

Remarks on non-Hamiltonian statistical mechanics: Lyapunov exponents and phase-space dimensionality loss

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Abstract. – The dissipation associated with nonequilibrium flow processes is reflected by the formation of strange attractor distributions in phase space. The information dimension of these attractors is less than that of the equilibrium phase space, corresponding to the extreme rarity of nonequilibrium states. Here we take advantage of a simple model for heat conduction to demonstrate that the nonequilibrium dimensionality loss can definitely exceed the number of phase-space dimensions required to thermostat an otherwise Hamiltonian system.

Nonequilibrium molecular dynamics has been used to establish a close link between microscopic dynamical phase-space instabilities and the macroscopic irreversible dissipation associated with the Second Law of Thermodynamics [1,2]. Both non-Hamiltonian and Hamiltonian methods have been used [3]. The simplest such connection between microscopic dynamics and macroscopic dissipation results when one or more Nosé-Hoover thermostats [4] are used to control nonequilibrium steady states. In the absence of nonequilibrium fluxes and with sufficient phase-space mixing, these thermostats generate Gibbs' and Boltzmann's canonical distribution. In cases which include nonequilibrium driving the instantaneous external entropy production rate (due to heat transfer with the thermostats) is proportional to the sum of the instantaneous Lyapunov exponents [5]:

$$\dot{S}/k \equiv - \sum \lambda = -\dot{\otimes} / \otimes .$$

The summed-up instantaneous exponents give the comoving rate of change (following the motion) of an infinitesimal phase-space hypervolume \otimes . The sum of the time-averaged Lyapunov

exponents, $\{\langle\lambda\rangle\}$, is necessarily negative, reflecting the irreversible dissipation described by the Second Law of Thermodynamics.

Despite the time reversibility of the underlying equations of motion, a symmetry breaking due to the enhanced stability of trajectories proceeding “forward” in time relative to their reversed twins, guarantees irreversibility and the formation of a phase-space strange attractor [5]. The dimensionality of such a strange attractor can be measured by computing the smallest number of time-averaged exponents (beginning with the largest one, $\langle\lambda_1\rangle$) with a negative sum. This “Kaplan-Yorke” dimension is identical to the “information dimension” in cases of physical interest [6].

Because Liouville’s theorem [7] establishes that the “extension in phase”, the hypervolume of the comoving element \otimes , cannot change in a motion governed by Hamiltonian dynamics, there has been some reluctance to accept this strange-attractor explanation of irreversibility. Very recently, Ramshaw has provided a particularly clear analysis of the generalized Liouville’s theorem required to describe nonequilibrium dynamics with time-reversible thermostats [8]. References [9] and [10] provided a useful computational model and a means to estimate the dimensionality loss, ΔD , the difference between the strange attractor’s information dimension and that of the phase-space in which it is embedded. It was shown that an accurate estimate for ΔD can be made, under certain conditions, which requires only a single exponent, not the whole spectrum. We use the whole spectrum here because we want to make the demonstration of dimensionality loss as convincing as possible.

In the “ ϕ^4 ” model an otherwise harmonic nearest-neighbor lattice, with Hooke’s law pair potential for particles i and j ,

$$\phi(r) = \frac{1}{2}(r - 1)^2; \quad r = |r_i - r_j| > 0,$$

has each particle tethered to its lattice site with a quartic potential, $\frac{1}{4}\delta r^4$. The quartic tethers prevent momentum conservation, so that Fourier heat conduction can be observed, and also can provide chaos, with one or more positive Lyapunov exponents. To model a nonequilibrium heat-conducting state, two or more of the particles are thermostated using feedback forces $\{-\zeta p\}$ which are linear or cubic in the friction coefficient ζ and the momentum p . Here we choose the simplest case, linear in both variables, the Nosé-Hoover thermostat. In one space dimension the thermostated equations of motion are

$$\dot{p} = F - \zeta p; \quad \dot{\zeta} = [(p^2/mkT) - 1]/\tau^2,$$

where τ is the characteristic response time of the thermostat force, $-\zeta p$. In two dimensions, where p^2 is a sum of x and y components, T is replaced by $2T$. The target temperature T for the thermostat is necessarily achieved whenever a stationary solution exists, such that the long-time-averaged value of $\dot{\zeta}$ vanishes. Because the long-time average of $\zeta\dot{\zeta} = (d/dt)\frac{1}{2}\zeta^2$ likewise vanishes, the heat transferred by any thermostated momentum can be directly related to the temperature:

$$\langle\zeta p^2/m\rangle \equiv \langle\zeta\rangle kT,$$

again explicitly writing only the one-dimensional case.

The 16-body system shown in fig. 1 has a cold particle at the lower left corner, a hot particle at the upper right corner, along with 14 Newtonian particles able to transmit heat from the hot particle to the cold one. This system (as well as many others) can exhibit dimensionality losses exceeding the 10 phase-space coordinates $\{x, y, p_x, p_y, \zeta\}$ required to describe the two thermostated particles. In the case shown in the figure, with cold temperature 0.001 and hot temperature 0.009, and a Nosé-Hoover relaxation time $\tau = 1.4$, the dimensionality loss is 12.5.

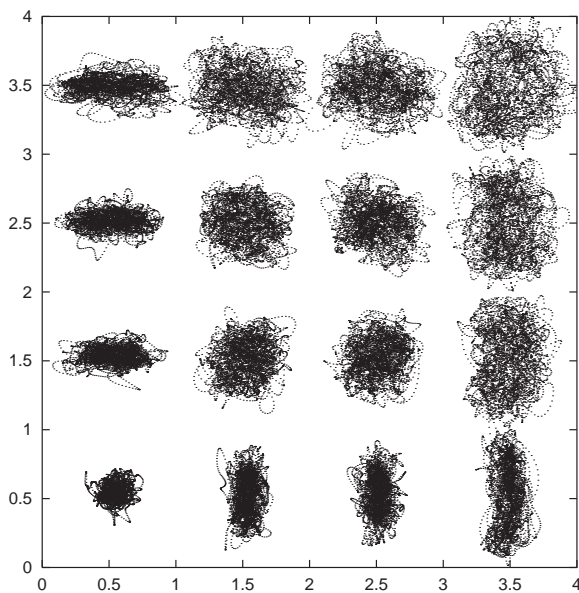


Fig. 1 – Stationary-state particle trajectories for a 16-particle system with dimensionality loss of 12.5 induced by two Nosé-Hoover thermostated particles at temperatures of 0.001 and 0.009.

This means that the sum of the 53 largest Lyapunov exponents, plus half the 54th, is zero. See fig. 2 for the spectrum of exponents. The strange attractor has an information dimension of 53.5, embedded in a 66-dimensional phase space, of which 56 dimensions represent the purely Hamiltonian particles.

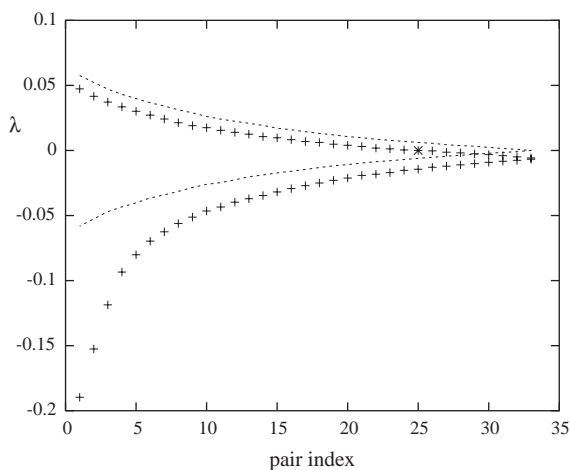


Fig. 2 – Lyapunov spectrum for the system shown in fig. 1. There are 24 positive exponents, a single vanishing exponent (emphasized here), and 41 negative exponents describing the motion in the 66-dimensional space. In the symmetric equilibrium situation (with the hot and cold temperatures equal) the exponents occur in 33 pairs, $\{\pm\lambda\}$, with a single pair of vanishing exponents. In the nonequilibrium case there is an overall shift toward more negative values, $\dot{S}/k \equiv -\sum \lambda > 0$.

This result establishes very clearly that the dissipation and overall contraction occurring in the thermostated part of the system can cause a loss in the Hamiltonian region too. Although we had been able to simulate systems with dimensionality losses barely exceeding the additional boundary phase-space coordinates [11], the present results are much more clearcut. Otherwise, one might imagine that the thermostat regions simply provide a time-dependent force, which for Hamiltonian dynamics can provide no dimensionality loss. The *feedback* linking the forces to the phase-space coordinates, not just to the time, makes the loss possible.

This situation is analogous to the dynamics of a one-dimensional damped harmonic oscillator with a *fixed* friction coefficient z , for which the logarithmic phase-space contraction rate,

$$\dot{\otimes}/\otimes \equiv (\partial\dot{q}/\partial q) + (\partial\dot{p}/\partial p),$$

occurs in the momentum direction only:

$$\begin{aligned} \dot{q} &= p; & \dot{p} &= -q - zp \longrightarrow \\ (\partial\dot{q}/\partial q) &= 0; & (\partial\dot{p}/\partial p) &= -z. \end{aligned}$$

The damped oscillator motion nevertheless collapses ($\otimes \rightarrow 0$) to the fixed point at the origin, ($q = 0, p = 0$) because the motion *rotates* the comoving phase volume. Phase-space rotation [12] in many-body systems increases rapidly with system size and is necessarily the mechanism through which the volume collapse can spread to directions without direct contraction.

In summary, thermostated heat flow, in a tethered harmonic lattice, shows conclusively that the dimensionality loss associated with irreversible processes can exceed the additional variables required to specify the thermal boundaries driving the system from equilibrium. This shows that the dimensionality loss is a real feature of nonequilibrium systems, not an artifact of a particular choice of thermostat. We believe that this finding clarifies a point which has been strenuously debated over the past decade [13]. There can be no doubt that advances in parallel computing will soon elucidate the precise way in which the large-system limit is obtained.

The approach we follow here connects irreversible entropy production to multifractal phase-space structures through time-reversible Nosé-Hoover thermostats. It is worth mentioning that there are now alternative connections, including some based on purely Hamiltonian mechanics [3].

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