrium. Thus the shear viscosities (stress σ_{xy} divided by strain rate $\dot{\epsilon} \equiv du_x/dy$) for 16 ergostated particles show no significant dependence on strain rate up to $\dot{\epsilon} \approx 1$. Symmetry suggests *quartic* strain-rate deviations from the quadratic prediction of irreversible thermodynamics. The deviations found here are nearly negligible. For this reason, we believe that the implications of our results from these simple systems have far-reaching significance. In the next section, we discuss and interpret our results.

V. DISCUSSION AND INTERPRETATION

Frederikson *et al.* provided a useful way to estimate the information dimension of phase-space attractors [20]. They called their estimate the "Lyapunov dimension." We adopt that terminology here. From this standpoint, the steady-state attractor is dimensionally larger than all those phase-space objects which grow in time and dimensionally smaller than all those objects which shrink. In the steady state the attractor neither grows nor shrinks. Any phase-space object of D dimensions, followed in time, grows or shrinks according to the sign of the sum of the largest D Lyapunov exponents.

By (the generally accepted) definition, a "chaotic system" possesses at least one positive Lyapunov exponent. Accordingly, for a *chaotic* system the one-dimensional object defined by the phase-space line linking two nearby trajectories grows, exponentially fast, at a rate given by λ_1. By (our own) definition, the phase-space volume occupied by a *dissipative* system *shrinks* with time. For a chaotic dissipative system, with time-reversible Gauss or

Nosé-Hoover equations of motion, the comoving phase-space volume with the complete dimensionality of the phase space necessarily shrinks [3-9] so that the complete sum of exponents $\sum_i \lambda_i$ has to be negative. Frederikson et al. defined the "Lyapunov dimension" estimate of the information dimension by finding the number of exponents required for the *incomplete* sum $\sum'_i \lambda_i$ to vanish. Figure 3 shows typical variations of the steady-state dimensionality loss with the degree of departure from equilibrium.

For a fixed value of the nonequilibrium flux (a mass, momentum, or energy current) the dissipation predicted by linear irreversible thermodynamics is extensive and, near equilibrium, is also approximately quadratic in the flux. We have verified this prediction numerically by considering several fields and strain rates, as detailed in the tables. Our numerical work verifies that for small (but by no means infinitesimal) gradients the dissipation remains nearly quadratic in the gradients. The Lyapunov exponents themselves reflect dynamic bifurcations in the many-body phase space. The magnitudes of the largest coefficients are of the order of a collision frequency. The distributions of the coefficients, for fluids or for solids, are relatively featureless, simpler in structure than the vibrational spectra characterizing solids. Because the sign of the strain rate is irrelevant to ΔD, the Lyapunov exponents likely vary quadratically with the deviation from equilibrium, but the fact that symmetry is broken suggests that a linear law is also possible.

In equilibrium a homogeneous ergostat does not affect the system at all. It is intuitively plausible, even in nonequilibrium states, that it provides the *least severe* modification necessary to keep the energy constant and hence the *least possible* dissipation. Our numerical investigations have confirmed this idea. A conjectured variational principle, that homogeneous constraints are the *least intrusive*, could join with many predecessors (see, for instance, Ref. [21]) and might also join them in prompting counterexamples. Nevertheless, our computational results so far bear the conjecture out.

As we *decrease* the number of degrees of freedom being ergostated the dissipation *increases* smoothly, at least until the disparity between the constrained and Newtonian particles becomes sufficiently large to lead to a structural change. The data in the tables support the view that any such structural change occurs relatively far from equilibrium.

Thus our numerical data support the views (at least sufficiently close to equilibrium) that the dissipation is *quadratic* in the gradients and *extensive,* that the Lyapunov spectrum varies no more than linearly with the deviation from equilibrium, and that the dimensionality drop, for nonequilibrium steady states, is minimum for homogeneous constraints. These three results together support the tentative conclusion that the fractional loss of phase-space dimensionality on a nonequilibrium strange attractor is a pure number, characterizing the material in question, and that the deviations which arise, farther from equilibrium, are at least linear in the deviation from equilibrium.

$$\Delta D / D \approx \dot{S} / N k \lambda_1 + O(\text{gradient}) .$$
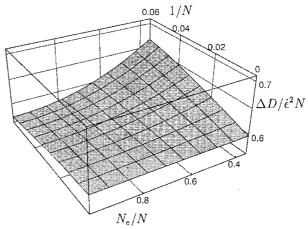

FIG. 3. Shows the variation of the steady-state dimensionality loss, $\Delta D \equiv D_{\text{equilibrium}} - D$, as a function of the number N_e of ergostated particles and of the inverse total number of particles, $1/N$, for a strain rate $\dot{\epsilon} = 0.25$. The $(\Delta D / \dot{\epsilon}^2 N)$ surface was generated by smoothing the respective data listed in Table II. It can be readily extrapolated to the hydrodynamic limit $1/N \to 0$ which demonstrates the extensivity of the dimension of the underlying strange attractor. Within the numerical uncertainty the limit $\lim_{N \to \infty} \Delta D / \dot{\epsilon} N \equiv d$ is even independent of the number of ergostated degrees of freedom (proportional to N_e). Since $\Delta D / N$ varies almost linearly with $1/N$ for fixed N_e / N, our numerical results suggest that the many-particle limit of ΔD is approached according to $\Delta D = a + dN$, where $a(N_e / N)$ depends only on the relative number of ergostated particles. For the homogeneous ergostat, $N_e = N$, $a(1)$ is negative. a eventually becomes positive if the relative number of ergostated degrees of freedom is reduced.

This means that the many-particle distribution functions, away from equilibrium but sufficiently close to it, are indeed multifractal in character, just as they are in smaller systems, so that the nonequilibrium Gibbs's entropy does indeed diverge.

VI. CONCLUSION

Because the near-equilibrium phase-space dimensionality loss is insensitive to the fraction of constrained particles and appears to be minimized when all degrees of freedom are similarly constrained, we have strong evidence that the phase-space attractor dimensionality reduction is real, persisting for large systems. The result of Sarman, Evans, and Morriss, for the homogeneous case, is fundamental to this demonstration and suggests as well that the large-system homogeneously thermostated nonequilibrium state provides the *hydrodynamic*-limit analog of the equilibrium *thermodynamic* limit.

[1] For an early review see W. G. Hoover and W. T. Ashurst, Adv. Theor. Chem. **1**, 1 (1975).

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

[3] W. G. Hoover, H. A. Posch, B. L. Holian, M. J. Gillan, M. Mareschal, and C. Massobrio, Mol. Sim. **1**, 79 (1987).

[4] B. L. Holian, W. G. Hoover, and H. A. Posch, Phys. Rev. Lett. **59**, 10 (1987).

[5] W. G. Hoover, Physica A **194**, 450 (1993).

[6] W. G. Hoover, *Computational Statistical Mechanics* (Elsevier, Amsterdam, 1991).

[7] H. A. Posch and W. G. Hoover, Phys. Rev. A **38**, 473 (1988). The Lagrange-multiplier method for determining Lyapunov exponents, outlined in W. G. Hoover and H. A. Posch, Phys. Lett. **113A**, 82 (1985), has since been rediscovered by I. Goldhirsch, S. A. Orszag, P. L. Sulem, and W. E. Wiesel, Physica D **27**, 311 (1987).

[8] For an application of the Chhabra-Jensen box-counting method see W. G. Hoover and B. Moran, Phys. Rev. A **40**, 5319 (1989).

[9] B. L. Holian, H. A. Posch, and W. G. Hoover, Phys. Rev. A **42**, 3196 (1990).

[10] S. Sarman, D. J. Evans, and G. P. Morriss, Phys. Rev. A **45**, 2233 (1992).

[11] W. G. Hoover, C. G. Tull (now C. G. Hoover), and H. A.

Posch, Phys. Lett. A **131**, 211 (1988).

[12] W. N. Vance, Phys. Rev. Lett. **69**, 1356 (1992).

[13] N. I. Chernov, G. L. Eyink, J. L. Lebowitz, and Y. G. Sinai, Phys. Rev. Lett. **70**, 2209 (1993).

[14] D. Jou and J. Casas-Vázquez, Phys. Rev. A **45**, 8371 (1992). See also a recent Comment on this work: W. G. Hoover, B. L. Holian, and H. A. Posch, Phys. Rev. E **48**, 3196 (1993).

[15] W. G. Hoover, A. J. C. Ladd, and B. Moran, Phys. Rev. Lett. **48**, 1818 (1982).

[16] For a critique of Jaynes's approach see W. G. Hoover, *Molecular Dynamics*, edited by H. Araki, W. Beiglböck, J. Ehlers, K. Hepp, R. Kippenhahn, H. A. Weidenmüller, and J. Zittartz, Lecture Notes in Physics Vol. 258 (Springer-Verlag, Heidelberg, 1986).

[17] L. V. Woodcock, Chem. Phys. Lett. **10**, 257 (1971).

[18] W. G. Hoover, D. J. Evans, R. B. Hickman, A. J. C. Ladd, W. T. Ashurst, and B. Moran, Phys. Rev. A **22**, 2798 (1980).

[19] W. G. Hoover, H. A. Posch, and L. W. Campbell, Chaos **3**, 1 (1993).

[20] P. Frederikson, J. Kaplan, E. Yorke, and J. Yorke, J. Differ. Equations **49**, 185 (1983).

[21] D. J. Evans and A. Baranyai, Phys. Rev. Lett. **67**, 2597 (1991).