10 November 1997

PHYSICS LETTERS A

ELSEVIER

Physics Letters A 235 (1997) 357–362

Multifractals from Hamiltonian many-body molecular dynamics

Wm.G. Hoover

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

Received 30 May 1997; revised manuscript received 3 July 1997; accepted for publication 12 August 1997
Communicated by A.R. Bishop

Abstract

Nonequilibrium simulations with time-reversible thermostats provide multifractal phase-space structures. But alternative stochastic approaches to temperature control rule out such fine-grained structures. Thus, the validity of the fractals has been questioned. I detail here the construction of the fully-Hamiltonian many-body problems which produce fractal structures isomorphic to those of the nonequilibrium simulations. © 1997 Published by Elsevier Science B.V.

About 10 years ago it was established that reversibly-thermostatted nonequilibrium steady states lead to multifractal phase-space structures. Such structures certainly give an appealing mechanical rationale for the second law of thermodynamics [1]. Nevertheless, as has been emphasized recently [2,3], the source of the fractal structures raises a question: "Do the fractals correctly represent the rarity of nonequilibrium states, or are they artifacts of particular time-reversible thermostatting techniques?" This very basic question was discussed at length recently [2], but no definite conclusion was reached. Here I construct two simple Hamiltonian many-body example problems, closely related to conventional field-driven "color conductivity" simulations [4], but with accelerating fields which vary with time. These examples, like their relatives for shear and heat flows, turn out to generate exactly the same fractal phase-space structures as do corresponding thermostatted nonequilibrium systems with constant accelerating fields. Thus the fractals describing many-body nonequilibrium thermostatted systems have identical twins, which can be generated by Hamiltonian systems with time-dependent external fields.

In what follows, I distinguish between thermostatted mechanics and conventional adiabatic Hamiltonian mechanics, citing both one-body and many-body examples of each. The two kinds of mechanics can be linked together. The many-body mass-flow example, emphasized here, has its conceptual roots in the one-body Galton board or Lorentz gas problem [5,6]. That one-body problem led first to the discovery of the multifractal phase-space structures and later to an analytical proof [6] confirming the results of the numerical investigations.

Analyses of the two-dimensional Galton board problem [5–8], the motion of a single particle moving in a triangular lattice of scatterers and accelerated by a constant external field, E_0, can lead to fractal phase-space structures for two kinds of thermostatted mechanics: (i) time-reversible isokinetic mechanics, or (ii) irreversible dissipative mechanics. Both one-body scattering problems include a friction coefficient ζ, and lead to exactly the same motion equation,

PII S0375-9601(97)00665-8

$$\dot{p} = F + E_0 - \zeta p .$$

Here F represents the force due to the scatterers and E_0 is the field strength. In discussing particular example problems I arbitrarily choose the accelerating field to lie in the x direction.

In the time-reversible isokinetic case, the friction coefficient varies with time. It is chosen so as to keep the moving particle's kinetic energy constant,

$$\zeta(t) \equiv (F \cdot p + E_0 \cdot p)/p^2 \Rightarrow \dot{K} = \dot{p} \cdot (p/m) = 0 .$$

$K = K_0$ is the kinetic energy of the moving particle. In the irreversible case, with a constant friction coefficient, ζ_0, the kinetic energy $K(t)$ fluctuates about its long-time average value. The multifractal phase-space structures which result, from either of the two types of dissipative one-body dynamical problems, time-reversible [5] or not [7], can be visualized easily. The structures correspond to sequences of scatterer collisions. The geometry of each such collision provides a single point located in a two- or three-dimensional "Poincaré section" of the one-body phase space [5]. The multifractal structures found in these sections evidently arise as consequences of long-time correlations induced by the accelerating field. These correlations emphasize phase-space states which have zero measure at equilibrium. It is in this sense that nonequilibrium states are relatively rare, even for such a one-body problem.

On the other hand, any long-time or long-distance correlations in many-body systems can be disrupted by adding noise at stochastic system boundaries [9]. It has been stated that stochastic boundary conditions inevitably lead to a continuous phase-space distribution [2]. It is certainly hopeless to try to visualize directly the topology of many-body phase-space distributions, so as to study their continuity. Nevertheless, it is possible to make accurate, but indirect, estimates of their fractal dimensions through analyses of the Lyapunov spectra. The Lyapunov exponents, $\{\lambda\}$, with $\lambda_i \geqslant \lambda_{i+1}$, which describe the orthogonal growth and decay rates of phase-space objects, can be used to locate the dimensional borderline separating objects which grow from objects which shrink. The borderline dimensionality, the "information dimension" is directly accessible from the spectra. It is simply the number of terms in the partial sum of exponents, $\sum' \lambda_i$, at which the sign of the sum changes from positive to negative.

Determinations of Lyapunov spectra for stationary nonequilibrium thermostatted systems, with up to 100 particles, strongly suggest a fractal dimensionality loss (the number of missing terms at the sign change of $\sum' \lambda_1$) which is "extensive", proportional to the number of particles, in the large-system limit [10]. The fractal structure of the distribution, revealed by these Lyapunov studies, is fundamentally important for statistical mechanics because it rules out the use of analytic expansions about the linear-response limit and likewise prohibits the use of Gibbs' entropies away from equilibrium. Such strong conclusions require support, based on simple examples, which can clarify the generality of the fractal structures away from equilibrium.

"Color conductivity" is the simplest example of a homogeneous nonequilibrium many-body problem [4]. It is a many-body model for mass currents driven by an external field. In the usual case, half the otherwise identical particles are driven to the right, and the remainder are driven to the left, by a fixed external field E_0. In the usual nonequilibrium simulations, a thermostatting force, $-\zeta p$, is added to the equations of motion to induce a stationary nonequilibrium state. For small fields it is possible to show that this procedure leads to a conductivity, $\kappa = \langle \pm v \rangle / E_0$, consistent with Green and Kubo's linear-response theory. For computations, it is simplest to imagine that the moving particles are hard disks, or spheres, because then the overall dynamics scales simply with temperature. Doubling all the particle velocities, and quadrupling the field strength, leaves the resulting trajectories $\{y(x)\}$ unchanged despite a fourfold increase in temperature. Members of a colliding pair of particles simply exchange relative radial momenta at the instant of their collision.

It is well established, when such a problem is thermostatted [11,12], that the phase-space distribution has a fractal information dimension linked to the Lyapunov spectrum, $\{\lambda\}$, as explained above. In addition, the complete sum of exponents is related to the external entropy production, $\dot{S}$, as well as to the time-averaged rate of divergence of the phase-space distribution function, $\mathrm{d}\ln f/\mathrm{d}t$,

$$-\sum \lambda_i = \dot{S}/k = \langle \mathrm{d}\ln f/\mathrm{d}t \rangle .$$

The Lyapunov exponents describe the time-averaged growth, or shrinkage, rates of the principal axes of a comoving, co-rotating ellipsoid centered on a typical phase-space trajectory [13]. The information dimension of the resulting fractal structure lies below that of the equilibrium distribution function by the "dimensionality loss" $\Delta D \simeq \dot{S}/k\lambda_1$, where λ_1 is the largest of the Lyapunov exponents. This relation becomes exact in the linear-response limit. Recent theoretical and numerical work has made these exponents accessible for hard disks and spheres [14,15].

It was already pointed out that the trajectories generated by the one-body Galton board problem coincide with those from the Hamiltonian dynamics of a particle in an exponentially-varying field, $\ln E(x) \sim x$ [8,16,17]. That is, the $y(x)$ trajectory of a conventional Hamiltonian particle moving in a conservative, but nonlinear, exponential field is isomorphic to a corresponding trajectory for an isokinetic thermostatted particle moving in a constant field E_0. Analogous many-body results, but with the spatial dependence, $E(x)$, replaced by a special time dependence, $E(K)$ or $E(t)$, can be established, as I show here. For small finite systems this dependence is relatively complicated. But it is plausible that it simplifies in the large-system limit, where fluctuations can be ignored. I have verified the corresponding trajectory isomorphisms for small systems and short times by carrying out detailed trajectory calculations, for both nonequilibrium mass currents and for the corresponding shear flows. A simple example calculation is described in more detail in the Appendix. Longer many-body simulations are under study by Oyeon Kum.

In the many-body case, Hamiltonian motion with a time-dependent "scaled" field, which depends explicitly on the kinetic energy, $E(K) \propto K(t)$, provides many-body trajectories isomorphic to those from isokinetic thermostatted many-body mechanics with fixed values of E_0 and K_0. See Table 1, where three related simulation types are compared. It is plausible that fluctuations can be ignored in the large-system limit. If this is so, the field's precise fluctuating dependence on the kinetic energy $K(t)$ can be replaced by the simpler analytic time dependence which follows from hydrodynamics,

$$E(K)/E_0 \doteq E(t)/E_0 \equiv (1 - t/\tau_0)^{-2}.$$

In the derivation of this relationship, given below, the relaxation time τ_0 is given a physical interpretation. It corresponds to the time required to extract an energy of order NkT_0 from a fixed external field E_0. A simple hydrodynamic analysis suggests that this time is sufficient for the logarithmic divergence of the number of collisions per particle.

Table 1
Three types of time-reversible color conductivity simulation compared. For them, the time dependencies of the field E and kinetic energy K are indicated, as is also the time-rate-of change of the phase-space density. The trajectories for the first two approaches are identical

Type	E	K	$\mathrm{d}\ln f/\mathrm{d}t$
isokinetic	E_0	K_0	$+2N\zeta(t)$
scaled field	$E_0[K(t)/K_0]$	$K(t)$	$-(E_0/K_0)\sum \pm(p_x/m)$
adiabatic	$E(t)$	$K(t)$	0

The estimated large-system hydrodynamic form just given for the time-dependent field, $E(t)$, suggests that the multifractal nature of nonequilibrium many-body phase-space distributions is not at all an artifact of the thermostatting procedure. Rather, it suggests that the structures seen in isokinetic simulations, which are identical to those generated with a field $E(K)$, can also be generated with conventional Hamiltonian mechanics, using $E(t)$. I sketch a proof of the trajectory isomorphism linking the isokinetic and scaled-field dynamics here. A numerical illustration appears in the Appendix.

The trajectory of a thermostatted hard disk or sphere is a sequence of curved arcs [5], punctuated by impulsive collisions. For hard disks or spheres the collision process is not affected by the field, so that it is sufficient to consider the streaming motion, between collisions, which is that of a system of mass points, thermostatted and subject to an external field, but free of other accelerations. The motion of such a set of particles follows trajectories *identical* to those found for the adiabatic Hamiltonian motion of unconstrained particles in a particular time-dependent scaled field, $E(K)$, thermostatted (1) and scaled field (2) in the present case, can most easily be shown to be identical by considering the curvatures of the individual particle trajectories. The trajectory slopes,

$$\{\mathrm{d}y/\mathrm{d}x \equiv p_y/p_x\},$$

vary along the particle's trajectories, as follows,

$$\{d^2y/dx^2 \equiv (d/dx)(p_y/p_x)$$
$$\equiv (1/\dot{x})(d/dt)(p_y/p_x)$$
$$= m(p_x\dot{p}_y - p_y\dot{p}_x)/p_x^3\}\,.$$

In the isokinetic case, (1), with a fixed field E_0, we find

$$\{d^2y/dx^2 = -mE_0p_y/p_x^3 = -(mE/p_x^2)\,dy/dx\}\,.$$

Thus, if an *adiabatic time-dependent* field $E(t)_{\text{adiabatic}} \equiv E(K)$ were chosen to be proportional to the total many-body kinetic energy, *exactly the same* individual particle trajectories would follow from the resulting adiabatic Hamiltonian mechanics. Hence, the corresponding many-body phase-space trajectories are isomorphic in configuration space, though they are traversed at different rates. It is remarkable that the thermostat forces make no contribution whatsoever to the curvatures $\{d^2y/dx^2\}$. This is a consequence of the fact that the constraint forces act parallel to the unconstrained trajectory directions.

Similar isomorphisms apply to shear flows, generated with Doll's or Sllod's algorithms, and to heat flows, generated using the Evans–Gillan algorithm [12]. In all three cases the adiabatic system energy increases with time as $(1-t/\tau_0)^{-2}$. The external field driving the current likewise varies as $(1 - t/\tau_0)^{-n}$, where n is 2 for a mass flow, 1 for a shear flow, and 0 for heat flow, all in the large-system limit, where fluctuations can be ignored.

The argument leading to these results is simplest to check for mass flow. Select initial velocities for a system of point particles and advance them forward in time, with fixed kinetic energy K_0, and fixed field E_0, according to the collisionless, but thermostatted, motion equations,

$$\{\dot{x} = p_x/m; \dot{y} = p_y/m; \dot{p}_x = \pm E_0 - \zeta p_x, \dot{p}_y = -\zeta p_y\}\,,$$
$$\zeta = \sum \pm E_0p_x \Big/ \sum p^2 \Rightarrow K \equiv K_0\,.$$

Then, set $dt = -dt$ and integrate the following adiabatic motion equations, which incorporate the kinetic-energy scaling of the field mentioned above, (backward) in time,

$$\{\dot{x} = p_x/m; \dot{y} = p_y/m; \dot{p}_x = \pm E(t); \dot{p}_y = 0\},$$
$$E(t) \equiv E_0K(t)/K_0\,.$$

Exactly the same $\{x, y\}$ trajectories are traced out, but in the reverse direction. Though we have here considered a field which responds deterministically to the kinetic energy, a simpler dependence, ignoring fluctuations, should apply as the system size is increased. In that case, the system energy should increase with time, due to the work done by the external field, in accordance with hydrodynamics,

$$N(D/2)k\dot{T} = E\sum \pm(p_x/m) \propto N\kappa E^2 \propto NT^{3/2}$$
$$\Rightarrow T/T_0 = E/E_0 = (1 - t/\tau_0)^{-2}\,.$$

Because the D-dimensional hard-particle conductivity κ varies as $T^{1/2}$, the characteristic time τ_0 is $DkT_0/\kappa_0E_0^2$. This limiting large-system case, with fluctuations ignored, should also correspond to a special irreversible *dissipative* dynamics, generated with a constant field E_0 and a constant friction coefficient ζ_0.

We see that pairs of isomorphic many-body trajectories can be correlated by a "time scaling", which links their underlying dynamics. The trajectory pairs considered here link steady-state isothermal and scaled-field evolutions, $0 < t < \infty$, to limiting large-system adiabatic evolutions with $0 < t_{\text{adiabatic}} < \tau_0$. These correlations are reminiscent of Nosé's use of time scaling to introduce temperature into Hamiltonian mechanics [18].

It is clear, because their thermostat contributions likewise have no effect on the trajectory curvatures, that shear flows and heat flows can be analyzed in much the same way. In the shear-flow case the strain rate $\dot{\epsilon} \equiv du_x/dy$ must vary as the square root of the kinetic energy to maintain an exact isomorphism. The heat-flow case is actually the simplest of the three types of transport, because the special Evans–Gillan field, which drives the heat flow, must be independent of kinetic energy, and so, independent of time, for isomorphic trajectories. In every case the large-system hydrodynamic time-dependence of the temperature has the same form, $\propto (1 - t/\tau_0)^{-2}$, with the system undergoing an infinite number of collisions per particle in a finite time τ_0.

The fundamental conclusion of this work is that the thermostatted nonequilibrium trajectories, as well as the multifractal distributions that they generate, are by no means unusual, at least for hard disks and spheres. The trajectories are in fact *identical* to trajectories

es are traced out, but
ve have here consid-
erministically to the
nce, ignoring fluctu-
m size is increased.
should increase with
he external field, in

$N\kappa E^2 \propto NT^{3/2}$

-2.

ard-particle conduc-
acteristic time τ_0 is
e-system case, with
correspond to a spe-
nics, generated with
nt friction coefficient

many-body trajecto-
scaling", which links
trajectory pairs con-
othermal and scaled-
imiting large-system
$_{\text{adiabatic}} < \tau_0$. These
sé's use of time scal-
to Hamiltonian me-

mostat contributions
rajectory curvatures,
can be analyzed in
-flow case the strain
e square root of the
ct isomorphism. The
implest of the three
pecial Evans–Gillan
, must be indepen-
ndependent of time,
very case the large-
dence of the temper-
$- t/\tau_0)^{-2}$, with the
nber of collisions per

this work is that the
jectories, as well as
hey generate, are by
d disks and spheres.
ical to trajectories

which can be generated with special adiabatic mechanics, when the mechanics includes external fields which generate mass, momentum, and energy currents. In the large-system limit, when fluctuations can be ignored, the isokinetic, scaled-field, and adiabatic mechanics should all generate similar phase-space distributions.

The careful reader may wonder how the fractal nature of the distribution could be consistent with Liouville's theorem, $\mathrm{d}\ln f/\mathrm{d}t \equiv 0$, which surely applies to the adiabatic cases. See Table 1. The explanation is simple. Though the *spatial* distribution becomes necessarily more and more localized as time goes on, the *momentum* distribution becomes correspondingly unbounded, just as is required to conserve overall phase volume. Thus the vanishing entropy of nonequilibrium states relative to equilibrium ones can be described by the continual phase-space shrinkage of "stationary" states, or by the growing unboundedness of the phase-space volume of the corresponding equilibrium adiabatic state.

Appendix

We demonstrate numerically the trajectory isomorphism discussed in the text, for a pair of hard disks in an external field. For two positively colored hard disks, the motion equations are as follows,

$$\{\dot{x} = p_x/m;\ \dot{y} = p_y/m;\ \dot{p}_x = F_x + E_0 - \zeta p_x;$$
$$\dot{p}_y = F_y - \zeta p_y\},$$
$$\zeta = (E_0/K_0)\sum(p_x/m) \quad \text{(isokinetic)};$$
$$\{\dot{x} = p_x/m;\ \dot{y} = p_y/m;\ \dot{p}_x = F_x + E_0(K/K_0);$$
$$\dot{p} = F_y\} \quad \text{(scaled field)}.$$

Here, the forces $\{F_x, F_y\}$ represent the hard-particle collisions. We choose a simple numerical example: the special case with E_0, K_0, the disk mass m, and the disk diameter σ all set equal to unity. The trajectories shown in Fig. 1 include a time-reversible elastic collision linking the velocities of two colliding disks:

$$\{(+1.0, 0.0); (-1.0, 0.0)\}$$
$$\leftrightarrow \{(0.0, -1.0); (0.0, +1.0)\}.$$

The collision occurs just as both disks reach the line $x = y$. Before and after the collision exactly the same curves, $\{y(x)\}$, are traced out, for either of the sets of motion equations just given.

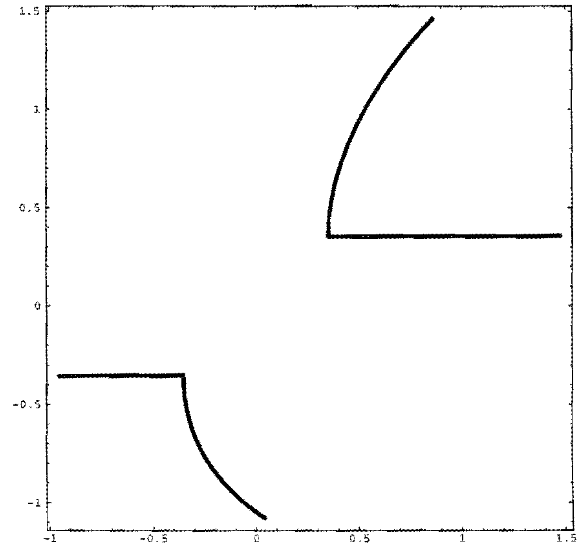

Fig. 1. Time-reversible hard-disk trajectories $\{y(x)\}$ according to both isokinetic and scaled-field dynamics, as is described in the appendix. Both disks have been "colored" so that the field accelerates them to the right. The collision occurs just as the disks reach the line $x = y$.

A number of colleagues have discussed with me the desirability of a many-body multifractal example free of thermostatting. To them, Aurel Bulgac, Brad Holian, Carol Hoover, Dimitri Kusnezov, Joel Lebowitz, Michel Mareschal, and Harald Posch, I extend thanks. I specially thank Christoph Dellago, who provided several valuable comments on the first version of this manuscript. Brad Holian, Carol Hoover, Oyeon Kum, Harold Posch, and Kris Wojiechowski kindly suggested useful clarifications, which are incorporated here. Work at the Lawrence Livermore National Laboratory was performed under the auspices of the University of California, through Department of Energy contract W-7405-eng-48, and was further supported by grants from the Advanced Scientific Computing Initiative and the Accelerated Strategic Computing Initiative.

References

[1] B.L. Holian, W.G. Hoover, H.A. Posch, Phys. Rev. Lett. 59 (1987) 10.
[2] See the discussions in: Microscopic Simulations of Complex Hydrodynamic Phenomena, eds. M. Mareschal, B.L. Holian, NATO ASI Series in Physics 292 (Plenum, New York, 1992).
[3] M. Mareschal, in: Microscopic Simulations of Complex Flows, eds. I. Prigogine, S.A. Rice, Advances in Chemical Physics, Vol. 100 (Wiley, New York, 1997) p. 317.
[4] D.J. Evans, W.G. Hoover, B.H. Failor, B. Moran, A.J.C. Ladd, Phys. Rev. A 28 (1983) 1016.
[5] B. Moran, W.G. Hoover, S. Bestiale, J. Stat. Phys. 48 (1987) 709.
[6] N.I. Chernov, G.L. Eyink, J.L. Lebowitz, Y.G. Sinai, Phys. Rev. Lett. 70 (1993) 2209.
[7] W.G. Hoover, B. Moran, Chaos 2 (1992) 599.
[8] W.G. Hoover, B. Moran, C.G. Hoover, W.J. Evans, Phys. Lett. A 133 (1988) 114.
[9] S. Goldstein, C. Kipnis, N. Ianiro, J. Stat. Phys. 41 (1985) 915.
[10] W.G. Hoover, H.A. Posch, Phys. Rev. E 49 (1994) 1913.
[11] W.G. Hoover, Computational Statistical Mechanics (Elsevier, Amsterdam, 1991).
[12] D.J. Evans, G.P. Morriss, Statistical Mechanics of Nonequilibrium Liquids (Academic Press, New York, 1990).
[13] H.A. Posch, W.G. Hoover, Phys. Rev. A 39 (1989) 2175.
[14] Ch. Dellago, H.A. Posch, W.G. Hoover, Phys. Rev. E 53 (1996) 1485.
[15] H. van Beijeren, J.R. Dorfman, E.G.D. Cohen, H.A. Posch, Ch. Dellago, Phys. Rev. Lett. 77 (1996) 1974.
[16] C.P. Dettmann, G.P. Morriss, Phys. Rev. E 54 (1996) 2495.
[17] C.P. Dettmann, G.P. Morriss, Phys. Rev. E 55 (1997) 3693.
[18] S. Nosé, Prog. Th. Phys. Supl. 103 (1991) 1.