Heat conduction in one-dimensional chains and nonequilibrium Lyapunov spectrum

H. A. Posch
Institute for Experimental Physics, University of Vienna, Boltzmanngasse 5, A-1090 Vienna, Austria

Wm. G. Hoover
Department of Applied Science, University of California at Davis–Livermore and Lawrence Livermore National Laboratory, Livermore, California 94551-7808

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We define and study the heat conductivity κ and the Lyapunov spectrum for a modified ''ding-a-ling'' chain undergoing steady heat flow. Free and bound particles alternate along a chain. In the present work, we use a linear gravitational potential to bind all the even-numbered particles to their lattice sites. The chain is bounded by two stochastic heat reservoirs, one hot and one cold. The Fourier conductivity of the chain decreases smoothly to a finite large-system limit. Special treatment of satellite collisions with the stochastic boundaries is required to obtain Lyapunov spectra. The summed spectra are negative, and correspond to a relatively small contraction in phase space, with the formation of a multifractal strange attractor. The largest of the Lyapunov exponents for the ding-a-ling chain appears to converge to a limiting value with increasing chain length, so that the large-system Lyapunov spectrum has a finite limit. [S1063-651X(98)11510-6]

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I. INTRODUCTION

Casati, Ford, Vivaldi, and Visscher introduced their ''ding-a-ling'' model in 1984 [1]. This one-dimensional model is, arguably, the simplest mechanical model to exhibit Fourier heat flow, with a well-defined thermal conductivity, $\kappa = -Q/(dT/dx)$, in the long-chain-length limit [2]. Here, Q is the heat flux, and dT/dx is the temperature gradient along the chain. In the original version of this model [1,2] all even-numbered particles were bound to their lattice sites with harmonic springs, while the odd-numbered particles were able to move freely, between their adjacent bound particles, transporting heat. The system was bounded by two stochastic heat reservoirs, which served to drive the chain into a nonequilibrium steady state. In a variant of this model, introduced by Prosen and Robnik [3], all interior particles are harmonically bound to lattice sites. The first and last particles move freely, coupling the chain of colliding oscillators to the terminating stochastic heat baths.

Recently, Hu, Li, and Zhao [4] considered one-dimensional Frenkel-Kontorova chains, consisting of particles connected by harmonic springs and, in addition, subjected to an external sinusoidal potential. They showed that this external potential (the ''lattice'') assumes the role of the bound lattice particles in the ding-a-ling model and that a strong phonon-lattice interaction, inducing phonon scattering on the lattice, is the key for the existence of a finite heat conductivity in the long-chain limit. Anharmonicity in the potential is not sufficient and can lead to a diverging conductivity as exemplified by the Fermi-Pasta-Ulam β model [5].

In studies of nonequilibrium steady states it is presently unclear to what extent the phase-space distribution function depends on the choice of boundary conditions [6]. It is quite reasonable, as we detail later, to expect boundary effects, of order $N^{-1/D}$ in D dimensions, where N is the number of particles. Such boundary effects can be sensitive to the details of their implementation. Using *deterministic feedback* to impose energetic or thermal constraints on boundary degrees of freedom, it has been established [9], even rigorously [10], that the phase-space distribution function can occupy a multifractal attractor, with an information dimension reduced well below that of the unconstrained equilibrium distribution. For *stochastic boundaries*, however, it has been stated that the distribution is absolutely continuous [6,7], without any fractal character. There are no numerical results confirming this idea, and the present work developed, in part, to test it. In a recent study of the phase space structure of a driven Lorentz gas with a partially stochastic boundary we have found numerical evidence suggesting that multifractal attractors may coexist with stochastic boundaries [8].

The noise introduced by stochastic boundaries is a complicating feature for any comparison with deterministic thermostatted boundaries. We are particularly interested in the chaotic properties of nonequilibrium steady states. It is of interest to determine, first of all, whether or not a Lyapunov spectrum exists for a system with stochastic boundaries. We have developed an approximate method for estimating such a spectrum and apply it here to a slightly modified version of the one-dimensional ding-a-ling model. We find that the resulting approximate spectra resemble those from other nonequilibrium steady-state simulations [6,9–12], with a negative overall sum corresponding to the collapse onto a phase-space strange attractor. However, the dimensionality loss is quite small, of order $1/N$ for a fixed temperature difference between the stochastic boundaries of the chain, due to the one-dimensional nature of the model.

The convergence of the Lyapunov spectrum for increasing system size in equilibrium is another interesting question. In two dimensions this convergence turned out to be delicate, [6] apparently depending on the details of the boundary conditions. There is numerical evidence for systems of hard disks in two dimensions [11], and for hard spheres in three [12], that the maximum exponent exists. Our results for the one-dimensional ding-a-ling model indicate that the largest Lyapunov exponent converges to a definite limit with increasing system size, as might be expected for the Einsteinlike localized-mode nature of the motion. In contrast, the Fermi-Pasta-Ulam β model, which is characterized by a diverging heat conductivity, seems to exhibit a logarithmic divergence of the maximum Lyapunov exponent with chain length [16] emphasizing the nonlocal character of its dynamical processes.

For the ding-a-ling model there is no special reason to use a harmonic binding potential for the particles bound to a lattice site. Here we modify the original model of Casati *et al.* by using a gravitational potential, $\phi = mg|x - x_0|$, rather than a harmonic one, for the even-numbered bound particles. Here, x stands for a bound-particle coordinate, and x_0 denotes the respective lattice site. The choice of a (one-dimensional) gravitational potential has the advantage that the times at which bound-free collisions occur can be found analytically, by solving quadratic equations. The simplified model has the same qualitative properties as the original one, but offers the advantage of superior computational efficiency. In Sec. II we introduce our model and describe an exact algorithm for the computation of Lyapunov spectra in tangent space. Particular emphasis is given to the proper treatment of stochastic boundaries on both ends of the chain. This allows the computation of full Lyapunov spectra for chains supporting stationary heat flow described by Fourier's law (in the long-chain limit). Our simulation results, both for equilibrium and stationary nonequilibrium chains, are presented in Sec. III. We conclude, in Sec. IV, with a few remarks.

II. MODIFIED DING-A-LING MODEL FOR HEAT CONDUCTION

At first glance it seems odd that a one-dimensional model could lead to (i) chaos, (ii) ergodicity, within the constraint $x_i \leqslant x_{i+1}$, and (iii) well-defined transport coefficients. But a sufficiently strong phase-space mixing, brought about by the phonon-lattice interaction, is enough for all three properties. The original ding-a-ling model, as well as the modification considered here, were specially constructed with chaotic mixing in mind. The bound particles can be made to vibrate rapidly, relative to the collision rates of their neighboring free particles, effectively randomizing the collisions. Casati, Ford, Visscher, and Vivaldi [1] used harmonic restoring forces and showed that for two-particle systems with periodic boundaries almost-K-system behavior is found for oscillator frequencies (their case $\omega = 3$), for which the ratio of the oscillator frequency, ν_B, to the bound-free collision frequency, ν_{BF}, may be estimated to $3\sqrt{3}/\pi$. Thus, a ratio equal to or exceeding this value generates enough mixing in phase space to allow Fourier's law to be valid in the long-chain limit [1,2]. This conclusion holds in spite of the fact that trajectory plots, like the sample shown in Fig. 1, indicate that repeated collisions, involving the same bound-free pair more than once, are relatively common. In such events the bound particle oscillates, colliding two or more times with the moving free particle, and ultimately reversing its direction of motion.

To avoid numerical root finding, we modify the original ding-a-ling model slightly and use gravitational forces for the bound particles instead of harmonic ones. The Hamiltonian is written as

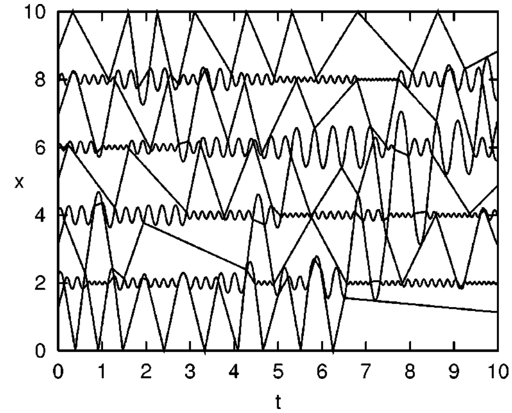

FIG. 1. Typical space-time trajectories for a gravitational ding-a-ling model with 9 particles, where the time is plotted along the horizontal axis. The boundary temperatures are 10 at the top, and 30 at the bottom, in units of $T^* = mg_0\sigma/k_B$. The gravitational field strength is $100g_0$.

$$H = \sum_{k=1}^{N} \left[\frac{p_k^2}{2m} + mg_k|x_k - k\sigma| \right] + \{\text{hard core}\},$$

where the gravitational acceleration $g_k = 0$ for the odd-numbered free particles, and $g_k = 100g_0$ for the even-numbered bound particles. x_k and p_k are the spatial coordinate and the momentum, respectively, of particle k. In the following we use reduced units for which the particle mass m, the mean interparticle spacing σ, and the gravitational constant g_0 are all unity. Our unit of time is $(\sigma/g_0)^{1/2}$, and the unit of energy is $m\sigma g_0$. Note that the gravitational field is 100 in our reduced units. Since also Boltzmann's constant k_B is taken as unity, all temperatures are measured in units of $T^* \equiv mg_0\sigma/k_B$. With a mean temperature of $20T^*$, the typical frequency ν_B of an oscillating bound particle is $\nu_B = 25/\sqrt{60}(g_0/\sigma)^{1/2}$. Since the thermal velocity is $\sqrt{20}(g_0\sigma)^{1/2}$, the bound-free collision rate ν_{BF} may be estimated as $4/\sqrt{20}(g_0/\sigma)^{1/2}$, and the ratio ν_B/ν_{BF} becomes $25/(4\sqrt{3})$. This number is almost twice that quoted above for the original model. Thus we expect mixing to be sufficient for Fourier's law to hold also in our case.

It is quite instructive to relate our reduced units to a typical atomic chain with $\sigma \sim 3\times10^{-10}$ m, $m \sim 4\times10^{-26}$ kg, and a bound frequency $\nu_B \sim 10^{12}$ Hz. For the unit acceleration one finds $g_0 \sim 3\times10^{13}$ ms^{-2}, and the temperature of $20T^*$ corresponds to about 500 K, a reasonable number. The temperature gradients, however, turn out to be quite large, as discussed later.

Trajectories were constructed by ordering all the collision times (including all those times when the bound particles return to their lattice sites, requiring a change in sign of the gravitational force) and choosing the smallest to update the system. In carrying out all our simulations, the momenta acquired by the first and last particles, on hitting the stochastic boundaries at $x_{\mathrm{hot}} = 0$ and $x_{\mathrm{cold}} \equiv L = (N+1)\sigma$, were selected from a one-sided equilibrium distribution $f(p) = (mkT)^{-1}|p|e^{-p^2/2mkT}$, where T is either T_{hot} or T_{cold}. Figure 1 shows a typical space-time trajectory segment for a nine-particle system. The time-averaged values of the particle kinetic energy and boundary heat flows were accumulated in order to obtain the temperature profile and the heat conductivity. Just as is suggested by elementary kinetic theory, we expected to find a heat conductivity varying as the square root of temperature, leading to a constant-flux profile, with the temperature proportional to the 2/3 power of the coordinate. Instead, the numerical results suggest quite a different power law. See Fig. 3. In the following section we explain the reason for this interesting finding.

The Lyapunov exponents, which can be used to determine the dimension of phase-space strange attractors [10], need special consideration in view of the stochastic boundaries. These exponents describe the tendency of satellite trajectories to separate from, or converge toward, a reference trajectory. They are obtained by following the dynamics of (infinitesimal) offset vectors in tangent space. Between consecutive instantaneous events, separated by a time interval τ, the offset-vector components $\{\delta x, \delta p\}$, associated with the position x and momentum p of a particle, evolve freely according to the motion equations

$$\delta x(\tau)=\delta x(0)+\tau\delta p(0)/m, \quad \delta p(\tau)=\delta p(0).$$

If at the end of a streaming period a bound particle crosses its lattice site, the constant force on this particle changes sign instantaneously, and the tangent-vector components for this particle immediately before $(-)$ and after $(+)$ the crossing are related according to the ''crossing map'' [11,13]

$$\delta x^{+}=\delta x^{-}, \quad \delta p^{+}=\delta p^{-}-2mg\,\delta x^{-}/|p|.$$

The components of all the other particles are unaffected. If the streaming is terminated by a collision between a bound (b) and a free (f) particle, the collision map relating their tangent-vector components immediately before $(-)$ and after $(+)$ the collision becomes [11]

$$\delta x_f^{+}=\delta x_f^{-}+(p_f^{-}-p_b^{-})\,\delta\tau/m, \quad \delta p_f^{+}=\delta p_b^{-}+m\tilde{g}\,\delta\tau,$$

$$\delta x_b^{+}=\delta x_b^{-}-(p_f^{-}-p_b^{-})\,\delta\tau/m, \quad \delta p_b^{+}=\delta p_f^{-}-m\tilde{g}\,\delta\tau,$$

where $\delta\tau=-m(\delta x_f^{-}-\delta x_b^{-})/(p_f^{-}-p_b^{-})$ denotes the delay time between the collision of the reference and the offset trajectories. $\tilde{g}=100g_0>0$, if the collision occurs to the left of the lattice site of the bound particle, and $\tilde{g}=-100g_0<0$ otherwise. All tangent-vector components of noncolliding particles are unaffected.

Finally, if the streaming is terminated by a boundary collision, two cases are distinguished: (i) If the boundary conditions are *adiabatic*, corresponding to a fixed phase-space volume, the respective collision map for the colliding particle with a hard wall becomes [11]

$$\delta x^{+}=-\delta x^{-}, \quad \delta p^{+}=-\delta p^{-}.$$

The resulting Lyapunov spectra then consist of pairs of exponents, $\{+\lambda,-\lambda\}$ summing to zero. Two of the exponents vanish because of energy conservation and nondivergent behavior in the flow direction.

(ii) In the nonequilibrium thermostated case, with a hot and a cold *stochastic* boundary, the statistical association of heat transfer ΔQ with phase volume $\delta\mathcal{V}$,

$$d\ \ln\ \delta\mathcal{V}/dt=\Delta Q/kT,$$

suggests that the components corresponding to the particle colliding with the stochastic boundary be scaled according to Gibbs' probability

$$(\delta x\,\delta p)^{+}/(\delta x\,\delta p)^{-}=e^{\Delta Q/kT},$$

leading to the collision map

$$\delta x^{+}=-\delta x^{-}, \quad \delta p^{+}=-\delta p^{-}e^{\Delta Q/kT}.$$

We show here that this procedure produces well-behaved nonequilibrium Lyapunov spectra. The sum of all the Lyapunov exponents vanishes for equilibrium systems, $T_{\mathrm{hot}}=T_{\mathrm{cold}}$, and is strictly negative for steady nonequilibrium heat flow for which $T_{\mathrm{hot}}>T_{\mathrm{cold}}$. Since no quantity is strictly conserved for stochastic boundaries, no vanishing Lyapunov exponents are found. The resulting spectra, along with our conductivity data, are described in the following section.

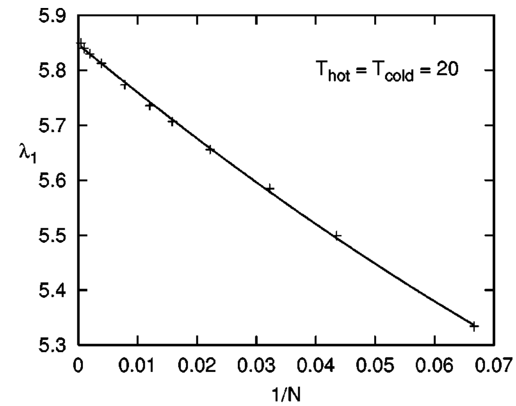

FIG. 2. Maximum Lyapunov exponent λ_1 for N-particle gravitational ding-a-ling chains at a temperature of 20 T^*. λ_1 is given in units of $(g_0/\sigma)^{1/2}$.

III. RESULTS

We consider equilibrium systems first, for which the temperatures of the stochastic boundaries on both ends of the chain are equal, $T_0=T_L=20T^*$. We have studied the maximum Lyapunov exponent for chains containing up to 2047 particles. Our simulation results are summarized by the crosses in Fig. 2. The smooth line constitutes a fit of a polynomial in $1/N$ to the data points,

$$\lambda_1=\left[5.85-8.9\left(\frac{1}{N}\right)+119\left(\frac{1}{N}\right)^2\right](g_0/\sigma)^{1/2}.$$

We find that the maximum exponent is well behaved in the long-chain limit. There is no indication of a divergence of λ_1 for $N\rightarrow\infty$ for this one-dimensional chaotic system. This result is in accord with our earlier results for hard disks in two dimensions [11], and for hard spheres in three [12]. We have found finite limiting exponents also for two-dimensional systems in nonequilibrium steady states with up to 32 000 [14] and 102 400 particles [15]. On the other hand, Searles *et al.* [16] interpret a weak, but persistent, increase of λ_1 with N for a Fermi-Pasta-Ulam β chain with up to 100 000 particles as a possible sign of a logarithmic divergence.

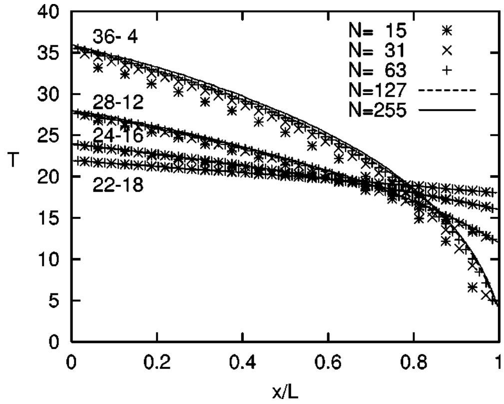

FIG. 3. Temperature profile for various chains with different lengths L and boundary temperatures. The labels indicate $T_{\text{hot}} - T_{\text{cold}}$. On the abscissa normalized particle coordinates x/L are used. The unit of temperature is $T^* = mg_0\sigma/k_B$.

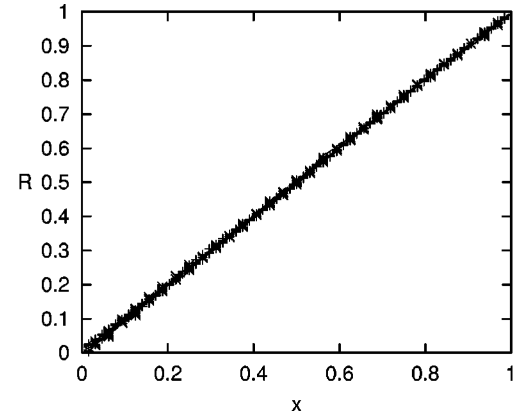

FIG. 4. Universal representation for various chains with different lengths L and boundary temperatures. The ratio $R \equiv [T(x)^{5/2} - T_0^{5/2}]/(T_L^{5/2} - T_0^{5/2})$ is plotted as a function of the reduced particle coordinate x/L for the profiles shown in Fig 3. Not included are the data for $T_{\text{hot}} - T_{\text{cold}} = (36-4)T^*$ for which, as is outlined in the main text, Fourier's heat conduction does not occur near the cold boundary.

Next we turn to the stationary nonequilibrium case. We determined the full Lyapunov spectra for systems with up to 63 particles. For larger systems $N > 127$ only the two largest exponents were obtained. The temperature for each particle was determined from its time-averaged kinetic energy. Temperature profiles for various chain lengths and temperature gradients are shown in Fig. 3, where a normalized particle coordinate x/L is used on the abscissa. The labels $T_{\text{hot}} - T_{\text{cold}}$ refer to the temperatures of the one-sided momentum distributions $f(p)$ used for the simulation. One observes (i) that for large temperature gradients (short chains) the extrapolated wall temperatures T_0 and T_L do not agree completely with T_{hot} and T_{cold}, respectively; (ii) that the temperature dependence of the conductivity $\kappa(T)$ gives rise to considerable nonlinearity in the profiles. The ansatz $\kappa = \kappa_0(T/T^*)^\alpha$, together with a constant space-independent heat flux $Q = -\kappa(dT/dx)$, leads to $\kappa_0(T/T^*)^\alpha dT = -Q dx$, which, integrated along the chain, yields

$$T(x)^{\alpha+1} = T_0^{\alpha+1} - \frac{(\alpha+1)Qx}{\kappa_0} T^{*\alpha}. \tag{1}$$

T_0 is the higher temperature at $x = 0$. From elementary kinetic-theory arguments we expected, initially, to find $\alpha = 1/2$. However, the experimental profiles are consistent with $\alpha = 3/2$. If the wall temperatures T_0 (hot) and T_L (cold) are determined from a fit of Eq. (1) to the experimental data, with $\alpha = 3/2$ fixed, one obtains a universal curve for all profiles by plotting $[T(x)^{5/2} - T_0^{5/2}]/(T_L^{5/2} - T_0^{5/2})$ as a function of x/L. See Fig. 4. The constant $\kappa_0 = (0.0236 \pm 0.0003)k_B(g_0/\sigma)^{1/2}$, the conductivity at unit temperature T^*, turns out to be independent of N for chains with $N \geqslant 15$. This result clearly shows that Fourier's law of heat conduction is obeyed for long gravitational ding-a-ling chains, thus confirming analogous conclusions for the original ding-a-ling model [2] or related models [3,4].

We were able to understand this dependence by solving a simple Master-equation kinetic-theory model for the temperature profile. The model assumes that the bound particles are characterized by temperatures while the free particles have momentum and energy fluxes determined by the temperature of their last collision with a bound particle. If these fluxes are then used to determine the energy flow between bound particles the power-law relation $\alpha = 3/2$ results from the resulting stationary state.

In Table I we have listed some of our nonequilibrium steady-state results for the gravitational ding-a-ling model: the extrapolated boundary temperatures T_0 and T_L, the heat flux Q, the time-averaged kinetic and potential energies per particle $\langle K \rangle/N$ and $\langle \Phi \rangle/N$, respectively, the thermal conductivity at unit temperature, κ_0, the maximum Lyapunov exponent λ_1, and, for the shorter chains, also the sum of all Lyapunov exponents $\Sigma_{l=1}^{2N}\lambda_l$. From these data one infers that the flux Q varies as $1/N$. Since, according to Fig. 3, also the temperature gradient is proportional to $1/N$, the conductivity κ approaches a finite limiting value for large N, as we had expected.

At this stage a short remark about the convergence of the simulation is in order. The simulation time must exceed the decay time τ_{therm} of a perturbation due to heat diffusion on a scale of the length of the chain. The latter may be estimated from $\tau_{\text{thermal}} \sim L^2/(\kappa/\rho C)$, where ρ, the mass density, and C, the specific heat, are of order unity, and $\kappa(T = 20T^*) \simeq 2k_B(g_0/\sigma)^{1/2}$. Most of our simulations were longer than 5×10^6 reduced time units, sufficient for the longest chains studied here. The Lyapunov exponents converge much faster than the local temperatures.

The Lyapunov spectra for nonequilibrium systems differ only slightly from equilibrium spectra of the same chain, for which both boundary temperatures are equal. As an example we show in Fig. 5 a spectrum for a 63-particle chain with boundary temperatures $T_{\text{hot}} = 28$ and $T_{\text{cold}} = 12$ in units of T^*. Although not noticeable on the scale of this figure, the sum of all exponents is negative. From the Kaplan-Yorke formula we deduce that the information dimension D_1 of the underlying strange attractor in phase space is 125.9954 ± 0.0001. This corresponds to a reduction in dimensionality $\Delta D = 0.0046 \pm 0.0001$. We observe from Table I and from Fig 6 that ΔD varies, for given $T_{\text{hot}} - T_{\text{cold}}$, as the heat flux Q and, consequently, is proportional to $1/N$. But also the driving temperature gradient decreases with $1/N$ if the length

TABLE I. Simulation results for nonequilibrium chains of N particles and length $L=(N+1)\sigma$. The left and right stochastic-boundary temperatures, T_{hot} and T_{cold}, and the extrapolated temperatures, T_0 and T_L, are given in units of $T^* \equiv mg_0\sigma/k_B$. κ_0, the conductivity at unit temperature, is given in units of $k_B(g_0/\sigma)^{1/2}$. Q is the heat flux (units: $mg_0^{3/2}\sigma^{1/2}$), λ_1 the maximum Lyapunov exponent [units: $(g_0/\sigma)^{1/2}$], and $\Sigma_{l=1}^{2N}$ is the sum over all exponents. $\Delta D = 2N - D_1$ is the dimensionality reduction, where D_1 is the Kaplan-Yorke (information) dimension. $\langle K\rangle/N$ and $\langle\Phi\rangle/N$ are the time-averaged kinetic and potential energies per particle, respectively, given in units of $mg_0\sigma$.

N	T_{hot}	T_{cold}	T_0	T_L	κ_0	Q	λ_1	$\Sigma_{l=1}^{2N}$	ΔD	$\langle K\rangle/N$	$\langle\Phi\rangle/N$
7	22	18	21.9	18.1	0.0234	0.972	4.782	−0.0098	0.00205	10.01	8.23
15	22	18	21.9	18.0	0.0233	0.503	5.334	−0.0051	0.00095	10.03	8.96
31	22	18	21.9	18.0	0.0233	0.253	5.585	−0.0026	0.00046	10.04	9.30
63	22	18	21.9	18.0	0.0237	0.130	5.709			10.04	9.46
127	22	18	21.9	18.0	0.0232	0.065	5.775			10.02	9.52
7	24	16	23.5	15.9	0.0232	1.932	4.781	−0.040	0.0084	10.04	8.25
15	24	16	23.7	15.9	0.0234	1.009	5.336	−0.021	0.0040	10.10	9.02
31	24	16	23.9	16.0	0.0233	0.516	5.590	−0.011	0.0020	10.18	9.41
63	24	16	24.0	16.0	0.0235	0.265	5.718	−0.006	0.0010	10.21	9.59
127	24	16	23.9	16.0	0.0236	0.131	5.784			10.17	9.63
255	24	16	24.0	16.0	0.0236	0.067	5.829			10.22	9.71
15	28	12	27.3	11.0	0.0235	2.054	5.344	−0.098	0.0183	10.46	9.29
31	28	12	27.6	11.4	0.0238	1.063	5.605	−0.051	0.0090	10.61	9.74
63	28	12	27.9	11.7	0.0238	0.544	5.741	−0.026	0.0046	10.72	9.98
127	28	12	28.0	11.8	0.0239	0.274	5.817	−0.014	0.0023	10.76	10.10
255	28	12	28.1	11.7	0.0230	0.134	5.867			10.79	10.16
15	36	4	33.8	0	0.025	4.270	5.36	−0.948	0.176	11.80	10.30
31	36	4	35.1	0	0.024	2.322	5.66	−0.516	0.091	12.40	11.10
63	36	4	35.9	0	0.025	1.206	5.81	−0.277	0.047	12.65	11.44
127	36	4	36.0	0	0.025	0.606	5.90	−0.136	0.023	12.74	11.58
255	36	4	36.3	0	0.025	0.308	5.96			12.88	11.73

of the chain increases. For a constant heat flux we deduce from Fig. 6 that for not too large temperature gradients the dimensionality reduction ΔD is proportional to N reminiscent of the extensivity found for dynamically thermostated homogeneous nonequilibrium systems [10]. Here we are limited to rather short chains (small N) to observe this extensive behavior. The reason is that the temperature gradients cannot be increased arbitrarily to allow for larger N, and that the temperate T_{cold} becomes so low in the process that the ratio ν_B/ν_{BF} is too small to support Fourier heat conduction near the cold boundary. This happens already for the largest gradients studied here for which $T_{\text{hot}}=36T^*$ and $T_{\text{cold}}=4T^*$ to

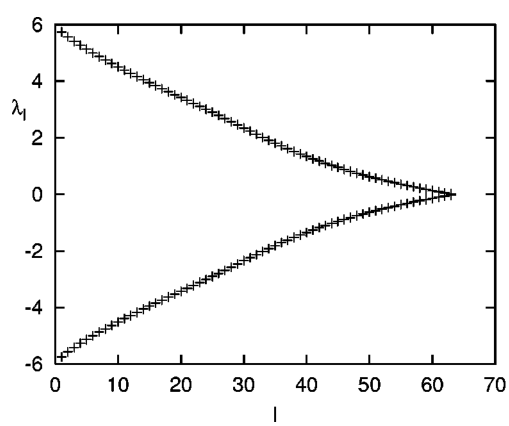

FIG. 5. Lyapunov spectrum for 63 ding-a-ling particles and for the boundary temperatures $T_{\text{hot}}=28$ and $T_{\text{cold}}=12$ in our reduced units $T^*=mg_0\sigma/k_B$. The sum over all exponents is negative as indicated in Table I. The Lyapunov exponents are given in units of $(g_0/\sigma)^{1/2}$.

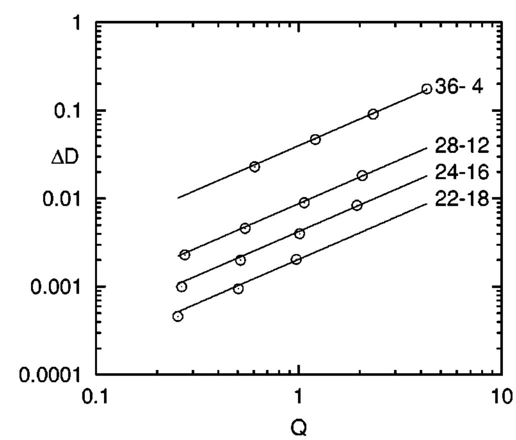

FIG. 6. Dimensionality reduction ΔD as a function of the heat flux Q for the boundary-temperature differences $T_{\text{hot}}-T_{\text{cold}}$ indicated by the labels (in units of $T^*=mg_0\sigma/k_B$). The straight lines are a fit of a linear relation $\Delta D = aQ$ to the data points. Along each line N varies parametrically.

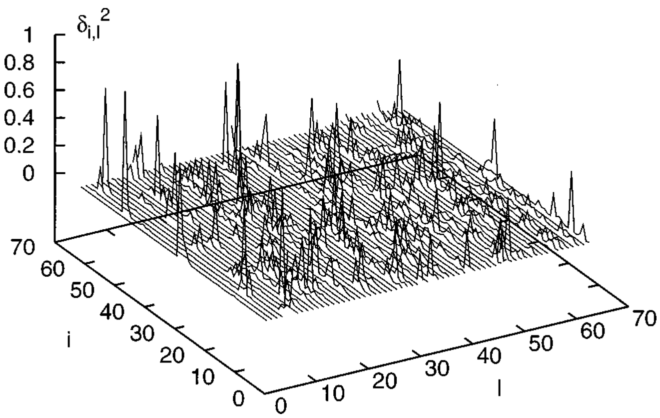

FIG. 7. Mean squared components $\delta_{i,l}^2$ for a gravitational ding-a-ling chain of 63 particles coupled to stochastic boundaries with $T_{\mathrm{hot}}=28T^*$, and $T_{\mathrm{cold}}=12T^*$. Only Lyapunov indices $1\leqslant l\leqslant 63$ associated with positive exponents are considered.

which the topmost line in Fig. 6 refers: For fixed Q, ΔD starts to increase much faster than proportional to N, once T_{cold} drops below $10T^*$. We also note that for a given length of the chain the reduction in dimensionality increases with the square of the temperature gradient, as expected. From an atomistic point of view the temperature gradients appearing here are extremely large.

In one dimension, the flow of heat, for a fixed temperature difference, is inversely proportional to system size. In two dimensions, for a square system, the heat flow is unchanged, while in three it increases. Thus the one-dimensional systems become more and more like equilibrium systems as the size is increased. The decreasing dissipation, with increasing system size, means that the reduction in phase-space dimensionality is largest for small systems.

In previous work [15,17,18] we have introduced so-called ''squared particle components'' $\delta_{i,l}$ defined as the projections of the offset vectors $\delta_l=\{\delta x_1,\delta p_1,\ldots,\delta x_N,\delta p_N\}_l$, associated with the Lyapunov exponent λ_l, onto the subspaces spanned by the phase variables of an individual particle i: $\delta_{i,l}^2\equiv\{\delta x_i^2+\delta p_i^2\}_l$. Since the offset vectors are taken as unit vectors in tangent space, the squared components obey the sum rule $\Sigma_{i=1}^N\delta_{i,l}^2=1$ for each l. They indicate to what extent a particular molecule i contributes to the phase-space expansion (contraction), as is quantified by λ_l, at any instant of time. In Fig. 7 we show $\delta_{i,l}^2$ for a stationary nonequilibrium chain of 63 particles, $1\leqslant i\leqslant 63$, and for all l associated with positive exponents, $1\leqslant i\leqslant 63$. For $l=1$ referring to the maximum exponent always a very localized active zone is observed to which only very few particles, sometimes only one or two, belong at any instant of time. It is a consequence of the competition between various colliding particles and a selection process introduced by the renormalization of the offset vectors in tangent space. An analogous behavior has been found in two dimensions for various dynamical systems [15,17,18] without stochastic boundaries, and has been also predicted from theoretical arguments [19]. The patterns of $\delta_{i,l}$ for larger l, may be much more complicated and less localized, and may involve various clusters of particles. In contrast to previous studies with two-dimensional dynamical systems [18] we do not find a coherent modelike structure for l belonging to the smallest positive exponents. This finding is partially due to the stochastic boundaries, but is mainly due to the lack of any long-wave acoustic modes.

IV. CONCLUSIONS

We have confirmed that the ding-a-ling model has a well-behaved heat conductivity. Likewise, it appears that the Lyapunov spectrum has a convergent large-system limit. We have developed an approach to the estimation of Lyapunov spectra for systems with stochastic boundaries, and used it to estimate the dimensionality loss of the strange attractor for a conducting ding-a-ling chain. The loss is limited in one dimension, where only two particles constitute the entire boundary. It is logical to expect that this same method, in two and three dimensions, would lead to a phase-space dimensionality reduction of order $N^{(D-1)/D}$ in D physical dimensions for given $T_{\mathrm{hot}}-T_{\mathrm{cold}}$. Although this latter dependence would seem inconsistent with an extensive dependence, $\Delta D\propto N$, as is suggested by irreversible thermodynamics, where the entropy production is proportional to the total volume of the system, any system that is both driven and thermostated at the boundary will have a dissipation rate proportional to a transport coefficient and to L^{D-2}. For hard particles the transport coefficient and the boundary driving can both increase, proportional to L, giving for the overall dissipation L^{D+1}. On the other hand, both the Lyapunov spectra and the boundary temperature increase, as L and L^2, respectively, so that the dimensionality loss should decrease as the surface/volume ratio.

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