

Liouville's theorems, Gibbs' entropy, and multifractal distributions for nonequilibrium steady states

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Liouville's best-known theorem, $\dot{f}(\{q,p\},t)=0$, describes the incompressible flow of phase-space probability density, $f(\{q,p\},t)$. This incompressible-flow theorem follows directly from Hamilton's equations of motion. It applies to simulations of isolated systems composed of interacting particles, whether or not the particles are confined by a box potential. Provided that the particle-particle and particle-box collisions are sufficiently mixing, the long-time-averaged value $\langle f \rangle$ approaches, in a "coarse-grained" sense, Gibbs' equilibrium microcanonical probability density, f_{eq} , from which all equilibrium properties follow, according to Gibbs' statistical mechanics. All these ideas can be extended to many-body simulations of deterministic open systems with nonequilibrium boundary conditions incorporating heat transfer. Then Liouville's compressible phase-space-flow theorem—in the original $\dot{f} \neq 0$ form—applies. I illustrate and contrast Liouville's two theorems for two simple nonequilibrium systems, in each case considering both stationary and time-dependent cases. Gibbs' distributions for incompressible (equilibrium) flows are typically smooth. Surprisingly, the long-time-averaged phase-space distributions of nonequilibrium compressible-flow systems are instead singular and "multifractal." The nonequilibrium analog of Gibbs' entropy, $S \equiv -k\langle \ln f \rangle$, diverges, to $-\infty$, in such a case. Gibbs' classic remedy for such entropy errors was to "coarse-grain" the probability density—by averaging over finite cells of dimensions $\Pi \Delta q \Delta p$. Such a coarse graining is effective for isolated systems approaching equilibrium, and leads to a unique entropy. Coarse graining is not as useful for deterministic open systems, constrained so as to describe stationary nonequilibrium states. Such systems have a Gibbs' entropy which depends, logarithmically, upon the grain size. The two Liouville's theorems, their applications to Gibbs' entropy, and to the grain-size dependence of that entropy, are clearly illustrated here with simple example problems. © 1998 American Institute of Physics. [S0021-9606(98)51235-4]

I. INTRODUCTION

Computer simulation is by now a familiar generator of equilibrium and nonequilibrium properties of classical many-body systems.¹⁻³ By linking microscopic mechanics to macroscopic thermodynamics, simulation has also facilitated theoretical analyses of systems far from equilibrium, and suggested new approaches to the foundational problems of statistical mechanics. Adopting the terminology used by Sklar, in a thorough and lively recent review,⁴ the accepted "orthodox" approach to reconciling time-reversible mechanics with the approach to equilibrium and irreversible thermodynamics relies on the differential equations of Hamiltonian mechanics and stresses the importance of suitably chosen initial conditions. This conservative approach is subject to the well-known recurrence and reversibility criticisms of Poincaré and Zermélo.

By contrast, it is an article of faith, shared by simulators and experimentalists, that the initial conditions are irrelevant, and that it is instead the boundary conditions which shape and determine flows.⁵ Simulators and experimentalists tend to analyze stationary nonequilibrium flows, rather than the

transients involved in equilibration. Curiously, even the imposition of boundary conditions, although certainly required for any nonequilibrium steady state, is not explicitly discussed by the orthodox school. In the equilibrium case such boundary conditions are regarded as "interventionist".⁴

The orthodox Hamiltonian approach entails solving two first-order differential equations of motion for each degree of freedom in the system:

$$\{\dot{q} = +\partial H(\{q,p\})/\partial p; \dot{p} = -\partial H(\{q,p\})/\partial q\},$$

where the generalized coordinates $\{q\}$ are paired with their conjugate momenta $\{p \equiv \partial L(\{q,\dot{q}\})/\partial \dot{q}\}$, which are given in terms of the underlying Lagrangian, $L(\{q,\dot{q}\}) \equiv K - \Phi$. In the usual case, where forces are nonlinear and the dynamics is chaotic so that analytic work is impractical, an approximate numerical solution of Hamilton's equations, giving $\{q(t), p(t)\}$, is generated at a series of discrete time steps $\{n\Delta t\}$, starting with initial values of the coordinates and momenta at time 0. In the absence of special boundary forces or nonequilibrium constraints, or driving fields, a typical sufficiently mixing system soon fluctuates about equilibrium. For stationary boundary conditions, the time series describing such a solution provides an approximation to Gibbs' ideal-

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ized probability density $f_{\text{eq}}(\{q,p\})$, with the approximation to the long-time average, $\langle f \rangle$, becoming exact in the long-time limit.

Gibbs' statistical mechanics applies to such equilibrium systems, provided only that the microscopic dynamics can reach all the $\{q,p\}$ states consistent with the fixed macroscopic variables characterizing the corresponding Gibbs' ensemble. In such equilibrium cases Gibbs replaces the detailed time averages of mechanical variables, such as the kinetic and potential energies, $\langle K \rangle$ and $\langle \Phi \rangle$, by time-independent phase averages, using the weighting function $\langle f \rangle = f_{\text{eq}}$ in preference to a detailed trajectory time series $\{q(n\Delta t), p(n\Delta t)\}$. Gibbs also showed that the equilibrium $\langle f \rangle$ itself, while not a dynamical variable like the energies, can be used to calculate the thermodynamic entropy, $S \equiv -k\langle \ln f \rangle$, where k is Boltzmann's constant. Because the instantaneous f is "invariant" to canonical transformations, the resulting entropy, from $\langle f \rangle$, does not depend upon the particular choice of generalized coordinates $\{q\}$.⁶ The probability, $f \Pi dq dp$, of occupying a particular region \otimes in phase space, $\otimes \equiv \Pi dq dp$, is independent of the chosen coordinate system, and is (apart from a multiplicative constant of order h^{-DN} in D dimensions) $\otimes e^{-S/k}$ for Gibbs' microcanonical ensemble and $\otimes e^{-(A-H)/kT}$ for his canonical ensemble. Here S , A , and H are, respectively, the entropy, the Helmholtz free energy, and the Hamiltonian. In addition to the independence of f and $\langle f \rangle$ to coordinate choice, the various projections of f onto subspaces with fewer than the total number of degrees of freedom, give additional "Poincaré invariants." These are likewise independent of the chosen phase-space coordinate system.⁷

There is a famous difficulty with this picture for entropy.^{4,8} Consider the expansion of an ideal gas, constrained initially by a piston to occupy exactly half of a large box of volume $2V$. The piston then moves, with a prescribed time history, so that the gas fills the entire volume $2V$ at a later time t . What then is the situation for times much greater than t , long after the piston has come to rest, so that the gas has equilibrated? If the expansion takes place so rapidly that the gas cannot keep up with the piston, and hence cannot do external work, a doubling of the volume should eventually leave the gas with an entropy increase of $k \ln 2$ per particle. On the other hand, if the expansion takes place so slowly that the gas remains near equilibrium throughout, the expansion is thermodynamically reversible, with no change in the entropy. For intermediate expansion programs, some portion of the maximum entropy gain, $Nk \ln 2$, occurs. The Gibbsian ensemble picture of these volume-doubling problems is different. Consider an equilibrium ensemble initially containing representatives of all phase-space states with energy E , occupying the volume V , and following the prescribed expansion program. Provided only that the motion of each ensemble member, following the doubling, obeys the same time-dependent Hamiltonian mechanics with the same piston motion, the ensemble phase-space volume and the corresponding Gibbs entropy of the ensemble must both be unchanged according to Liouville's incompressible-flow theorem. Similar considerations hold for gaseous effusion, in which a small hole is bored in a motionless piston at time 0.

According to the equilibrium version of Liouville's incompressible theorem, $\dot{f} = 0$, as discussed in Sec. II, the fine-grained f cannot change with time. Thus Gibbs' entropy $-k\langle \ln f \rangle$ can neither increase nor decrease. Thus Gibbs' "fine-grained" ensemble entropy cannot possibly reproduce the inexorable entropy increase described by the second law of thermodynamics. That law requires an increasing entropy for any system subject to noticeably time-dependent forces. A way to avoid the Gibbs' entropy difficulty, at least for some situations, is to use "coarse graining",^{4,8} a division of the phase space into small cells $\{\Pi \Delta q \Delta p\}$. The resulting coarse-grained entropy approximates the proper equilibrium value, just as a trapezoidal-rule summation approximates an integral. It is tempting to use this same picture not only at equilibrium, but also away from equilibrium. But a decade of research has established a severe difficulty with such a coarse-graining remedy: nonequilibrium distribution functions are typically "multifractal" distributions, singular everywhere, with "multifractal" signifying a density which varies locally as a fractional power of the small cell size, never giving a convergent entropy, even in the small-cell limit. Thus these multifractal nonequilibrium systems have divergent Gibbs' entropies.^{9,10}

In Sec. II, I develop Liouville's theorems with both $\dot{f} = 0$ and $\dot{f} \neq 0$. Although these theorems are generally attributed to Liouville's 1838 exposition,¹¹ a simpler, older, path to them is the many-dimensional version of Euler's continuity equation, $d \ln \rho / dt \equiv -\nabla \cdot v$, where the density ρ of a conserved quantity (mass or probability) flows through the appropriate space (either three-dimensional or many-dimensional) with velocity v . Liouville's theorems can be applied both at, and away from, equilibrium. In considering the compressible case, away from equilibrium, the three articles by Andrey make interesting reading.¹²⁻¹⁴ He begins by focusing on the $\dot{f} \neq 0$ theorem as a possible explanation of the Second law. Four years later his thoughts are clearer and more concise.¹³ Finally, in an admirably clear article¹⁴ he gives Liouville credit for both the theorems: "a reading of great old masters is very beneficial." See also the related articles in Refs. 15-17. In Sec. II, I also discuss the implications of applying the compressible $\dot{f} \neq 0$ theorem to a time-reversible nonequilibrium flow, where such a flow is inevitably characterized by a chaotic repeller-attractor pair in the phase space. I relate the overall time-averaged contraction of such a phase-space flow to the corresponding Lyapunov spectrum, which is in turn directly related to the time-rate-of-change of Gibbs' entropy, and to its dependence on the "grain size" of a coarse-grained approach. In Sec. III, I briefly consider the dependence of Gibbs' equilibrium entropy on the physical units, the grain size, and the boundary conditions, setting the stage for detailed nonequilibrium calculations. In Sec. IV, I describe general relationships between isomorphic pairs of solutions to the motion equations, one solution thermostatted and the other not. In Sec. V, I illustrate compressible phase-space flow for the simplest relevant example, a harmonic oscillator, either damped, or subject to an equivalent time-dependent force. In Sec. VI, I recall the properties of the "Galton Board" problem, a particle

scattered by a regular lattice, in the presence of an accelerating field. For this problem, I display the grain-size dependence of Gibbs' entropy. In Sec. VII, I summarize our present understanding of Liouville's theorems, and entropy, for nonequilibrium states.

II. TIME-REVERSIBLE HEAT FLOW IN PHASE SPACE

Hamilton's motion equations can describe isolated systems as well as systems confined by time-dependent, but velocity-independent, potentials. Although they can be implemented in any set of generalized coordinates $\{q, p\}$, it is usually convenient to choose Cartesian coordinates, with the Hamiltonian a separable sum of potential and kinetic parts,

$$H(\{q, p\}) = \Phi(\{q\}) + K(\{p\}) \\ \rightarrow \{\dot{q} = p/m; \dot{p} = F(\{q\})\}.$$

The choice of coordinates can affect no physical properties of such a system.

To describe thermally "open" systems, interacting with sources or sinks of heat, additional velocity-dependent accelerations are necessary. Accordingly, those particles interacting with external heat sources or sinks are affected by corresponding "thermostat forces." The simplest such forces are deterministic and time reversible. When the additional velocity-dependent thermostat forces are obtained from mechanical variational principles, such as Gauss' principle of least constraint or Hamilton's principle of least action, they typically involve a Lagrange multiplier, ζ , are linear in the momenta, and retain the property of time reversibility, with the equations of motion having the form:^{2,3,18}

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

These time-reversible "thermostatted" motion equations do not follow from a Hamiltonian. With them, it is still usual, but not necessary, to choose Cartesian coordinates and momenta for the $\{q, p\}$. The additional Lagrange multiplier, or "friction coefficient," ζ , imposes a thermal constraint on the selected degrees of freedom in such a way as to preserve the overall time reversibility of the system of equations with both ζ and the $\{p\}$ changing sign along a time-reversed trajectory segment.

It is sometimes desirable—steady heat flow is one example—to use two or more friction coefficients to impose separate kinetic temperatures on separate sets of degrees of freedom. In the absence of sources or sinks of probability, whether or not such thermal constraints are present, it is evident that the local comoving phase-space probability, $f(\{q(t), p(t)\}) \otimes$ [where \otimes is an infinitesimal comoving and corotating volume element, $\Pi dq dp$, centered on a trajectory] must be conserved by the flow. It follows that the change in a differentiable probability density, f , at any fixed phase-space location $\{q, p\}$, is given by the divergence of the local flux:

$$\partial f / \partial t = - \sum [\partial(\dot{q}f(\{q, p\}) / \partial q \\ + \partial(\dot{p}f(\{q, p\}) / \partial p].$$

This form of Liouville's theorem, which applies to both cases, compressible and incompressible, is simply the "Eulerian" (laboratory-frame) form of Euler's continuity equation, which has to be obeyed by any differentiable density of a conserved quantity (usually these are the mass, momentum, and energy densities). It is more usual to consider the "Lagrangian" (comoving-frame) form of the time dependence of f , $df/dt \equiv \dot{f}$. This is the time dependence following the flow:

$$\dot{f} \equiv \partial f / \partial t + \sum [\dot{q}(\partial f / \partial q) + \dot{p}(\partial f / \partial p)]$$

$$= -f \sum [(\partial \dot{q} / \partial q) + (\partial \dot{p} / \partial p)]$$

$$\rightarrow d \ln f / dt = -d \ln \otimes / dt$$

$$\equiv - \sum [(\partial \dot{q} / \partial q) + (\partial \dot{p} / \partial p)].$$

This form too applies to both cases, compressible and incompressible. With Hamilton's equations of motion each of the terms $(\partial \dot{q} / \partial q) + (\partial \dot{p} / \partial p)$ vanishes, giving the more familiar incompressible Liouville's theorem: $\dot{f} = 0$; otherwise we have the more general result: $\dot{f} \neq 0$. In the presence of deterministic thermostating forces $-\zeta p$, f changes with time in a definite way:

$$\dot{f} = -f \sum (\partial \dot{p} / \partial p) \equiv f \sum [\partial(\zeta p) / \partial p] \approx f \sum \zeta.$$

The last approximate equality follows because the dependence of ζ on $\{p\}$ is typically weak, of order $1/N$ for an N -body system.^{2,3}

Evidently positive dissipative friction leads to divergence of $\langle \ln f \rangle \sim +t$ and the consequent vanishing of the comoving phase volume $\ln \otimes \sim -t$. Negative friction would cause f to vanish, and \otimes to diverge, with $\langle \ln f \rangle \sim -t$. It is clear that only the former possibility, increasing f : $\langle \dot{f} \rangle > 0$ and decreasing \otimes : $\langle \dot{\otimes} \rangle < 0$, is consistent with a bounded phase-space volume. This observation is the mechanical analog of the Second law of thermodynamics.^{9,10} Time averages are required by the presence of microscopic fluctuations.

We see that a superficially small change in the dynamics, just adding time-reversible friction, actually induces a qualitative change in the resulting phase-space distribution as well as a (time-averaged) one-way "arrow of time," with $\langle \ln f \rangle \rightarrow \infty$.^{9,10} The qualitative difference between incompressible and compressible phase-space flows was clearly emphasized by Ramshaw,¹⁵ who built on Andrey's work,¹³ but did not discuss the crucial property of time reversibility. Necessarily, something dramatic happens in the case, typical for nonequilibrium steady states, that $\langle \ln f \rangle$ diverges. This is the formation of a fractal phase-space object, a "strange attractor." In the nonequilibrium steady state, $\langle f \rangle$ becomes a multifractal attractor, with a density which is everywhere singular, and with a dynamics which is both "chaotic" (long-time expo-

nential separation of nearby trajectories) and “attractive,” converging onto an object with information dimension strictly less than that of the equilibrium distribution.^{9,10} In a variety of example problems, one of which¹⁹ is worked out in detail in Sec. V, the fractal structure can be verified by computing the cell-size dependence of the local cell measures $\{\mu\}$, giving the coarse-grained entropy,

$$S_{CG} \left(\prod \Delta q \Delta p \right) / k = - \sum \mu \ln \mu;$$

$$\mu \equiv f_{cell} \prod \Delta q \Delta p \rightarrow \sum \mu = 1,$$

on the phase-space cell size, $\prod \Delta q \Delta p$.²⁰ If, as is usual and also useful, the equations of motion are time reversible, the time-reversed forward trajectory must correspond to a topologically similar mirror-image ($\{+p\} \rightarrow \{-p\}$) “repellor” structure corresponding to the past:

$$f_A(\{q, +p, +t\}) \Leftrightarrow f_R(\{q, -p, -t\}).$$

The attractor, rather than the repellor, is actually observed in any numerical solution because the flow in its vicinity is more stable than that near the repellor.

Flow stability can be quantified through the Lyapunov exponents, $\{\lambda\}$, which describe the rates of increase (or decrease) of trajectory separations parallel to the principal axes of a corotating hypersphere centered on a system trajectory. Worked-out examples show that the individual instantaneous exponents depend upon the choice of generalized coordinates,²¹ while the instantaneous sum, $\sum \lambda \equiv d \ln \mathcal{O}/dt \equiv -d \ln f/dt$, which is directly related to probability, and hence to a Poincaré invariant, does not.

An alternative method for imposing boundary conditions, so as to simulate nonequilibrium systems, is stochastic.^{4,22–25} Then, velocities for particles reaching a stochastic boundary are chosen from the corresponding one-sided Maxwell–Boltzmann distribution. This choice introduces discontinuities into the particle trajectories, making a Lyapunov analysis difficult, and making use of Liouville’s theorem at the least difficult, and perhaps impossible. Because physical phenomena ought not to depend upon the boundary details for large systems, this situation seems paradoxical. It is likely a case of nonuniform convergence, with the fractal distributions characteristic of deterministic thermostats emerging as large-system limits when stochastic boundaries are used.^{24,26}

III. GIBBS’ ENTROPY FROM THE DISTRIBUTION FUNCTION

It is important to emphasize that the catastrophic divergence of Gibbs’ entropy, associated with nonequilibrium steady states, occurs completely independently of the mild inconvenience associated with the necessary choice of either an absolute or a relative entropy scale. The entropy computed from the probability density $\langle f \rangle$ corresponds, at equilibrium, to the thermodynamic entropy, according to Gibbs. Because f is independent of the particular choice of coordinates $\{q\}$, this equilibrium entropy can only depend, logarithmically, upon the units of action. It is usual to appeal to

Bohr’s correspondence principle, making f dimensionless by dividing by Planck’s constant, h , for each degree of freedom. Otherwise, a change from centimeter-gram-second (cgs) to meter-kilogram-second (mks) units, for instance, would change the energy scale, and the probability density, by a factor of 10^7 , causing a decrease in S of $7k \ln 10$ per degree of freedom. A wholly classical alternative is to measure entropy relative to that of a corresponding ideal gas:

$$\Delta S = k[\ln(f_{ideal}/f_{real})].$$

In a mixing system it is expected that the probability density will eventually approach all allowed points of the phase space arbitrarily closely. Thus a time averaging, or an instantaneous average over fixed phase-space cells, can give the equilibrium distribution. The expanding-gas example, discussed in Sec. I, illustrates this possibility. On the other hand, the very definition of a fractal, a distribution in which the density varies as a power law in the vicinity of each point, suggests that the corresponding Gibbs’ entropy would depend upon cell size. An example confirming this expectation is worked out in Sec. VI.

IV. ISOMORPHISMS LINKING THERMOSTATED AND ADIABATIC SYSTEMS

Although the difference between conservative Hamiltonian mechanics and reversibly thermostated nonequilibrium mechanics is qualitative, it is possible to find particular many-body trajectories which can be described by either mechanics. Thus, these pairs of special trajectories are isomorphs, the same with or without thermostats. In the thermostated case the occupied phase space neither shrinks nor grows as time goes on. The process is steady, with all segments of the trajectory equally likely. On the other hand, the phase space of a system driven strongly from equilibrium can grow without limit, by virtue of an ever-increasing energy.

By using an external driving field and impulsive hard-particle forces, ensembles of pairs of isomorphic trajectories can be generated.^{27,28} Not just any driving will do. Any fixed strength for the driving forces would eventually lead to a high-temperature equilibrium. On the other hand, a driving which increases sufficiently rapidly with time, or in space, can be chosen to maintain a fixed ratio of the driving and inertial forces, resulting in a stationary nonequilibrium state.

An example of the isomorphic pairs of trajectories can be based on the Galton board problem, discussed in more detail for conventional equilibrium and thermostated simulations in Sec. V. The conventional Galton board contains a particle accelerated, in the x direction, by a constant external field, E . With impulsive hard-particle forces, the equations of motion between collisions,

$$\dot{x} = p_x/m; \dot{p}_x = E; \dot{y} = p_y/m; \dot{p}_y = 0,$$

lead to curved trajectories, with

$$\begin{aligned}
 d^2x/dy^2 &= (d/dy)(p_x/p_y) \\
 &= (m/p_y)(d/dt)(p_x/p_y) \\
 &= (m/p_y^3)[(p_y\dot{p}_x) - (p_x\dot{p}_y)] = mE/p_y^2.
 \end{aligned}$$

For simplicity, choose a constant-energy solution of these equations with a vanishing initial energy, $K + \Phi = p^2/2m - Ex = 0$. Then, the curvature of the trajectory depends upon the ratio of the driving force, $\dot{p}_x = -d\Phi/dx$, to the kinetic energy, which is in turn the negative of the field energy, $p^2/2m = -\Phi = Ex$. Thus an exponential field leads to a steady-state trajectory $y(x)$ with stationary curvature fluctuations. Exactly the same trajectory results if the dynamics is carried out, not at constant energy but with the kinetic energy constrained to its initial value, by a varying time-reversible friction force $-\zeta p$:

$$\begin{aligned}
 \dot{x} &= p_x/m; \dot{y} = p_y/m; \dot{p}_x = F_x + E - \zeta p_x; \\
 \dot{p}_y &= F_y - \zeta p_y; \zeta \equiv (F \cdot p + Ep_x)/p^2.
 \end{aligned}$$

Exactly similar isomorphic pairs of many-body trajectories can be constructed for (i) driven systems without thermostats, and (ii) nonequilibrium thermostatted systems with dissipative mass, momentum, or energy flows.²⁷ Thus, the dissipative fractal phase-space structures can apply with or without thermostating forces. An example, based on the Galton board problem,^{19,26,29} is described in Sec. VI.

V. EXAMPLE: THE DAMPED HARMONIC OSCILLATOR

Let us examine Liouville's \dot{f} theorems in detail for a simple example. Consider a critically damped harmonic oscillator with unit mass and force constant and initial coordinate q_0 and momentum p_0 . The equations of motion,

$$\dot{q} = p; \dot{p} = -q - 2p,$$

have the solution $q = [q_0 + (q_0 + p_0)t]e^{-t}$. In Fig. 1 I consider the special case in which the initial conditions are $\{q_0, p_0\} = \{1, 1\}$:

$$q = (2t + 1)e^{-t}; p \equiv \dot{q} = (1 - 2t)e^{-t};$$

$$\ddot{q} = (2t - 3)e^{-t} = -q - 2\dot{q} = -q - 2p = -q + (4t - 2)e^{-t}.$$

Liouville's compressible $\dot{f} \neq 0$ theorem shows that the comoving phase-space probability density diverges exponentially in time: $f(q, p, t)/f(1, 1, 0) = e^{+2t}$. The corresponding comoving phase volume vanishes: $\otimes(q, p, t)/\otimes(1, 1, 0) = e^{-2t}$. Remarkably, the same trajectory is also the solution of the undamped, but driven, oscillator motion equations:

$$\dot{q} = p; \dot{p} = \ddot{q} = -q + F(t); F(t) = (4t - 2)e^{-t},$$

where the external force $F(t)$ has been chosen to reproduce the damped trajectory without using a velocity-dependent force. Now, Liouville's incompressible theorem applies. Figure 1 confirms that the latter equations of motion show none of the dissipation of the former, although the two sets have a common solution.

This example indicates the impossibility of directly determining Lyapunov exponents from a single trajectory, as

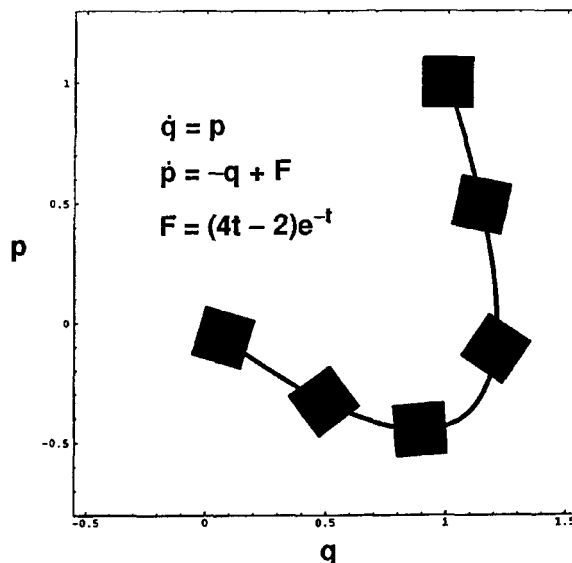


FIG. 1. Motion of an ensemble of harmonic oscillators obeying Liouville's $\dot{f}=0$ theorem. The initial ensemble, a square centered on $(x \equiv q_0 = 1, \dot{q} \equiv p_0 = 1)$, eventually circles the origin. Snapshots are shown at $\{t\} = \{0.0, 0.2, 0.6, 1.5, 2.5, 5.0\}$. Only the trajectory at the center of the comoving square phase volume (heavy line) is critically damped by the force $F(t)$. See Ref. 2.

was stressed by Farmer *et al.*²⁰ It also illustrates the utility of the exponents in describing phase-space compressibility. With a frictional force the two exponents are both -1 and the flow is compressible. With a time-dependent driving force the two exponents both vanish and the flow is incompressible. This instructive analysis of the harmonic oscillator cannot easily be extended to nonlinear chaotic systems. For these, numerical calculations are required. Let us turn next to the simplest chaotic example.

VI. EXAMPLE: THE GALTON BOARD

The equilibrium Galton board describes the field-free scattering of a particle by a fixed array of scatterers.^{19,26,27,29} Figure 2 shows collisions resulting when the scatterers make up a regular triangular lattice of hard disks. The successive collisions undergone by a scattering particle, a moving mass point, can be described by the two angles, $\{\alpha, \beta\}$. α gives the location of a collision relative to the field direction, while β gives the direction of the outgoing velocity relative to the radius vector, at each collision. In the equilibrium case, with no driving field, all collisions $\{\alpha, \sin\beta\}$ are equally likely, and, because the dynamics is mixing, the coverage in the Poincaré plane tabulating these collisions is uniform. Although the motion obeys Liouville's $\dot{f}=0$ theorem, the coarse-grained entropy, shown as the series of dots parallel to the abscissa in Fig. 3, is essentially independent of cell size. The distribution of 3 000 000 successive collisions is essentially uniform, as the number of phase-space cells is increased from 1 to 65 536, as is indicated in Fig. 3.

Consider next a nonequilibrium finite-field sequence of 3 000 000 collisions generated with isokinetic thermostat

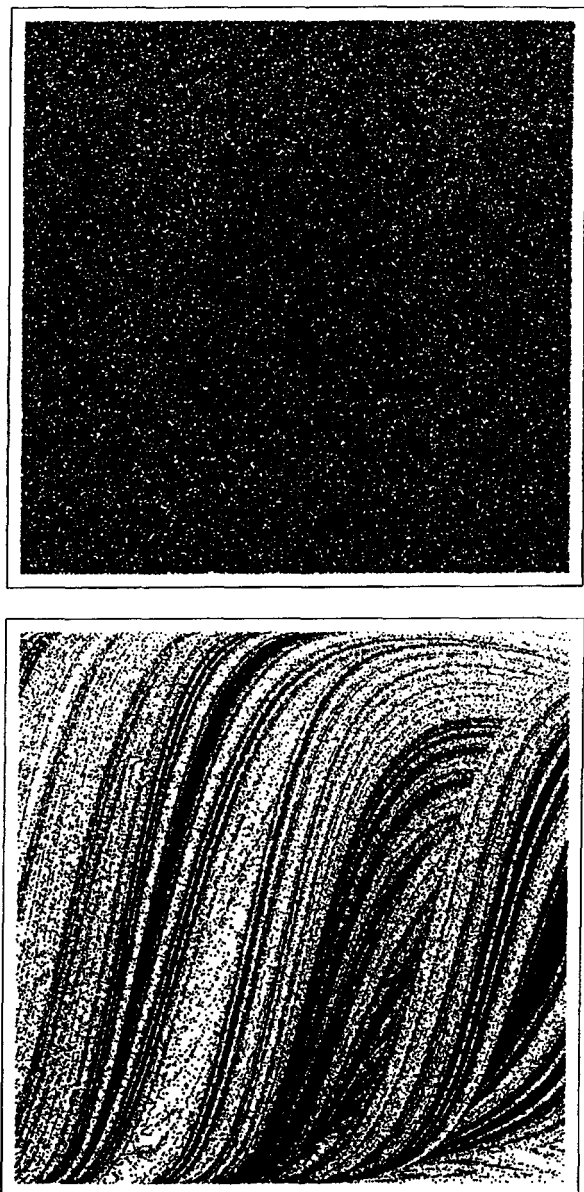


FIG. 2. Collision sequences for the isoenergetic and isokinetic motions of a mass-point particle in a "Galton board." The sequences are sets of the collisional functions, $\{0 < \alpha < \pi, -1 < \sin \beta < +1\}$. The two cases illustrated correspond to driving fields of 0 (isoenergetic) and $3p^2/m\sigma$ (isokinetic), both at four-fifths the close-packed scatterer density. The scatterers are disks of diameter σ and 300 000 collisions are shown. The isokinetic sequence of collisions could also be obtained without friction or constraints, by using an exponentially increasing field. See W. G. Hoover, B. Moran, C. G. Hoover, and W. J. Evans, Phys. Lett. A 133, 114 (1988).

forces, which constrain the kinetic energy, providing a multifractal phase-space structure with an entropy which varies with the logarithm of the cell size. 300 000 points, in a Poincaré section through the multifractal structure, are shown in Fig. 2. Now Liouville's compressible theorem applies. This section produces a Gibbs' entropy with an essential dependence on the cell size (see Fig. 3). The slope indicates that $\langle \ln(f/f_{\text{ideal}}) \rangle$ varies as $0.15 \ln(1/\epsilon)$, where ϵ is the cell width.

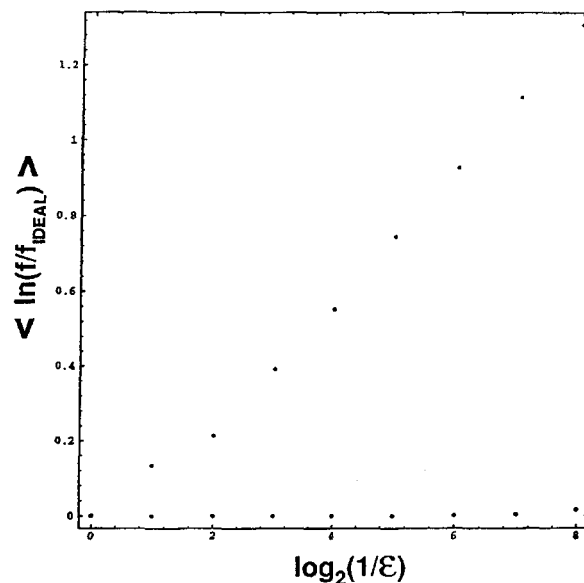


FIG. 3. Cell-size dependence of the coarse-grained distribution function for collision sequences ten times the length of those shown in Fig. 2. The Poincaré sections of Fig. 2 have been divided into ϵ^{-2} cells, with $\epsilon = 1, 0.5, 0.25, 0.125, \dots$. The coarse-grained value of $\langle \ln(f/f_{\text{ideal}}) \rangle$, where f_{ideal} is the uniform distribution, is plotted as a function of $\log_2(1/\epsilon)$.

This example shows that coarse graining does not cure the diverging entropy which inevitably accompanies deterministic chaos away from equilibrium. These same trajectories also result from a special time-dependent field, and then obey Liouville's incompressible theorem.

Breyman *et al.* have rightly emphasized that the derivatives of coarse-grained entropy, with respect to external variables, can be useful even when the entropy itself is not. Likewise, in dealing with systems open to mass flow, the division of entropy change into separate convective and comoving parts can be useful in drawing a correspondence with irreversible thermodynamics.³⁰⁻³²

VII. CONCLUSIONS

Liouville's incompressible flow theorem, $\dot{f}=0$, usually applied to equilibrium systems, is better known than the nonequilibrium compressible theorem, $\dot{f} = -f \sum \partial \dot{p} / \partial p$. The compressible Liouville theorem usefully links fractal dimensionality, dissipation, and the Lyapunov spectrum for deterministically driven systems, and in a way which simplifies theoretical analysis. But Gibbs' entropy, $S = -k \langle \ln f \rangle$, which corresponds, in equilibrium thermodynamics, to the force driving systems toward equilibrium, is a casualty of this analysis. Gibbs' entropy seems to have no fundamental interpretation away from equilibrium, although in some situations derivatives of its coarse-grained analog may be useful. Is there a way to characterize the nonequilibrium fractals so as to form a nonequilibrium potential as useful as the free energies associated with equilibrium states? No one knows.

The singular multifractal nature of thermostatted phase-space distributions is qualitatively different to the smooth nature which one might expect to apply with stochastic

boundaries. Because the number of boundary particles is small and the dimensionality decrease appears to be extensive,³³ it seems likely that the multifractal structure will emerge only gradually. But no one knows for sure. A definitive test would be welcome. Likewise, an experimental or computational technique for the determination of Lyapunov exponents, or a stochastic analog of these exponents from a time series alone, would be welcome. Although formal embedding techniques, using time-delay coordinates, are effective in problems involving only a few variables, a useful computational many-body analog is badly needed, as are also laboratory experiments.

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