One-Dimensional Classical Many-Body System Having a Normal Thermal Conductivity

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By numerically computing orbits for a chaotic, one-dimensional, many-body system placed between two thermal reservoirs, we verify directly that its energy transport obeys the Fourier heat law and we determine its thermal conductivity K. The same value of K is independently obtained by use of the Green-Kubo formalism. These numerical studies verify that chaos is the essential ingredient of diffusive energy transport, and they validate the Green-Kubo formalism.

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Neither phenomenological nor fundamental transport theory can predict whether or not a given classical many-body Hamiltonian system yields an energy transport governed by the Fourier heat law. Indeed, transport theory circumvents this quite deep dynamical problem by explicitly postulating that the many-body problem is analytically unsolvable and that dynamics can be replaced by suitably chosen probability assumptions which are, by definition, unverifiable in terms of first principles.

In this paper we shall use results from contemporary nonlinear dynamics to select a many-body system which, by direct numerical integration of its equations of motion, can be shown to obey the Fourier heat law. Recall that heat flow obeys a simple diffusion equation which can be regarded as the continuum limit of a discrete random walk.[1] Thus, randomness is an essential ingredient of thermal conductivity. Fortunately, dynamics has established the existence[2] of a class of Hamiltonian systems—called K systems—almost all of whose orbits are, in fact, deterministically random despite the seeming contradiction of these words.[3] Thus, for the first time, the possibility exists of obtaining the Fourier law from dynamics, a problem which Peierls[4] has called one of the outstanding unsolved problems of modern physics.

In seeking a simple model which can be shown to obey the Fourier heat law, we have been forced to meet two requirements. First, we must select a deterministically random system, and second, we must choose a system of sufficient simplicity that numerical analysis is feasible. Thus, we immediately exclude integrable, near integrable, ergodic (only), and mixing (only) systems since they are not deterministically random; in fact, diffusive energy transport has never been observed in these systems.[5,6] But let us recall that even systems obeying the Fourier heat law can transport energy in the form of slowly decaying coherent excitations such as soundlike pulses and solitary waves. In numerical experiments which unavoidably consider only a small number of particles, this phenomenon is quite troublesome. Specifically, though K or almost K systems[7] guarantee[3,6] that these soundlike solutions will eventually decay, we must find a small chaotic system in which this decay rate is sufficiently rapid.

In consequence, we have selected a many-body system which exhibits, as a parameter is varied, the full range of behavior from integrable to almost K and which at the same time has no problem with energy-bearing, long-lived, solitonlike pulses. Figure 1(a) reveals our model to be a one-dimensional array of equal mass, hard-point particles. We insisted on a one-dimensional system to eliminate higher dimensionality as a crucial element in obtaining a normal thermal conductivity. The even-numbered particles in Fig. 1(a) form a set of equally spaced lattice oscillators with each oscillator being harmonically bound to its individual lattice site and with all oscillators vibrating at the same frequency ω. The odd-numbered particles are free particles constrained only by the two adjacent even-numbered oscillators. Because each free particle moves like a clapper between two bells, we have come to call the system in Fig. 1(a) the "ding-a-ling" model. Aside from the appropriateness of the onomatopoeia, this name reflects the seeming ridiculousness of

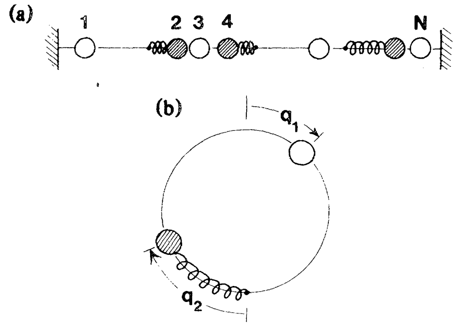

FIG. 1. (a) The N-particle ding-a-ling model. (b) The two-particle, periodic system. Here the springs merely symbolize the harmonic restoring force on each bound particle and they should not be regarded as actually existing.

presuming that the ding-a-ling model could have any relevance to physics. The Hamiltonian for the N-particle ding-a-ling model may be written

$$H=\frac{1}{2}\sum_{k=1}^{N}(P_k^2+\omega_k^2 q_k^2)+\text{hard point core}, \quad (1)$$

where ω_k equals ω for even k and zero for odd k and where all particles have unit mass. It may be shown that the dynamics governed by the Hamiltonian (1) is uniquely determined by the ratio $E/\omega^2 l_0^2$, where E is the energy per particle and l_0 is half the lattice distance between two bound particles. In consequence, we may let ω be the fundamental parameter of our model after setting $l_0=1$ and $E=1$. As ω tends to zero in Hamiltonian (1), the system tends to the well-known integrable hard-point gas. As ω increases from zero, a smooth transition to almost-K-system behavior is observed. To illustrate the effect of varying ω for fixed particle number, in Fig. 2 we display surfaces of section for the periodic, two-particle ding-a-ling model shown in Fig. 1(b). Kolmogorov-Arnold-Moser curves cover much of Fig. 2(a) at $\omega=0.2$, while chaos dominates in Fig. 2(b) at $\omega=3.0$. Moreover, we have verified that the ω value at which almost-K-system behavior occurs decreases dramatically with increasing particle number. Turning now to the question of attenuation for solitonlike pulses, as a pulse propagates through the lattice of Fig. 1(a) it gives a fraction of its energy to each bound particle is passes. As ω increases, it may be shown that the propagation distance to extinction decreases rapidly. In summary, the ding-a-ling model exhibits a transition to almost-K-system behavior with controllable attenuation of soundlike pulses.

We have established the validity of the Fourier heat law for our model in two ways. In the first, we

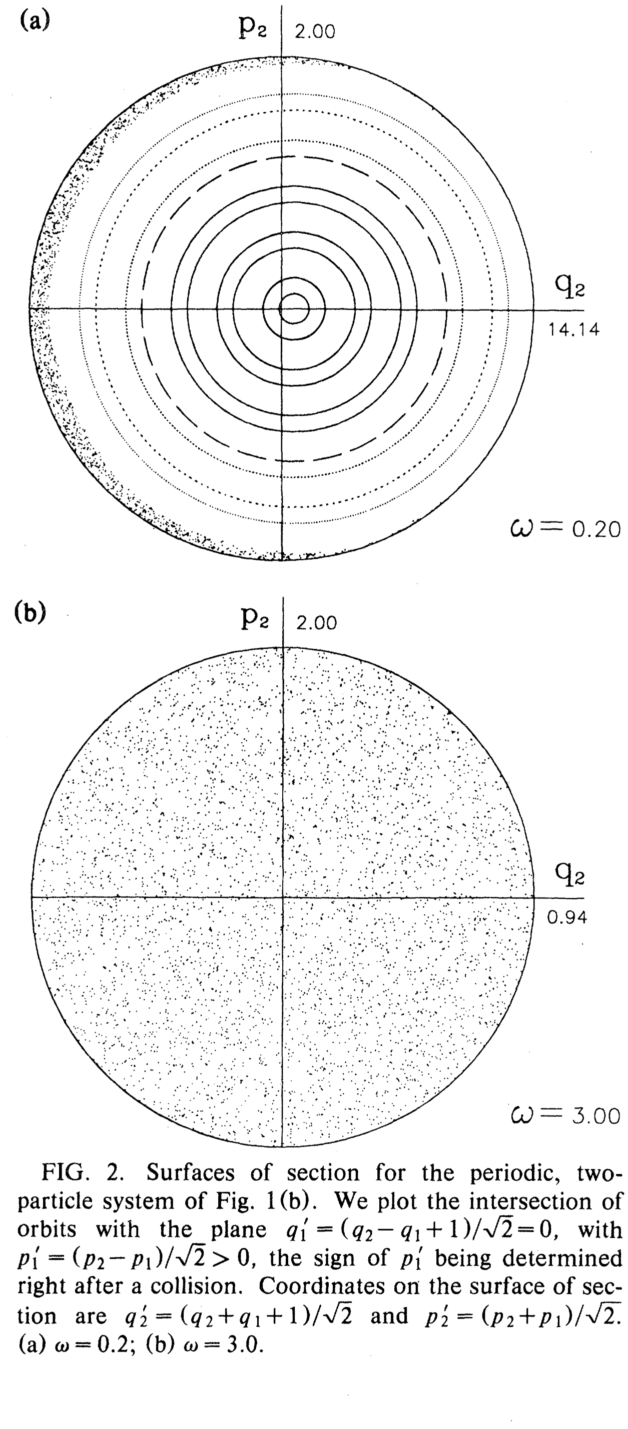

FIG. 2. Surfaces of section for the periodic, two-particle system of Fig. 1(b). We plot the intersection of orbits with the plane $q_1'=(q_2-q_1+1)/\sqrt{2}=0$, with $p_1'=(p_2-p_1)/\sqrt{2}>0$, the sign of p_1' being determined right after a collision. Coordinates on the surface of section are $q_2'=(q_2+q_1+1)/\sqrt{2}$ and $p_2'=(p_2+p_1)/\sqrt{2}$. (a) $\omega=0.2$; (b) $\omega=3.0$.

let N be odd in Eq. (1) and place the freely moving end particles of the ding-a-ling model in contact with two thermal reservoirs at temperatures $T_L=2.5$ (left) and $T_R=1.5$ (right), in arbitrary units. These reservoirs are taken to be "Maxwellian" gases characterized by the velocity distribution

$$f(v)=(|v|/T)\exp(-v^2/2T). \quad (2)$$

When either of the free end particles passed through an arbitrarily defined system boundary it was absorbed by the relevant reservoir and then emitted back into the system with a velocity determined by the probability distribution of Eq. (2). The amount of energy ΔE exchanged with the reservoir in this way is used to compute the dimensionless average flux $\langle J \rangle$ at each system boundary, where

$$\langle J(t)\rangle = t^{-1}\sum_{i=1}^{n} \Delta E_i, \tag{3}$$

with ΔE_i denoting the energy transfer at the ith reservoir interaction and $n = n(t)$ the number of interactions up to the time t. Equality of these two boundary fluxes signals the onset of a stationary state. Then, after defining the particle temperature to be twice its average kinetic energy, we computed the value of the steady-state internal temperature gradient ∇T by obtaining a least-squares straight-line fit to the temperature data. Finally, we calculated at $\omega = 10$ the thermal conductivity K via the Fourier heat law $\langle J \rangle = -k\nabla T$. Because ω is large here, we are at liberty to use very short lattices and relatively long computation times which greatly reduces statistical fluctuations. We have considered two distinct lattices having five and nine moving particles. The results are summarized in Table I. Since for $N > 4$ the critical ω value for the onset of chaos is extremely small, one might expect to verify the Fourier law for very small ω. However, as mentioned earlier, decreasing ω below a certain value permits solitonlike pulses to transport appreciable amounts of energy. Thus for given ω, the lattice size must be chosen long enough to thwart the effect of solitons to carry energy. In Fig. 3 we display the behavior of the thermal conductivity at $\omega = 1$. Here a normal conductivity indpendent of length is obtained only when the number of moving particles is greater than or equal to 11.

As an independent means of verifying our results we have computed the thermal conductivity K using a Green-Kubo formula which expresses transport coefficients as integrals of autocorrelation functions.[8] In particular, the thermal conductivity K for a one-dimensional system of length N and temperature T is given by

$$K = (\beta/TN)\int_{t_0}^{t} \langle J(t')J(t_0)\rangle\, dt', \tag{4}$$

where J is an average heat current, β is the usual inverse temperature, angular brackets denote an equilibrium average, and where, for finite systems Eq. (4) is valid only for times smaller than the sound transit time across the lattice. Specializing Eq. (4) to our model, it may be shown[6] that

$$K = \frac{1}{NT^2(t-t_0)}\sum_{i=1}^{N/2}\sum_{j=1}^{N/2} c_{ij}\langle \Delta Q_i \Delta Q_j\rangle, \tag{5a}$$

where

$$c_{ij} = \begin{cases} \frac{1}{2}; & |i-j| < N/4, \\ 0; & |i-j| = N/4, \\ \frac{1}{2}; & |i-j| > N/4. \end{cases} \tag{5b}$$

ΔQ_i means the change in energy between time zero and t in that portion of the lattice between particle i and particle $i + N/2$.

To evaluate Eq. (5), we have numerically integrated orbits for a 48-particle lattice with periodic boundary condition, i.e., 48 particles moving on a ring as in Fig. 1(b). In Fig. 4 we display the behavior of the function $K(t-t_0)$, computed via Eq. (5), for $\omega = 10$ and $\omega = 0.1$, respectively. For $\omega = 10$ the least-squares straight-line fit gives an average slope $s = 0.995$, very close to the theoretical value $s = 1$ expected for diffusive energy transport. The corresponding value of the conductivity

TABLE I. K, ∇T, and $\langle J \rangle$ for $N = 5, 9$.

N	K	∇T	$\langle J \rangle$
5	0.374 ± 0.008	−0.180	0.0672
9	0.376 ± 0.022	−0.105	0.0396

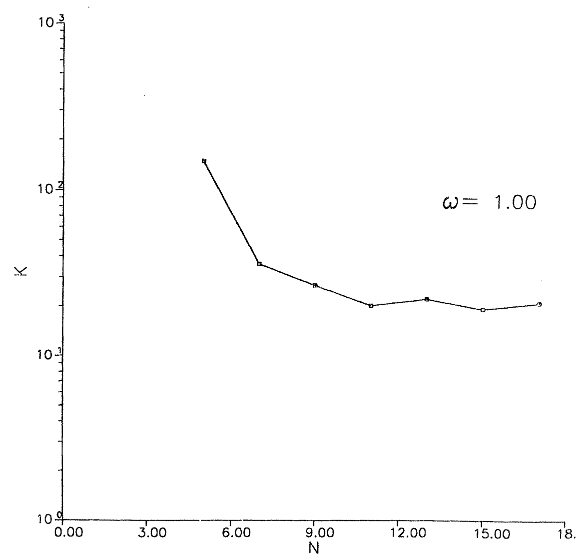

FIG. 3. Behavior of the coefficient of thermal conductivity as a function of the particle number N.

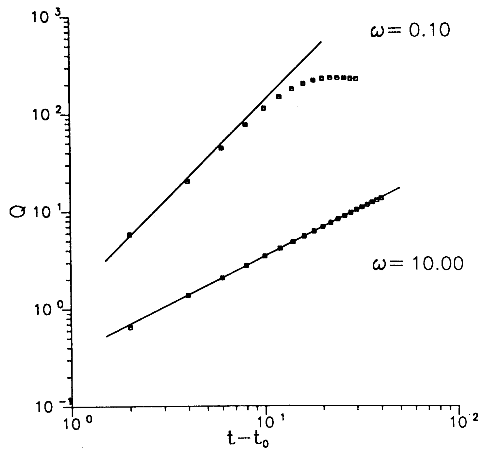

FIG. 4. Integrated heat current Q as a function of time, for a 48-particle lattice with periodic boundary conditions. Diffusive energy transfer (lower curve, slope $s=1$) is observed for $\omega=10$, while the energy initially propagates like sound for $\omega=0.1$ (upper curve, slope $s=2$).

$K=0.353\pm0.026$ is in excellent agreement with the reservoir value for K in Table I and thus confirms the validity of the Green-Kubo formula. For $\omega=0.1$, the initial slope agrees with that predicted for soundlike energy propagation characteristic of the hard-point gas ($s=2$, solid line). For longer times the slope decreases, since an increasing amount of energy is transported diffusively. However, the full transition to normal thermal conductivity can be barely observed because the data saturate for $t-t_0>10$, as a result of finite lattice size.

In this work we have established the validity of the Fourier law of heat conduction for a one-dimensional nonlinear system via direct integration of Hamilton's equations. Two independent approaches to the problems were used. First, if the system is placed between two thermal reservoirs at different temperatures, the steady-state heat flux is proportional to the temperature gradient, the coefficient of thermal conductivity being the negative of their ratio. Second, we have verified that the mean square energy change of Eq. (5a) grows linearly with time, as required for diffusive energy transport, and thence have computed the thermal conductivity K via a Green-Kubo formula. The fact that the same conductivity was obtained in these two cases provides striking mutual confirmation of both results. Moreover, it provides a major vindication of the Green-Kubo formalism.

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