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Heat transfer between two degrees of freedom

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A particularly simple chaotic nonequilibrium open system with two Cartesian degrees of freedom, characterized by two distinct temperatures T_x and T_y, is introduced. The two temperatures are maintained by Nosé–Hoover canonical-ensemble thermostats. Both the equilibrium (no net heat transfer) and nonequilibrium (dissipative) Lyapunov spectra are characterized for this simple system.

I. INTRODUCTION

Lyapunov instability is fundamental to an understanding of the microscopic source of macroscopic thermodynamic irreversibility. The Lyapunov *spectrum*[1–3] $\{\lambda\}$ measures the deformation of phase-space hypervolumes, based on the sum of the first n exponents (with $\lambda_1 \geqslant \lambda_2 \geqslant \lambda_3 \geqslant \cdots$) giving the time-averaged growth rate of an n-dimensional phase-space object. In the *equilibrium* case (steady state with no net heat transfer) the spectrum is a symmetric set of "Smale pairs," with each positive exponent corresponding to a negative exponent with the same absolute value. The phase-space hypervolume is thus, in accord with Liouville's theorem, a constant of the motion. In the *nonequilibrium* case (open system with net heat transfer) the spectrum has a roughly similar shape, at least close to equilibrium, but the sum of the exponents is *necessarily negative*, and corresponds to the rate of irreversible entropy production: $-\ \Sigma\lambda \equiv \dot{S}/k$. So far, only a few results for nonequilibrium steady states are available.[4–7] Evans, Morriss, and Cohen, following up earlier work of Dressler[8] have related the equilibrium and nonequilibrium spectra for a class of *homogeneously* thermostatted systems in which all particles are thermostatted in the same way. For such systems they showed that nonequilibrium dissipation induces precisely equal shifts of each Smale pair of Lyapunov exponents.

In our nonequilibrium studies we focused on the distributions of Lyapunov exponents for "many" bodies, up to 32 atoms in three dimensions and 49 in two. These systems are sufficiently complex to frustrate theoretical analysis. Here, we introduce a simpler prototypical system so as to elucidate steady nonequilibrium heat flow with the least number of degrees of freedom possible. We consider an *angle-dependent* two-dimensional oscillator with different horizontal and vertical temperatures T_x and T_y. We introduce and analyze the model in Sec. II, summarizing our conclusions in Sec. III.

II. MODEL

We consider the motion of a mass m in a two-dimensional Hooke's law potential, generalized by making the harmonic force constant vary periodically with the polar angle θ:

$$\phi(r,\theta) = (\kappa r^2/2)[1 + 0.5\cos(3\theta)].$$

The resulting Hamiltonian system is a relative of the classic Hénon–Heiles system, which also exhibits threefold rotational symmetry. In polar coordinates the dynamics of the system takes place in a three-dimensional subspace of the four-dimensional $\{r,\theta,p_r,p_\theta\}$ phase space, conserving the energy, $H \equiv (p^2/2m) + \phi$. By introducing a pair of canonical Nosé–Hoover thermostats[5,9] this system can be forced to undergo an irreversible transfer of heat between the x and y coordinate directions. The flow of heat always takes place from the higher to the lower temperature, in just such a way as to match the predictions of the Second Law of Thermodynamics.[10,11] In *Cartesian* coordinates, the phase space $\{x,y,p_x,p_y,\zeta_x,\zeta_y\}$ for the thermostatted system is augmented to include the two additional thermostat variables ζ_x and ζ_y. The corresponding Cartesian equations of motion are

$$m\frac{dx}{dt} = p_x;\quad \frac{dp_x}{dt} = F_x - \zeta_x p_x;\quad \frac{d\zeta_x}{dt} = \frac{[(p_x^2/m) - kT_x]}{(kT_x\tau_x^2)}$$

$$m\frac{dy}{dt} = p_y;\quad \frac{dp_y}{dt} = F_y - \zeta_y p_y;\quad \frac{d\zeta_y}{dt} = \frac{[(p_y^2/m) - kT_y]}{(kT_y\tau_y^2)},$$

where, for convenience in what follows, the oscillator mass m, Boltzmann's constant k, the force constant κ, and the thermostat relaxation times $\{\tau\}$ will all be chosen equal to unity. The phase space for this system is six dimensional, $\{x,y,p_x,p_y,\zeta_x,\zeta_y\}$ and can have as many as five nonzero Lyapunov exponents (only four in the nondissipative equilibrium case with $T_x = T_y$). Figure 1 shows typical trajectories for both the equilibrium case (no heat transfer) and the nonequilibrium case (including heat transfer from the higher to the lower temperature). Note that the symmetry with which the three potential valleys are explored disappears when the horizontal and vertical temperatures differ.

We wish to study the nonequilibrium shift of the Lyapunov-exponent pairs as the temperatures T_x and T_y are varied. In a seminal paper, Evans, Morriss, and Cohen showed[8] that in a nonequilibrium system in which all particles obey the same thermostatted equations of motion, the various pairs of exponents will all have the *same* (negative) shift, with $\lambda_1 + \lambda_6 \equiv \lambda_2 + \lambda_5 \equiv \lambda_3 + \lambda_4$. In the present calculations the average temperatures associated with the x and y degrees of freedom are distinct, away from equilibrium, so that the shifts can differ.

The spectrum of Lyapunov exponents $\{\lambda\}$ can be obtained in a variety of ways. We have compared two of these approaches, using Lagrange multipliers[3] in order to force six "satellite" trajectories to maintain an orthonormal relationship to one another, as well as using repeated Gram–Schmidt orthonormalization of the phase-space basis vectors to maintain these constraints, as was first suggested by Benettin's work.[1] Independent calculations were carried out in Livermore and Vienna.

In the equilibrium case, with $T_x \equiv T_y \equiv 1$, the spectrum was determined by using the fourth-order Runge–Kutta method to follow a fifty million time step run ($dt = 0.01$). The results, with initial conditions $\{x,y,p_x,p_y,\zeta_x,\zeta_y\} = \{1,1,1,1,0,0\}$, were as follows:

$$\{\lambda_{\rm eq}\} = \{+0.135, +0.050, +0.003, -0.003, -0.050, -0.135\},$$

with an uncertainty of ± 0.01 in the individual exponents. The spectrum shows the expected Smale-pair symmetry and resembles in shape the shapes of spectra recently found for chains and strings of coupled pendula[6] with many degrees of freedom. Test runs with time steps of 0.05 and 0.10 confirmed these results, and were also used to determine the uncertainty quoted above.

This simple equilibrium system becomes a prototypical *nonequilibrium steady state* when *different* values are chosen for the two temperatures T_x and T_y, allowing for a net heat transfer from the higher to the lower temperature. With a fourfold difference in temperature, $T_x = 2$; $T_y = 1/2$, the spectrum is considerably changed. A ten-million-time-step simulation with $dt = 0.10$ and a hundred-million-time-step simulation with $dt = 0.01$ confirm the values

$$\{\lambda_{\rm neg}\} = \{+0.117, +0.043, +0.001, -0.008, -0.067, -0.200\}.$$

The two simulations suggest that these exponents have uncertainties no larger than ± 0.01. Thus this nonequilibrium spectrum establishes shifts $\Delta\lambda \equiv \lambda_{\rm neg} - \lambda_{\rm eq}$ for the Smale pairs of $+0.117 - 0.200 = -0.08_3$ and $+0.043 - 0.067 = -0.02_4$, with the larger pair of nonzero exponents shifting more than twice as much as does the intermediate pair of exponents. *Reversing* the temperatures, so that energy flows from the y direction to the x, with $T_y = 2$ and $T_x = 1/2$, gives another nonequilibrium spectrum of exponents, again calculated from independent ten- and hundred-million-time-step simulations with a total time of 1 000 000:

$$\{\lambda_{\rm neg}\} = \{+0.031, +0.001, -0.005, -0.043, -0.128, -0.216\}.$$

These data likewise indicate a definite disparity in the shifts of the nonzero Smale pairs, $\Delta\lambda \equiv \lambda_{\rm neg} - \lambda_{\rm eq}$: -0.18_5 vs -0.12_7 vs -0.04_8.

III. CONCLUSION

By adding the possibility for heat transfer to a simple problem resembling the Hénon–Heiles model, and with only two degrees of freedom, a nonequilibrium steady state, with a hot-to-cold heat flow obeying the Second Law of Thermodynamics can be achieved and characterized. The thermostatting in our simple open-system model is *inhomogeneous,* with different control variables $\{\zeta_x,\zeta_y\}$ and different average values, $T_x \neq T_y$, characterizing the two temperature reservoirs. Although the Lyapunov spectra for such inhomogeneous steady states *do* retain a resemblance to the spectrum for the corresponding equilibrium case there appears to be no simple relation, such as that discovered by Evans, Morriss, and Cohen,[8] linking the shifts of the individual Lyapunov-exponent Smale pairs to the overall thermodynamic dissipation.

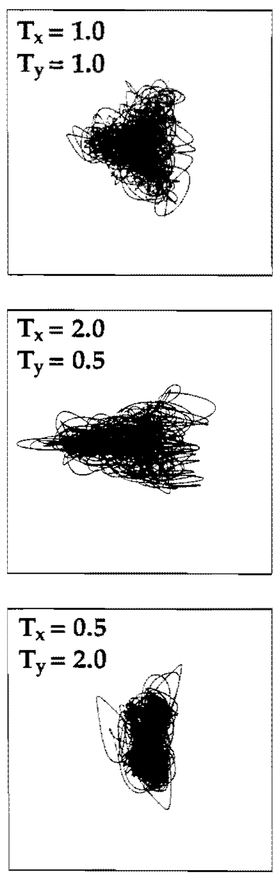

FIG. 1. Typical chaotic trajectories for both equilibrium (no net heat flow) and nonequilibrium (net hot-to-cold heat flow) simulations. In the top equilibrium illustration the horizontal and vertical temperatures are equal to unity. The other two trajectories correspond to nonequilibrium steady states with $\{T_x,T_y\} = \{2.0,0.5\}$ and $\{0.5,2.0\}$. In all three simulations the temperatures were enforced with Nosé–Hoover thermostats having characteristic relaxation times of unity. The trajectories shown are one thousand times shorter than those used in computing the Lyapunov spectra.

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