Heat Conduction in Chains of Nonlinear Oscillators

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We numerically study heat conduction in chains of nonlinear oscillators with time-reversible thermostats. A nontrivial temperature profile is found to set in, which obeys a simple scaling relation for increasing the number N of particles. The thermal conductivity diverges approximately as $N^{1/2}$, indicating that chaotic behavior is not enough to ensure the Fourier law. Finally, we show that the microscopic dynamics ensures fulfillment of a macroscopic balance equation for the entropy production. [S0031-9007(97)02611-2]

The approach to nonequilibrium statistical mechanics through the introduction of microscopically time-reversible models has been shown to be rather powerful in the context of many-particle dynamics [1]. If the reversibility property is supplemented by the so-called *chaotic hypothesis*, the tools developed for strictly hyperbolic systems allowed making general statistical predictions that have been successfully tested [2]. Among the achievements of this approach, we recall the derivation of the Onsager reciprocity relations [3] and the expression of entropy production in terms of a self-generated dissipation rate [4].

So far, however, most of the numerical efforts in this area have been restricted mainly to the description of gases and fluids, where the thermostats, introduced to keep the energy constant, affect each particle [1] (with a few exceptions, such as Refs. [3,5,6]). In the present Letter we investigate the possibility of extending the above approach to a chain of coupled nonlinear oscillators, with specific reference to heat-conduction properties of insulating solids. In this context, the most natural choice is to put only the chain extrema in contact with two thermal baths at different temperatures.

A further motivation for the present work is the lack of convincing results about the validity of the Fourier conduction law in 1D systems. Let us briefly review the current state of the arts. In the simplest case of coupled harmonic oscillators, it was rigorously shown [7] that, if the extrema of the chain are put in contact with stochastic heat reservoirs operating at different temperatures, a nonequilibrium stationary state sets in with no temperature gradient in the bulk. As a result, thermal conductivity κ turns out to be proportional to the number of oscillators N. Such a divergence simply follows from the existence of extended waves (phonons) freely traveling and carrying energy along the lattice without attenuation.

Afterwards, the role of impurities has been taken into account, since it was expected that phonon waves should be damped by the scattering processes due to defects, thus possibly removing the divergence of κ. Unfortunately, it was found that although isotopic disorder in a harmonic chain yields a nonzero temperature gradient in the bulk [8,9], it still implies a diverging conductivity ($\kappa \approx N^{1/2}$) [10,11]. A finite κ has been obtained only by placing all the oscillators in contact with independent thermal baths [12]. As a result, one can conclude that no physically sound description of Fourier law can be obtained with harmonic chains.

More than disorder, anharmonicity has been invoked as the key feature of real solids responsible for normal heat conduction [13]: Nonlinearities make phonons interact among themselves, thus impeding free propagation. In the spirit of the general theory of dynamical systems, nonintegrability, rather than anharmonicity, is the property that should be responsible for a finite conductivity. In fact, nonlinear normal modes (solitons) freely transport energy along the chain. Our numerical simulations performed with a Toda chain [see Eqs. (1) and (2) for the precise definition of the model] do reveal the same scenario as for linear chains (see also [14]).

Numerical experiments for chains with chaotic smooth potentials [14,15] have been performed with too few particles to allow, even in the most detailed investigation [16], a conclusive study of the dependence of κ on N. The same can be said for the case where both anharmonicity and disorder have been simultaneously included [17,18].

Finally, we must recall two somehow artificial models that lead to contradictory conclusions: The first one is a chain of harmonic oscillators with an infinite barrier set at a given distance [19]; the second is the so-called ding-a-ling model, where harmonic oscillators alternate with free particles [20]. While in the former case the conductivity has again been found to diverge, in the latter the authors found convincing evidence that it attains a finite value.

In this Letter we study the Fermi-Pasta-Ulam (FPU) model, which represents the simplest anharmonic

approximation of a monoatomic solid. Specifically, we consider a chain of N oscillators, indicating with q_i the displacement of the ith particle from its equilibrium position. Fixed boundary conditions are assumed ($q_0 = q_{N+1} = 0$), while the dynamics of the central $N - 2$ oscillators is ruled by the equations of motion

$$\ddot{q}_i = f_i - f_{i+1}, \tag{1}$$

where $f_i = -V'(q_i - q_{i-1})$ and $V(x) = x^2/2 + \beta x^4/4$ is the interaction potential (β has been fixed equal to 0.1). Nosé-Hoover thermostats [1,21] act on the first and the last particle, keeping them at temperature T_+ and T_-, respectively,

$$\ddot{q}_1 = -\zeta_+ \dot{q}_1 + f_1 - f_2, \quad \dot{\zeta}_+ = \frac{\dot{q}_1^2}{T_+} - 1,$$
$$\ddot{q}_N = -\zeta_- \dot{q}_N + f_N - f_{N+1},$$
$$\dot{\zeta}_- = \frac{\dot{q}_N^2}{T_-} - 1. \tag{2}$$

The dynamical equations are left invariant under time reversal composed with the involution $p_i \rightarrow -p_i$. Recent numerical observations [22] show that time-reversible nonequilibrium dynamics yields results compatible with the predictions of Ref. [2], despite the fact that the system under investigation is not strictly Anosov. We expect that this should hold also for our model at sufficiently high temperatures. However, we shall not further address this point here; this will be the subject of a forthcoming paper [23].

We have performed extensive numerical simulations with several values of N and $T_\pm$, integrating the equations of motion with an improved fourth-order Runge-Kutta-Ghil algorithm. The first clear result is the convergence to a well defined spatial profile of the local temperature $T_i = \langle p_i^2 \rangle$ ($\langle \cdot \rangle$ denoting time average). The asymptotic stationary state satisfies the local equilibrium condition, as confirmed by the fluctuations of T_i that are in agreement with the canonical ones. The only exceptions are represented by the particles close to the boundaries, where the temperature profile seems to exhibit a singularity. Globally, the profiles satisfy a simple scaling relation, as clearly shown in Fig. 1, where the values of T_i, corresponding to different chain lengths (and the same boundary temperatures), are plotted versus i/N. The adoption of the above scaled units is tantamount to considering the continuum limit with the lattice spacing a equal to $1/N$. However, this is to be taken only as a formal interpretation, as the mass density obviously diverges when $N \rightarrow \infty$; conversely, if the equations are rescaled in such a way that both energy and mass densities are kept constant, one finds that the nonlinearity coefficient β should diverge.

The nonlinear shape of the profiles could be interpreted as an indication of a temperature-dependent conductivity, but this is incorrect, since simulations done with such small temperature differences as $T_+ - T_- = 4$ still reveal clear deviations from linearity. This is rather an indication of
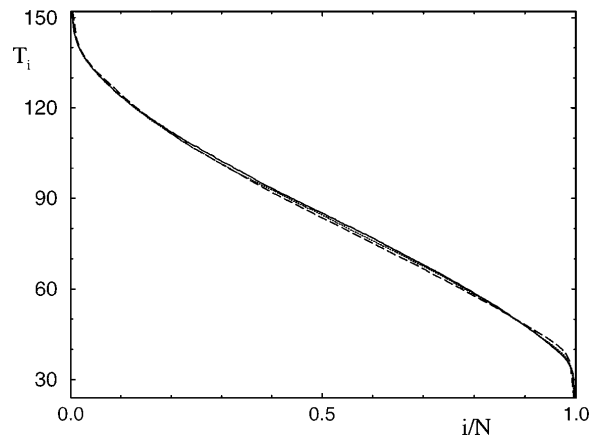

FIG. 1. Scaling of the temperature profiles for the FPU β model. The imposed temperatures are $T_+ = 152$ and $T_- = 24$, and chain lengths are $N = 128$, 194, and 256 (dashed, dotted, and solid lines, respectively). Averages are carried over a time interval $\approx 10^6$, after a transient $\approx 10^4$.

the relevant role played by boundary conditions; indeed, a seemingly square-root-type singularity in the temperature profile is always observed at the chain extrema.

The next result concerns the local heat flux $J(x,t)$, which is implicitly defined by the continuity equation,

$$\dot{H}(x,t) + \mathrm{div}J(x,t) = 0, \tag{3}$$

where $H = \sum_i H_i \delta(x - x_i)$, $H_i = p_i^2/2 + V(q_i - q_{i-1})$ and $x_i = ia + q_i$. By Fourier transforming (in space) Eq. (3), and upon expanding in powers of the wave number k, one eventually finds that the heat flux at the ith position is given by [23,24]

$$J_i(t) = a p_i f_{i+1}, \tag{4}$$

where $p_i f_{i+1}$ has the simple interpretation of the flow of potential energy from the ith to the neighboring particle. We have checked that $J \equiv \langle J_i(t) \rangle$ is independent of the lattice position i, as it should indeed be for a stationary nonequilibrium state.

The only physically meaningful setting for the comparison of heat fluxes for different values of N is achieved by fixing $a = 1$, as it is the case in real systems where the lattice spacing is determined by the mutual interactions. The data reported in Fig. 2 shows that J scales to zero as $N^{-\alpha}$, with $\alpha = 0.55 \pm 0.05$. The same scaling behavior has been obtained for different choices of the temperatures T_+ and T_-, provided that they are sufficiently large to ensure a chaotic behavior. This implies that the conductivity,

$$\kappa = \frac{J}{dT/dx}, \tag{5}$$

diverges as $N^{1-\alpha}$, since the temperature gradient vanishes as N^{-1}. Therefore, we are forced to conclude that
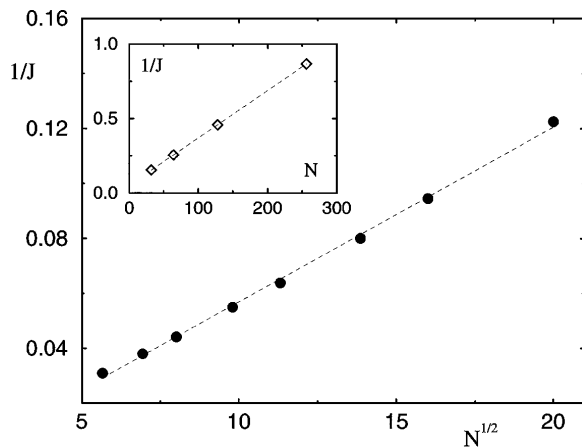
FIG. 2. Scaling of the heat flux J with the number of oscillators N for the FPU β model (same temperatures as in Fig. 1). The inset refers to the case of an imposed constant gradient $(T_+ - T_-)/N$ (see text) with the same boundary temperatures: Scaling with N^{-1} implies that the conductivity is constant.

Fourier law is not satisfied in the present framework and that chaoticity is not sufficient to ensure its validity. Surprisingly, the above behavior is similar to the one found in harmonic chains with random masses [11], as if disorder and anharmonicity played the same role. However, we have no explanation for this fact.

Two further remarks should be added as a comment to the scaling behavior of J. First, from the very definitions [Eqs. (4) and (5)], one realizes that the assumption $a = N^{-1/4}$ implies an asymptotically finite κ, but this is no more than just a formal statement. Second, notice that in the present philosophy, which is the standard one adopted in the literature, T_+ and T_- are kept fixed while N diverges, so that the temperature gradient (i.e., the external field) goes to 0. Accordingly, in the limit of large N, the chain gets closer and closer to equilibrium so that, independently of $(T_+ - T_-)$, a linear regime (in the Green-Kubo sense) is eventually attained. This is at variance with other physical settings, such as electric charge transport, where the external field is a free parameter whose magnitude can be fixed independently of the system size. Accordingly, it is not obvious how to study nonlinear corrections in this framework, if they are relevant at all.

As a last comment on thermal conductivity in FPU chains, we want to stress that a truly finite κ is observed when each particle is thermostated independently, according to a linear temperature profile. Obviously, in this case, $\langle J_i(t) \rangle$ depends on the lattice site, but its average value over all sites is found to scale as N^{-1} (see the inset of Fig. 2). This is analogous to what was found in Ref. [12] with stochastic heat baths. Needless to say, this result sounds a bit artificial, as the profile is imposed from the outside.

Returning to the usual case, the energy balance at the chain extrema implies that

$$J = -\langle \zeta_\pm p_{1,N}^2 \rangle = -\langle \zeta_\pm \rangle T_\pm, \qquad (6)$$

where the last equality is obtained from the condition $\langle d\zeta_\pm^2/dt \rangle = 0$. The above equation expresses the general scenario arising in time-reversible models that a nonequilibrium stationary state corresponds to a spontaneous emergence of dissipation [2,4]. The global volume contraction rate γ in phase space is given by the average of the divergence of the velocity field, i.e., $\gamma = \langle \zeta_+ + \zeta_- \rangle$. In all simulations we checked that $\gamma > 0$, as long as $T_+ \neq T_-$, consistently with a theorem recently proved by Ruelle [25]. In any case, $\langle \zeta_+ \rangle$ is always negative (provided that $T_+ > T_-$), as indeed prescribed by energy balance. In fact, the energy is pumped in from the hot reservoir, flows through the chain, and is eventually absorbed in the cold reservoir. Dynamically, it is at least bizarre that the hot thermostat is characterized by a local expansion of volumes: This is completely opposite to the approach in terms of stochastic baths, where dissipation is always assumed. To what extent this peculiar feature is physically meaningful is unclear; nevertheless, the interpretation in terms of entropy production makes perfect sense. In fact, Eq. (6) can be rewritten as

$$\langle \zeta_+ \rangle + \langle \zeta_- \rangle = J\left(\frac{1}{T_-} - \frac{1}{T_+}\right), \qquad (7)$$

with the convention that $J > 0$ is an incoming flux. Equation (7) can be physically interpreted as a balance relation for the global entropy production. According to the general principles of irreversible thermodynamics, the local rate of entropy production σ in the bulk is given by

$$\sigma(x) = J\frac{d}{dx}\left(\frac{1}{T(x)}\right). \qquad (8)$$

Upon integrating Eq. (8), the right-hand side of Eq. (7) is obtained, which can thus be interpreted as the global production rate of entropy in the bulk. On the other hand, according to general arguments on reversible thermostats [2], the left-hand side of Eq. (7) is identified with the entropy production from the heat baths. Equation (7) has been numerically tested in a wide range of temperatures.

A relevant consequence of Eq. (6) is that $\zeta_\pm$ are proportional to J, so that not only the fluxes but also the dissipation γ vanish in the thermodynamic limit $N \to \infty$. This is indeed a remarkable difference with respect to other models of gases and fluids studied, e.g., in Refs. [2,4,5], where the dissipation is always extensive. In our opinion, this is due to the vanishing of dT/dx, and not to the fact that thermostats act only at the boundaries. Indeed, by globally thermostating the two halves of the lattice at two different temperatures [26], we find that γ,

which is now the sum of N contributions, still goes to zero as $N^{-1/2}$.

Although it is generally believed that nonlinearity yields a finite thermal transport coefficient, we have shown that this is not true in FPU chains equipped with time-reversible thermal baths. The specific choice of the thermostat does not affect the generality of our conclusions since the repetition of some simulations with isokinetic (Gaussian) thermostats [1] lead to similar results. Another possible explanation of the divergence of κ could be the dimensionality of the system: It might be that solitonlike propagation is generically favored in 1D systems. At the present stage this is only a speculation that needs further investigation. Another item that should be seriously taken into account concerns boundary conditions. If, as we suspect, the nonlinear shape of the profile stems from the peculiar functioning of the thermostats, it is not to be excluded that a different setup could lead to more physically meaningful results. Some preliminary simulations performed by thermostating a number of $\mathcal{O}(N)$ particles on both the left and right sides suggest a possible slow convergence to a finite κ value. In any case, the anomalous behavior of the conductivity is presumably to be attributed to the almost free evolution of the small-wave-number Fourier modes even at high energies [27]. In fact, the small coupling of such modes with the rest of the chain suggests the possible existence of perturbations traveling almost undamped along the chain.

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