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Multifractals from stochastic many-body molecular dynamics

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Abstract

Nonequilibrium simulations with time-reversible thermostats provide multifractal phase-space structures. Alternative stochastic approaches to thermal boundaries would seem to rule out such fine-grained structures. Here we discuss the meaning of this difference and illustrate a possible resolution of it for a hybrid stochastic-and-deterministic version of the two-dimensional Galton board problem. © 1998 Elsevier Science B.V.

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More than 10 years ago it was established, computationally, that reversibly-thermostatted nonequilibrium steady states lead to multifractal phase-space structures. The relative rarity of nonequilibrium states implied by this fractal structure is consistent with the second law of thermodynamics [1,2]. On the other hand, there are equally long-standing theoretical results suggesting that nonequilibrium steady states give rise to continuous phase-space distributions [3,4]. How could both these results – fractal on the one hand, and continuous on the other – be true? To shed some light on this question we consider here the simplest model which combines chaos with dissipation so as to provide an interesting steady state, the "Galton board". The model is based on the periodic lattice of scatterers which Sir Francis Galton used to study probability densities, beginning in 1873 [5]. In our version of the Galton board, a single moving mass point is accelerated through a periodic two-dimensional triangular-lattice array of scatterers. Nonequilibrium steady states can be achieved for this model by incorporating in it a "thermostat" capable of removing the energy gained from the accelerating field [6–12].

If we choose the x axis parallel to the field direction, and perpendicular to one of the three sets of lines of scatterers, then the conventional Hamiltonian equations of motion for the moving mass point are as follows [6,7],

$$\dot{x} = p_x/m , \quad \dot{y} = p_y/m , \quad \dot{p}_x = F_x + E , \quad \dot{p}_y = F_y .$$

The force F describes the interaction of the moving mass point with the periodic array of hard-disk scatterers and the accelerating field is E. The energy gained from the field can be extracted – so as to obtain a nonequilibrium steady state – by introducing into the equations of motion (i) a frictional force, $-\zeta p$, with either constant [8] or time-reversible [6,7,9] friction

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coefficient ζ, or (ii) inelastic scattering, as described by a coefficient of restitution [10]. Each of these approaches leads to a multifractal phase-space distribution [11,12], as evidenced by numerical analyses of the Poincaré sections describing the collisions.

The information dimension D of such a section can be estimated by dividing the Poincaré section into bins of width ϵ. Then, the limiting small-ϵ bin-size dependence of the probability density f, or, equivalently, the measure μ, gives the information dimension [13,14],

$$D \ln \epsilon \leftarrow \langle \ln \mu_\epsilon \rangle \equiv \sum \mu_\epsilon \ln \mu_\epsilon$$
$$\doteq \int f \ln f \, d\vec{\Gamma}_{\text{Section}} .$$

Thus the information dimension follows from the apparent phase-space probability for occupying a bin of width ϵ and sectional volume $d\vec{\Gamma}_{\text{Section}}$,

$$f_\epsilon \, d\vec{\Gamma}_{\text{Section}} \equiv \mu \propto \epsilon^D .$$

In the isokinetic Galton board, the information dimension so found varies smoothly with the field strength E, decreasing quadratically from the zero-field dimension, $D(0) = 2$, for small fields, and, for larger fields, gives rise to limit cycles, with dimensionality zero in the Poincaré section.

As Lebowitz (see the discussions in Ref. [3]) pointed out to us, Goldstein, Kipnis, and Ianiro [4] have proved that the fine-grained probability density $f_\Gamma \propto \mu$ is continuous for a particular many-body problem with stochastic thermal boundaries. And it is certainly plausible that choosing just the right sequence of "random" velocities at a thermal boundary could lead to any conceivable phase-space configuration. On the other hand, it seems to be usual that a multifractal phase-space distribution requires, for its support, the entire accessible phase-space dimensionality, so that the "embedding dimension" of the multifractal is the same as that at equilibrium, while the "information dimension", discussed further below, is smaller. Such a situation occurs in the case of the isokinetic Galton board [6,7].

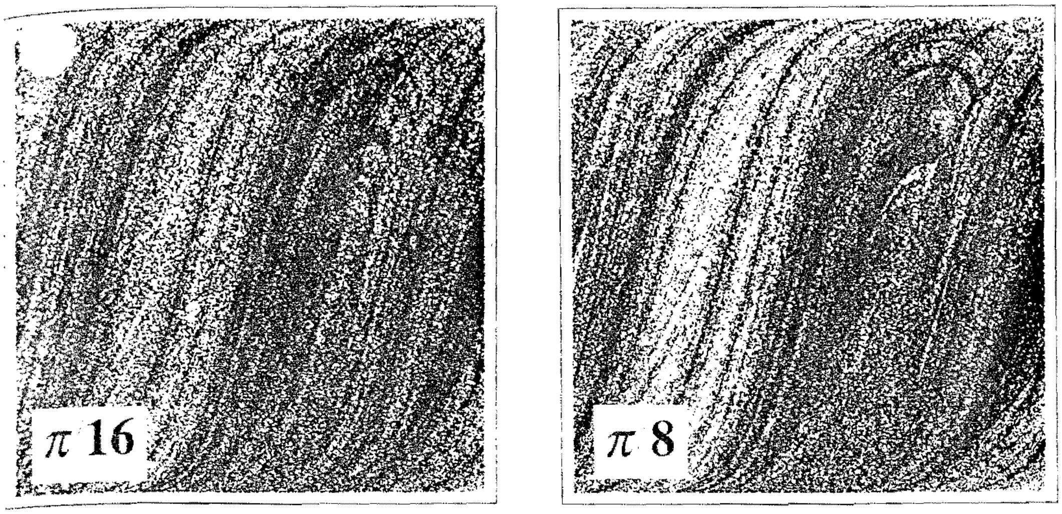
In "isokinetic" Galton board simulations [6,11], the motion is entirely deterministic, but with a (time-reversible) frictional force, $-\zeta p$, added to the equations of motion to keep the kinetic energy constant. This restriction confines the possible collisions to a two-dimensional region. Each collision, between the moving mass point, at r_{point}, and one of the fixed scatterers, at $r_{\text{scatterer}}$, can be characterized by the pair of angles, $\{\alpha, \beta\}$, where α, with $0 < \alpha < \pi$, gives the direction of the vector $r_{\text{ps}} \equiv r_{\text{point}} - r_{\text{scatterer}}$, relative to the field direction, and β, with $-\frac{1}{2}\pi < \beta < \frac{1}{2}\pi$, gives the direction of the point's velocity just after colliding, relative to the same vector r_{ps}.

In systems with "stochastic" boundaries, the motion suffers a discontinuous velocity change at those boundaries: the old particle velocity is replaced by a new one, chosen from a Maxwell-Boltzmann distribution characteristic of the boundary. This is the case for which a theoretical analysis, establishing the continuity of the resulting phase-space distribution for heat conduction, has been completed [4]. To caricature a "stochastic" boundary in the mass flow described by the Galton board problem, we divide the possible hard-disk scattering collisions into two classes: (i) deterministic and elastic for $\alpha_{\min} < \alpha < \pi$, with the radial momentum reflected and the energy conserved, and (ii) "stochastic" for $0 < \alpha < \alpha_{\min}$, with the moving point's post-collisional direction – given by the angle β – random, but with the post-collisional speed for the stochastic collisions a fixed constant, p_0/m. Though the kinetic energy varies in this caricature problem, we continue to use the two-dimensional Poincaré section for displaying the point-scatterer collisions. Such a projection operation would tend to reduce, rather than enhance, any fractal character in the distribution. The projection operation is analogous to combining strictly isokinetic distributions, but with slightly different fields. The collisions shown, from a long time series, are all equally likely. See Fig. 1, which shows typical sequences of 100 000 collisions, generated in this way, for two different locations of the boundary angle, $\alpha_{\min}$, which separates the deterministic collisions from the stochastic ones. There is a strong visual resemblance between these distributions for stochastic hybrid dynamics and the more familiar [6] isokinetic multifractals, one of which is shown in Fig. 2.

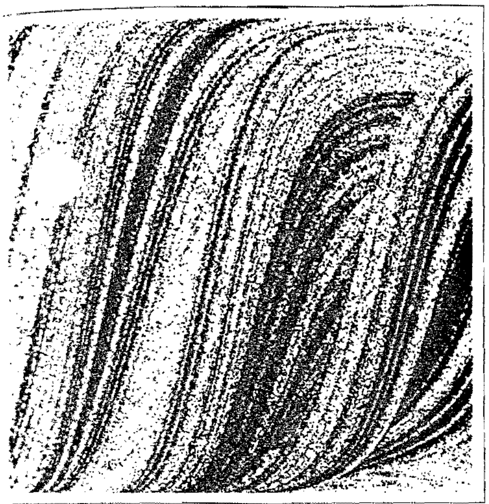
The approximate information dimensions, $\{D_\epsilon\}$, for million-collision data sequences similar to those illustrated in these two figures, were estimated from the quotients [14],

$$D_\epsilon \equiv \langle \ln \mu_\epsilon \rangle / \ln \epsilon ,$$

and are given in Table 1. The convergence of the numerical analysis strongly suggests that the distribu-



Collision sequences, $\{\alpha, \sin\beta\}$, for a reduced field strength of 3.0, using two different widths for the stochastic region, $\pi < \{\frac{1}{16}, \frac{1}{8}\}$. Within the stochastic strip, which is not shown in the figure, the speed just after collision is set equal to p_0/m direction is chosen at random. The density of the scatterers is $\frac{4}{5}$ the close-packed density. The abscissas correspond to the region $\alpha < \pi$ and the ordinates to the range $-\frac{1}{2}\pi < \beta < \frac{1}{2}\pi$.



Typical collision sequence, $\{\alpha, \sin\beta\}$, for a reduced field ...th of 3.0, using the usual isokinetic thermostat, which con- ... the moving particle's speed to the fixed constant p_0/m. ...ensity of the scatterers is $\frac{4}{5}$ the close-packed density. The ... corresponds to the region $0 < \alpha < \pi$ and the ordinate to ...nge $-\frac{1}{2}\pi < \beta < \frac{1}{2}\pi$.

...s are multifractal. The numerical work is best car- ... out by scaling the deterministic portion of the ...caré section into a unit square. The resulting nu- ...ical values are quite consistent with a visual impression: not only the fully-deterministic isokinetic Poincaré section, but also its stochastic cousins, appear to be multifractals, though the information dimensions of the stochastic sections are considerably closer to that of the full space. See again Table 1. Because kinetic energy varies in the stochastic case, a complete description of such collisions would require a third dimension, such as speed. We believe that this additional information cannot alter the conclusion that our caricature of a "stochastic" phase-space distribution is a multifractal.

In response to one referee's suggestions we wish to emphasize that many results in statistical mechanics apply strictly only in limiting cases, such as truly infinite sampling times or an infinite number of degrees of freedom. The deviations from such limits can be quite small, of order e^{-t} or e^{-N} or an inverse power of t or N. Thus numerical results can appear to approach such limits even though they differ by small terms. The results presented here suggest that stochastic boundaries may well give phase-space distributions resembling known multifractal distributions. Assessing this suggestion is an outstanding, quite difficult, theoretical task. We agree with the referee that the numerical work cannot be wholly convincing, particularly in view of the fact that the numerical informa-

Table 1
Information dimension as determined with equal rectangular bins, using the collision data of Figs. 1 and 2, expanded to one million collisions. The apparent information dimensions $D = \langle \ln \mu_\epsilon \rangle / \ln \epsilon$ are tabulated for 16^2, 32^2, and 64^2 Poincaré section bins. The first two calculations are stochastic, while the last, with no stochastic region, is isokinetic. The angle $\alpha_{\min}$ describes the width of the stochastic boundary region, as is described in the text. All the data are for a field strength of $3p_0^2/m\sigma$, where σ is the scatterer diameter and the scatterer density is four-fifths the close-packed density.

$\alpha_{\min}$	D_{16}	D_{32}	D_{64}
$\frac{1}{8}\pi$	1.961	1.960	1.960
$\frac{1}{16}\pi$	1.974	1.973	1.972
0.0	1.861	1.850	1.844

tion dimensions are not so far removed from the embedding dimension. The results are both suggestive and provocative. Since completing this work we have studied the heat conductivity of a one-dimensional anharmonic tethered chain resembling the "dingaling" model [15]. By using the heat transfer at the chain's hot/cold stochastic boundaries to estimate the local phase-space expansion/contraction we have obtained numerical results quite consistent with a multifractal distribution.

How could a stochastic boundary generate a multifractal section? Even though Hamiltonian motion conserves phase-space volume, it distorts the shapes of comoving volume elements. Thus, in the stochastic replacement of an old velocity distribution by a new equilibrium one, the projection of changed velocities, into momentum space, can give a net increase or decrease in phase volume. This violation of Liouville's theorem is confined to the stochastic regions of phase space. Though such a replacement does not immediately destroy the continuity of a smooth distribution, it seems conceivable that repeated iterations of the stochastic-collision process, like iterations of the generalized baker map, can lead to multifractal limiting distributions. Such an explanation is consistent with the stochastic Galton board data, presented here. If stochastic boundaries can violate Liouville's theorem locally, leading, with iteration, to multifractal structures, it is also possible that the apparent conflict between the stochastic and deterministic approaches to nonequilibrium steady states can be resolved definitively, through careful analyses of examples similar to those considered here. The situation seems to us analogous to a dissipative map, in which the volume change associated with dissipation is provided by the boundary mapping.

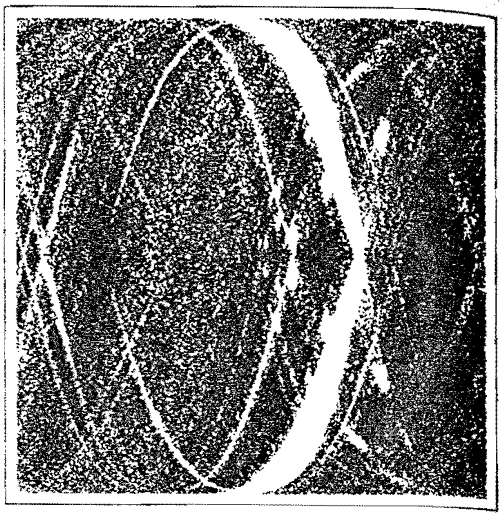


Fig. 3. Subset of a typical collision sequence, $\{\alpha, \sin\beta\}$. The points shown are taken from those trajectories with 80 or more successive collisions in the deterministic region, omitting the first five and the last five points, under the conditions of Fig. 1 with $\alpha_{\min} = \frac{1}{16}\pi$.

It seems also likely that the phase-space structures found here can be related to the "escape-rate theory" for open systems, discussed by Dorfman, Gaspard, and Nicolis [16,17]. In that theory, the rate of information gain about the initial condition, the "Kolmogorov–Sinai entropy", associated with phase-space flows, is separable into two parts, (i) that described by the positive Lyapunov exponents and (ii) that described by the "escape rate". This rate is also directly related to a thermodynamic dissipation rate, $\dot{S}_{\text{external}}/k$. In the present stochastic model the rate of "escape", into the stochastic "boundary" region, is determined by the magnitude of the angle $\alpha_{\min}$. The collision sequences which can avoid that stochastic region indefinitely evidently make up a "chaotic-saddle repellor", with an information dimension D less than that of the embedding space. The Galton board with stochastic boundaries can be viewed as an open system: a particle reaching the thermostat region $0 < \alpha < \alpha_{\min}$ escapes and is replaced by another particle with a thermalized momentum. A first approximation to such a saddle reellor is shown in Fig. 3, where only those Poincaré points are shown which belong to uninterrupted sequences of at least 80 consecutive elastic collisions.

It should be mentioned that our attempts to create similar repellor structures through straightforward generalizations of time-reversible maps [18], including stochastic strip regions, failed. We expect that, with further diligence, such a map could be constructed, to complement the many significant and highly interesting studies carried out by Breymann, Tél, and Vollmer [19,20], but we have not yet found such a map.

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