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# Normal and anomalous heat transport in one-dimensional classical lattices

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We present analytic and numerical results on several models of one-dimensional (1D) classical lattices with the goal of determining the origins of anomalous heat transport and the conditions for normal transport in these systems. Some of the recent results in the literature are reviewed and several original "toy" models are added that provide key elements to determine which dynamical properties are necessary and which are sufficient for certain types of heat transport. We demonstrate with numerical examples that chaos in the sense of positivity of Lyapunov exponents is neither necessary nor sufficient to guarantee normal transport in 1D lattices. Quite surprisingly, we find that in the absence of momentum conservation, even ergodicity of an isolated system is not necessary for the normal transport. Specifically, we demonstrate clearly the validity of the Fourier law in a pseudo-integrable particle chain. © *2005 American Institute of Physics.*
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**The study of how heat is transported through solids has a history dating back to antiquity and culminating, in the regime of classical physics, in the Fourier law of heat conduction, which asserts that the flux of heat (the "heat current") is proportional to a constant times the gradient of the temperature. This "normal transport" of heat corresponds to "diffusion" of the heat through the system and is observed in most physical systems. In some mathematical models and in certain specially prepared experiments, one can observe "anomalous" transport of heat. Strictly speaking, one uses the term anomalous transport to describe anything that is not "normal," up to and including the case in which the heat propagates ballistically through through the system. Numerous prior studies have sought to understand the origins of both normal and anomalous transport and to isolate key features of the systems that lead to each type of transport. A particularly important set of studies developed from the original Fermi–Pasta–Ulam (FPU) study of the (supposed) equipartition of energy in a one-dimensional chain of coupled *nonlinear* classical oscillators. Just as the study of the time evolution of the FPU system revealed the surprising result that there was no apparent evolution towards equipartition but instead a tendency towards the recurrence of the initial state, so the study of transport in FPU-like systems revealed that their thermal conductivity was indeed anomalous. In the present article, we explore systematically the conditions that lead to normal or anomalous conductivity in classical, one-dimensional chains ("lattices"). We find an interesting interplay among the consequences of translation invariance (momentum conservation), nonlinearity, complete integrability, and deterministic chaos, and demonstrate the particularly surprising result that chaos is neither necessary nor sufficient for normal conductivity in these systems.**

## I. INTRODUCTION

The related issues of thermalization, transport, and heat conduction in one-dimensional (1D) classical lattices have been sources of continuing interest (and frustration) for several generations of physicists, particularly since the pioneering computational study of Fermi, Pasta, and Ulam (FPU) revealed the remarkable "little discovery"[1] that even in a strongly nonlinear 1D lattice recurrences of the initial state prevented the equipartition of energy and consequent thermalization. The complex of questions that has developed from the FPU work involves the interrelations among equipartition of energy (the questions like: Is there equipartition? In which modes?), local thermal equilibrium (Does the system reach a well-defined temperature locally? If so, what is it?), and the transport of energy/heat (Does the system obey Fourier's/Ficke's heat law? If not, what is the nature of the abnormal transport?). Review articles spread over nearly three decades have provided snapshots of the understanding (and confusion) at different stages of this odyssey.[2–8]

In this article, we will explore a subset of these questions dealing with the transport of energy/heat in 1D classical lattices. In particular, we will focus on the many studies that have attempted to verify the validity of Fourier's law of heat conduction

$$\langle \mathbf{J} \rangle = -\kappa \nabla T \tag{1}$$

in 1D classical lattices or "chains."

Here, $\kappa$ is the transport coefficient of thermal conductivity and is supposed to be an *intensive* observable, i.e., inde-

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pendent of the size of the system. Strictly speaking, $\kappa$ is well defined only for a system that *obeys* Fourier's law and for which a *linear* temperature gradient is established. Further, since in general $\kappa$ is a function of temperature, the relative temperature variation across the chain should be small for $\kappa$ to be truly constant.

In the literature, the dependence of $\kappa(L)$ on the size $L$ of the system has also been used to characterize the (degree of) anomalous transport. However, the definition of $\kappa$ for an anomalous conductor, where no *internal* temperature gradient may be established, is highly ambiguous. Usually, one defines it as $\kappa_G(L) \equiv JL/\Delta T$ where $\Delta T$ is the total temperature drop between the two thermal baths. In this article we shall call such a definition of $\kappa_G$ a *global thermal conductivity*, in contrast to another definition of the so-called *local thermal conductivity* $\kappa_L = J/\nabla T$, which may depend on the position in the lattice, since $\nabla T = dT(x)/dx$ and is unique only in the case of a linear themperature profile. We note that the global and local thermal conductivities are proportional, namely $\kappa_L = c\kappa_G$ where $c$ does not depend on the size $L$, *if and only if* the temperature profile is scaling, i.e., $T(x) = \tau(x/L)$ where $\tau(\zeta)$ again does not depend on $L$. We will confront these subtle distinctions at several points in the ensuing discussion.

To place our work in the larger context, it is useful to recall that the issues of equipartition/thermal equilibration and heat conduction/energy flow, although clearly related, can in fact be studied separately. For instance, although an integrable system will never reach a thermal equilibrium ensemble unless it is started in one, the concept of "soliton statistical mechanics" is not an oxymoron: assuming that the system is in a thermal equilibrium ensemble, one can study what other aspects of statistical mechanics remain valid and, in particular, what role solitons play in the response of the system to external perturbations. Similarly, the study of thermal transport (Fourier's/Ficke's heat law), is the search for a *nonequilibrium steady state* in which heat flows across the system, and the flow is typically analyzed *assuming* the Green–Kubo formalism of linear response,[9] in terms of correlation functions in the thermal equilibrium (grand canonical) state, independent of whether a particular system can actually reach this state. Indeed, systems exhibiting "anomalous conductivity" are precisely those in which this analysis does *not* lead to Fourier's law.

We shall focus here on heat conduction but will attempt to make clear whenever our results impact (or depend on) the existence of equipartition and local thermal equilibrium.

Previous studies have led to bewildering array of partial results and conjectures:

- harmonic chains,[10] showing $\kappa_G \sim L^1$, a result understood by the stability of linear Fourier modes, absence of mode–mode coupling, with the rigorous consequence that no thermal gradient can be formed in the system;
- integrable models,[3] $\kappa_G \sim L^1$, a result understood by the presence of *nonlinear* stable modes (the solitons) and complete interability;[3]
- nonintegrable models with smooth potentials: (1) the FPU models, leading eventually to claim that chaos was necessary and sufficient for normal conductivity ($\kappa_G \sim \kappa_L \sim L^0$), Ref. 8, a claim that has been countered by strong numerical evidence for anomalous conductivity in FPU chains ($\kappa_G \sim \kappa_L \sim \sim L^\alpha$, where $\alpha \approx 0.37$);[11,12]; (2) the diatomic Toda chain, where initial results claiming $\kappa_G \sim L^0$, Ref. 13 have recently been refuted by a study showing $\alpha \approx 0.4$, Ref. 14; (3) the Frenkel–Kontorova model, which shows (at least for low temperatures) $\kappa_G \sim \kappa_L \sim L^0$, Ref. 15; and
- noninterable models with hard-core potentials (1) the "ding-a-ling" model[16] and (2) the "ding-dong" model,[17] both showing convincingly that $\kappa_G \sim \kappa_L \sim L^0$.

This bewildering array of results has recently been greatly clarified in a series of independent but overlapping studies. The numerical studies of Hu, Li, and Zhao[15] and of Hatano[14] show that *overall momentum conservation* appears to a key factor in anomalous transport in 1D lattices. Lepri *et al.*[18,19] and Hatano[14] have argued that the anomalous transport in momentum conserving systems can be understood in terms of low frequency, long-wavelength "hydrodynamic modes" that exist in typical momentum conserving systems and that *hydrodynamic arguments may explain the exponents observed in FPU*[18,19] *and diatomic Toda*[14] *lattices.* Later on, several othe papers appeared which tried to formalize the statement that momentum conservation implies anomalous transport.[20–22]

In the present article, we review these recent results and extend them on several fronts, using numerical simulations of several different models. First, we present a counterexample showing that converse of the earlier statement is not true: namely, anomalous conductivity does *not* imply that the model is momentum conserving. Second, we present convincing numerical data showing that chaos is neither necessary nor sufficient for normal conductivity, providing counterexamples to prior claims.[8] Finally, we present some (hopefully well-motivated) speculations on the necessary and sufficient conditions for *normal* conductivity in 1D lattice systems.

The class of models we study is described by the quite general 1D classical lattice Hamiltonian with single-particle and two-particle interactions

$$H \equiv \sum_n \left[ \frac{p_n^2}{2m_n} + U_n^{\mathrm{os}}(q_n) + V_{n+1/2}^{\mathrm{ip}}(q_{n+1} - q_n) \right]. \qquad (2)$$

Here, the particles moving in 1D have "absolute" coordinates $x_n = na + q_n$, where $a$ is the average lattice spacing and the relative coordinates $q_n$ designate the particles' displacements from their equilibrium (average) positions. We will either consider the particles to be on a ring with periodic boundary conditions (in this case $x_N \equiv x_0 + Na$, $q_N \equiv q_0$), or we will place the system between two thermal reservoirs (at possibly different temperatures) by coupling the edge particles 1 and $N$ to canonical stochastic "heat" baths. To present our analytic results in the most general context, we will consider arbitrary "disorder": the masses, $m_n$, can depend on lattice stite $n$, as can both the *on-site* potential $U_n^{\mathrm{os}}$ (which represents a "phonon-fixed lattice" interaction) and the *interparticle* potential $V_{n+1/2}^{\mathrm{ip}}$ (="phonon–phonon" interaction).

We begin our detailed discussion in Sec. II with a survey of several different models (mostly previously studied) that fit into the general class described by the Hamiltonian in Eq. (2). The models are presented in a general sense of increasing "normality," starting with (highly pathological) linear/harmonic chains, moving to (still pathological) integrable models, and finally treating (supposedly) "normal" chaotic models. Already from this survey we obtain two important results. First, we show that momentum conservation is not *necessary* for anomalous transport. The harmonic *optical* chain, which does not conserve momentum but does exhibit anomalous transport, provides one clear example of this, and an integrable model first introduced by Izergin and Korepin provides another. Second, by reviewing recent results in the FPU chain, which is known to exhibit chaos but also clearly displays anomalous conductivity, we can conclude that chaos is not sufficient for normal conductivity, in constrast to previous claims.[8] In Sec. II, we discuss some of the recent theoretical work on the relation between the total momentum conservation and anomalous heat transport. We show that one can relate momentum conservation to the divergence of a particular form of the Kubo formula corresponding to a nonequillibrium system of spatially uniform density. However, uniform pressure, as required by the stationary state, produces the gradient of the density (or gradient of the chemical potential) which drives the ballistic current in the oposite direction to the temperature gradient. The two ballistic contributions thus cancel and the resulting next order term typically gives anomalous superdiffusive transport. In Sec. III we define and study the family of "bing-bang" models, which are constructed by considering purely *hard-wall* potentials $U^{\rm os}$ and $V^{\rm ip}$. The bing-bang models are in fact equivalent to $N$-dimensional polyhedral billiards, which have vanishing Lyapunov exponents and therefore zero Kolmogorov–Sinai entropy. Hence, the bing-bang models are never chaotic in a sense of positive Lyapunov exponents. Nonetheless, we present convincing numerical evidence of *normal* (diffusive) heat transport in a (pseudo-integrable) nonchaotic but momentum nonconserving bing-bang model with an on-site potential. This demonstrates that *chaos*, at least in the sense of exponential instability of generic trajectories, is not necessary for the validity of the Fourier law. Taken together with the results from Sec. I, this shows the surprising result that chaos is neither necessary nor sufficient for normal conductivity in 1D classical lattices. In Sec. IV we summarize our results and conclude by discussing possible precise necessary and sufficient conditions for normal and anomalous transport.

## II. PARTIAL SURVEY OF PREVIOUS MODEL STUDIES

As this article is not a review of the very broad topic of anomalous transport,[7,23] the ensuing survey of previous model studies is not intended to be exhaustive, but rather merely illustrative, of the variety of models and results.

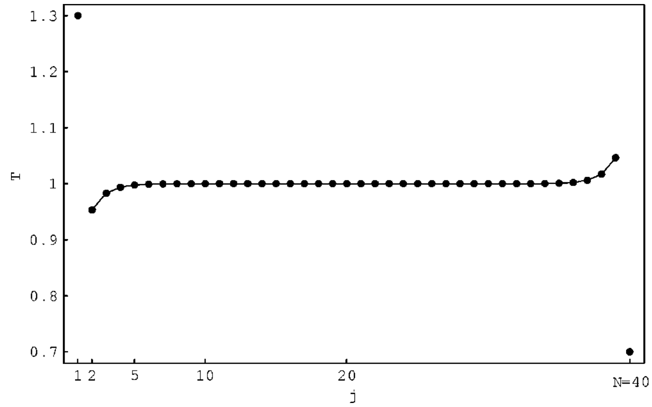


FIG. 1. Temperature profile for the linear *optical* chain with the parameter $\tilde{\nu}=0.25$ and with reservoir temperatures $T_L=1.3$, $T_R=0.7$. The size of the lattice here is $N=40$. As discussed in the text, this profile is the same as for the linear acoustic chain discussed in Ref. 10.

### A. Linear models

#### 1. The linear acoustic chain

One of the first and few rigorous results on the issue of thermal conductivity is due to Rieder, Lebowitz, and Lieb,[10] who studied a linear (acoustic) chain of $N$ (equal) harmonically coupled particles, where

$$U^{\rm os}(q) = 0, \quad V^{\rm ip}(q) = \tfrac{1}{2}\omega^2 q^2, \tag{3}$$

which are placed between two heat baths at temperatures $T_1$ and $T_N$. Rieder *et al.*[10] show that the transport is ballistic, with the average heat current $J$ which is proportional to the *difference* of the temperatures of the two heat baths and independent of the size of the system

$$J = \gamma(T_N - T_1). \tag{4}$$

They also calculate the temperature profile $T_j$, $j=1,2\ldots N$, proving that it is asymptotically flat at the value of the average temperature $T(0<j/N<1)\to\frac{1}{2}(T_N+T_0)$, as $N\to\infty$. However, close to the boundaries of the system the temperature profile exhibits exponentially attenuated jumps to satisfy the boundary conditions. Surprisingly, these jumps are in the opposite direction from the temperatures of the corresponding heat baths (see Fig. 1). Therefore, in the linear, *momentum-conserving* (acoustic) chain we find $\kappa_G=L^1$. But note that since the temperature profile is exponentially close to a flat profile, $\kappa_L\propto\exp(c_0L)$.

#### 2. The linear optical chain

Particularly in light of recent discussions on the role of on-site potential and total momentum conservation in heat conduction,[15,20] it is natural to pose the following simple question: what happens to the analysis of Rieder *et al.* if a harmonic (quadratic) on-site potential is added, thereby breaking the momentum conservation of the model but retaining its linearity? Remarkably, we have been unable to find a previous reference in which this question was studied, so we present the results briefly here. The model is effectively a discretized massive Klein–Gordon system or linear *optical* chain, with

$$U^{\mathrm{os}}(q) = \tfrac{1}{2}\Omega^2 q^2, \quad V^{\mathrm{ip}}(q) = \tfrac{1}{2}\omega^2 q^2. \tag{5}$$

The formalism of Ref. 10 applies to the general class of linear chains, so it can be applied to the case of the linear on-site potential (5). Because the analysis is straightforward, we merely quote the results here. The momentum *nonconserving* linear optical chain also exhibits ballistic ($\kappa_G \sim L^1$) heat transport. Indeed, this optical model behaves in essentially the same way as the acoustic chain. The general shape of the temperature profile [Eq. (4.2) of Ref. 10] and the expression of the heat current [Eq. (4.6) of Ref. 10] remain exactly the same, the only difference being that the dimensionless parameter $\nu \propto \omega^2$ of the linear acoustic chain[10] is replaced by

$$\tilde{\nu} = \nu + \frac{\Omega^2}{\omega^2}, \tag{6}$$

for the linear optical chain. Note that this simple analysis already provides a nontrivial result: anomalous transport does *not* imply momentum conservation, so that momentum conservation is not a necessary condition for anomalous transport.

We should note that linear chains are also highly pathological in the additional sense that many of their dynamical properties depend on the spectral properties of model of the heat baths. This is a simple consequence of the existence of time conserved normal modes. It has been pointed out in Ref. 24, that in the case of the linear chain with disordered masses, one can obtain super diffusive $\alpha > 0$, diffusive $\alpha = 0$, or even subdiffusive $\alpha < 0$, behavior for different choices of heat baths.

### B. Nonlinear but integrable models

#### 1. The Toda lattice

As an example of a nonlinear but integrable momentum-conserving model, we consider the celebrated Toda lattice,[2,25] for which

$$U^{\mathrm{os}}(q) = 0, \quad V^{\mathrm{ip}}(q) = \exp(-q). \tag{7}$$

Mokross and Büttner[26] have shown by numerical simulation that the temperature profile is almost flat and that the heat current is proportional to the difference of the bath temperatures (4). Hence they find numerical evidence for ballistic heat transport, with $\kappa_G(L) \propto L^1$, and $\kappa_L(L) \propto \exp(c_0 L)$, for this *integrable* and *momentum-conserving* but *nonlinear* chain. For a discussion of the role of solitons in this anomalous transport, see Ref. 3, and for the propagation of shock waves, see Ref. 27.

#### 2. The Izergin–Korepin discrete sine-Gordon model

The natural class of models to consider next is a nonlinear but integrable chain that does not conserve momentum, i.e., has $U^{\mathrm{os}}(q) \neq 0$. There are not many known models with such properties. However, one such model has been proposed by Izergin and Korepin[28] in the context of ultraviolet regularization of integrable quantum field theories in $1+1$ dimensions. They introduced a spatially discrete version of the famous sin($h$)-Gordon model (we shall call this IK–SG model) which has the following properties: it preserves the integrability of the continuum limit and it has an on-site potential [sin $\phi$ (for unimodular complex field) or sinh $\phi$ (for real field)]. The classical Hamiltionian formulation of the model has been described in detail by Tarasov in Ref. 29. For simplicity, we consider here the case of real field variables $\phi_j^{\pm}(t)$, $j \in \mathbb{Z}$, which corresponds in the continuum limit to the sinh-Gordon model with a confining anharmonic on-site potential. Unfortunately, the model cannot be cast exactly in the usual kinetic plus potential energy form of (2) except as an approximation to leading order in lattice discreteness (see later). Nonetheless, the model provides important insight into the question of the role of $U^{\mathrm{os}}$ in anomalous conductivity. Referring to Ref. 29, we find that the Hamiltonian of the discrete IK–SG model reads

$$H = \sum_n h_n, \quad h_n = h_n^+ + h_n^-, \tag{8}$$

$$h_n^{\pm} = \frac{(\phi_{n\mp1}^{+} \cos\delta - \phi_{n\pm1}^{-} \sin\delta)(\phi_n^{-}\cos\delta - \phi_n^{+}\sin\delta)}{(1+\phi_{n\pm1}^{-}\phi_n^{+})(1+\phi_{n\mp1}^{+}\phi_n^{-})} + \frac{2}{\sin 2\delta},$$

where the parameter $\delta$ is related to a *lattice spacing* $\Delta$ via $\Delta = 2\sin 2\delta$. For the *real* field variables $\phi_n^{\pm}$, the Poisson bracket is defined as

$$\{\phi_n^{-}, \phi_m^{+}\} = \frac{1}{4\cos 2\delta}\phi_n^{+}\phi_n^{-}(\phi_n^{+}\cos\delta - \phi_n^{-}\sin\delta)^2\delta_{nm},$$

$$\{\phi_n^{+}, \phi_m^{+}\} = \{\phi_n^{-}, \phi_m^{-}\} = 0. \tag{9}$$

The field variables can be transformed to conventional (discretized) canonical fields, $u(x)$, $u_n = u(x_n)$ and canonical momentum field $\pi(x)$, $\pi_n = \pi(x_n)$, $p_n = \pi_n \Delta$, and $x_n = n\Delta$, by the transformation

$$\phi_n^{\pm} = \frac{\exp\left(\mp\frac{1}{2}u_n\right)\cos\delta + \exp\left(\pm\frac{1}{2}u_n\right)\sin\delta}{\sqrt{1+\cosh(u_n)\sin 2\delta}}\exp\left(\frac{1}{4}p_n\right), \tag{10}$$

$$\{u_n, p_m\} = \delta_{nm}.$$

In fact, the discrete Hamiltonian (8) can be written explicitly as an expansion in $\Delta$ of the continuum sinh-Gordon Hamiltonian as

$$H = \sum_n \left\{ \left[\frac{1}{2}\pi_n^2 + \frac{1}{8}(u_{n+1} - u_{n-1})^2 + \cosh u_n\right]\Delta + \frac{1}{2}\cosh(u_n)\pi_n\Delta^2 + \mathcal{O}(\Delta^3)\right\}. \tag{11}$$

Izergin and Korepin have shown that the earlier discretized sinh-Gordon model (8) is completely solvable by the method of inverse scattering, and hence, they have explicitly demonstrated its integrability.

We have used the earlier exact completely integrable model (8) in order to check the nature of energy transport in

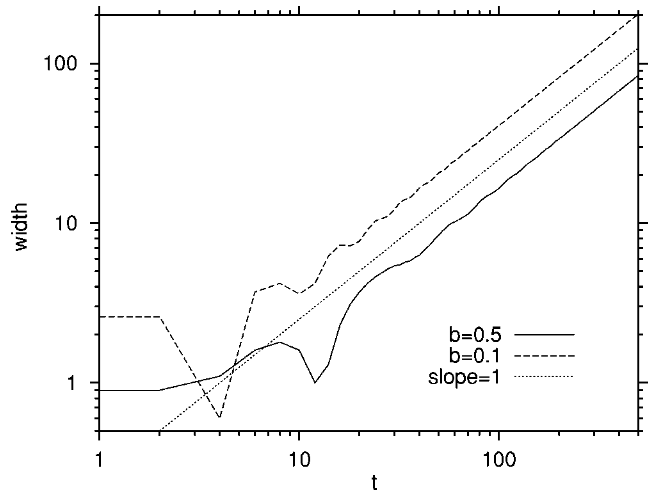


FIG. 2. The width, $\sigma(t) \equiv \sqrt{(\Sigma_n n^2 h_n)/(\Sigma_n h_n)}$, of a pulse spreading from an initial single-site disturbance as a function of time in the IK–SG model for two different values of parameter $b = \tan\delta$. The initial excitation is delta-like with $\phi_0^+ = 2, \phi_0^- = 3, \phi_n^{\pm} = 0, n \neq 0$. A finite lattice of length $N = 800$ with periodic boundary conditions has been used in the simulation. The line with slope 1 is used to guide the eye: the figure provides clear evidence of ballistic transport, $\sigma(t) \sim t$.

an IK–SG lattice. Since we have not found any natural intuitive way of coupling the variables $\phi_n^{\pm}$ (for $n = 1, N$) to the heat baths, we have decided to study the propagation of an initially localized pulse in an autonomous (isolated) lattice of very large size $N$ and with periodic boundary conditions $\phi_0^{\pm} \equiv \phi_N^{\pm}$. We start by initially exciting field variables at only one site (say $n = n_0 = N/2$) and setting all the others to the ground state (vacuum) value $\phi_{n \neq n_0}^{\pm} = 0$. Then we measure, numerically, after time $t$, the spatial spreading of the disturbance

$$\sigma^2(t) = \frac{1}{E} \sum_n (n - n_0)^2 h_n(t), \quad E = \sum_n h_n(t) = \text{const}. \tag{12}$$

For the numerical integration we use the adaptive step-size fourth order Runge–Kutta algorithm from Ref. 30. Clearly, for *diffusive* energy transport, one would find $\sigma(t) \propto t^{1/2}$, whereas for *ballistic* transport, $\sigma(t) \propto t$. In Fig. 2 we show results of two numerical experiments with different values of the lattice parameter ($\delta$ or $\Delta$); both show very clearly that (independent of the lattice parameter) the transport is ballistic, $\sigma(t) \propto t$.

This strongly suggests that integrability alone (the existence of an infinite number of independent conserved quantities in one-to-one correspondence with the set of degrees of freedom) is enough to yield anomalous (in fact, ballistic) heat transport, irrespective of the presence of on-site potential. This provides a second illustration, this time in a nonlinear context, of the result that momentum conservation is not necessary for anomalous transport.

## C. Chaotic models with smooth potentials

### 1. Chaotic but momentum conserving: The FPU models

In a series of recent studies[11,12,18,19] of the celebrated FPU $\beta$ chain,[1,8] for which

$$U^{\text{os}}(q) = 0, \quad V^{\text{ip}}(q) = \frac{1}{2}q^2 + \frac{1}{4}\beta q^4, \tag{13}$$

several groups have shown by careful numerical analyses that despite strongly chaotic behavior (characterized by almost everywhere positive Lyapunov exponents), the model exhibits power-law divergence of thermal conductivity in thermodynamic limit, $\kappa_L \sim L^{\alpha}$, with $\alpha \approx 0.4$. Hatano has shown[14] that for the diatomic Toda chain [same as (7) but for different (dimerized) masses, $m_{2n} = m_2 \neq m_{2n+1} = m_1$] there exists practically the same scaling with $\alpha \approx 0.4$ as for FPU models. More recently, a similar scaling has been shown for two other models: namely, for 1D chains where $V^{\text{ip}}(q)$ has the form of Lennard–Jones or Morse potentials.[31] These results suggests possible universality of the scaling exponent $\alpha \approx 0.4$ (perhaps $2/5$) of the divergence of thermal conductivity for strongly chaotic, momentum conserving lattices. This universality has been partially explained by Hatano[14] using hydrodynamic arguments or by Lepri *et al.*[7,18,19] using mode-coupling theory.[32]

However, recently Narayan and Ramaswamy[21] proposed another "thermodynamic" approach to mode–mode coupling theory, which using a mapping to Burgers equation and the renormalization group predicts the universal exponent for the divergence of heat conductivity to be $\alpha = 1/3$. It should be mentioned that there exist other models with no on-site potential which should conform to 1D hydrodynamics in the thermodynamic limit, for example diatomic hard-point gas in 1D, which seems to have a smaller exponent $\alpha$. Depending on the range and type of simulation[22,33,34] one finds values in the range $\alpha \in [0.25, 0.35]$.

On the other hand, there exist certain momentum conserving particle chains which seem to exhibit normal heat conduction to a very high numerical accuracy. This is the case for the so-called rotator model,[35,36] with no on-site potential $U^{\text{os}} \equiv 0$, and cosine interparticle potential $V^{\text{ip}}(q) = V_0 \cos q$. This model has a characteristic feature, namely it cannot support a nonvanishing pressure, and thus the infinite-wavelength phonons cannot carry any energy current,[20] but it is not clear why it should be excluded from the universality arguments.[21] Thus there remain still unsettled issues in connection to the heat transport in momentum conserving though chaotic lattices. For some recent progress see, e.g., Refs. 37 and 38.

In any case, note that the existence of anomalous conductivity in models that exhibit strong chaos proves that chaos is not sufficient for normal conductivity, refuting earlier claims.[8] In Sec. III, we shall show the still more surprising result that chaos is also not necessary for normal conductivity.

### 2. Chaotic but momentum nonconserving: The Frenkel–Kontorova model

Apart from a few more or less artificial models, such as ding-a-ling[16] and ding-dong[17] chains, which combine smooth and hard-core potentials, only one chaotic momentum nonconserving model with a smooth potential has been studied recently: namely, the Frenkel–Kontorova (FK) chain, with

$$U^{\mathrm{os}}(q) = U_0 \cos q, \quad V^{\mathrm{ip}}(q) = \tfrac{1}{2}q^2. \tag{14}$$

The numerical results of Hu, Li, and Zhao[15] establish convincingly that this model exhibits *normal* heat transport—$\kappa_L \sim L^0$—*provided* that the temperature is low enough: specifically, the thermal energy ($\sim k_B T$) must be smaller than the amplitude of the on-site potential barrier [$U_0$ in Eq. (14)]. However, for temperatures well above $U_0/k_B$, the mean free path of the phonons becomes (exponentially) large, so the Fourier law is no longer simple to observe numerically. Very recently, Ref. 39 reports on extensive numerical simulations which appears to confirm the normal heat transport in FK chain even for temperatures above $U_0/k_B$.

## III. MOMENTUM CONSERVATION AND ANOMALOUS TRANSPORT

In this section we discuss some interesting and important connections between momentum conserving lattices and anomalous heat transport in 1D which follow from considering Kubo formula and the linear response theory.

In the absence of an on-site potential, the general Hamiltonian of Eq. (2) becomes

$$H_{\mathrm{MC}} = \sum_{n=0}^{N-1} \left[ \frac{1}{2m_n} p_n^2 + V_{n+1/2}(q_{n+1} - q_n) \right], \tag{15}$$

where $V_{n+1/2}(q)$ is an arbitrary (generally nonlinear) interparticle interaction and the subscript "MC" stands for momentum conserving. As in Eq. (2) the interparticle potential, $V_{n+1/2}(q_{n+1}-q_n)$, and the masses, $m_n$, may depend on the site label $n$. However, there is now *no* on-site potential, $U^{\mathrm{os}}(q_n)$, depending on the individual coordinates. Thus, $H_{\mathrm{MC}}$ is invariant under translations $q_n \to q_n + b$ for *arbitrary* $b$, and this spatial translational symmetry corresponds to total momentum conservation. As before, we consider the (finite) system to be defined on a system of length $L = Na$ with periodic boundary conditions $(q_N, p_N) \equiv (q_0, p_0)$, where the actual particle positions are $x_n = na + q_n$.

We may write the Hamiltonian in Eq. (15) as $H_{\mathrm{MC}} = \Sigma_{n=0}^{N-1} h_{n+1/2}$, where $h_{n+1/2}$ is the Hamiltonian density

$$h_{n+1/2} = \frac{p_{n+1}^2}{4m_{n+1}} + \frac{p_n^2}{4m_n} + V_{n+1/2}(q_{n+1} - q_n). \tag{16}$$

Our aim is to estimate $\kappa$, the coefficient of thermal conductivity. Using the standard Kubo formula expression for $\kappa$ of linear response (see, e.g., Ref. 40):

$$\kappa = \lim_{T\to\infty} \lim_{L\to\infty} \frac{\beta}{L} \int_{-T}^{T} dt \langle J(t) J \rangle_\beta, \tag{17}$$

then one can show, from very elementary arguments,[20] that $\kappa = \infty$ provided the thermodynamic pressure $\phi$ (i.e., average force between an arbitrary pair of particles) is nonvanishing. Here $\langle\ \rangle_\beta$ denotes a canonical phase space average at inverse temperature $\beta$. The approach of Ref. 20 has been criticized[21,23] by the claim that the heat current of the Kubo formula (17) needs a modification for the case of a system with Gallilean invariance: Namely, the center of mass motion should be subtracted from the current, or one should put oneself into the frame where the total momentum is zero.

However, the formulation of Ref. 20 was based on a slightly nonstandard, though thermodynamically completely equivalent heat current, namely the so-called *lattice current*

$$J = \sum_{n=0}^{N-1} j_n, \tag{18}$$

where $j_n$ is the heat current density,[15] is given by

$$j_n = \{h_{n+1/2}, h_{n-1/2}\} \tag{19}$$

$$= \frac{p_n}{2m_n}[V'_{n+1/2}(q_{n+1} - q_n) + V'_{n-1/2}(q_n - q_{n-1})]. \tag{20}$$

$\{,\}$ is the usual canonical Poisson bracket. Note that this form of $j_n$ does correspond to the intuitive definition that the time rate of change of the energy at location $n$ which should be given by the (net) force $\sim [V'_{n+1/2}(q_{n+1} - q_n) + V'_{n-1/2}(q_n - q_{n-1})]$ times the velocity $p_n/2m_n$. More importantly, the current density $j_n$ by construction satisfies the continuity equation

$$\frac{d}{dt} h_{n+1/2} = j_{n+1} - j_n. \tag{21}$$

Since the usual derivation of linear response and Kubo formula are based on the *real-space heat current* $J_{\mathrm{rs}} = \Sigma_n \frac{1}{2} m_n v_n^3$, where $v_n = p_n/m_n$ is the velocity of $n$th particle, one needs to rederive carefully the linear response formalism for the lattice current. This has been done in Ref. 22. Now, we wish to stress that the lattice current $J$ and the real-space current $J_{\mathrm{rs}}$ are only equivalent if the center of mass motion is zero, precisely as required by the arguments of Refs. 21 and 23. In other words, adding a nonvanishing center-of-mass motion to the current $J_{\mathrm{rs}}$, does not change the lattice current $J$. Still, as shown in Ref. 22 the Kubo formula (17) does not refer to the proper perturbation of the equilibrium state so it does not describe the steady heat current between two heat baths.

This result is quite interesting and consistent with the interpretation given in Refs. 21 and 23. The unmodified Kubo formula (17), with the current (19), is the correct one if one considers a particular kind of nonequillibrium initial state, namely such with a *spatially uniform density* (or uniform chemical potential). This we call the *isochoric* initial state, and in such a case we find rigorously[20] that

$$\frac{\beta}{L} \int_0^T dt \langle J(t) J \rangle_\beta \geqslant \frac{t_0}{a\overline{m}} \phi^2 T, \tag{22}$$

so the transport is ballistic.

However, such a state cannot approximate a *steady state* of a large piece of the lattice between two heat baths at sligthly different temperatures. In such a physical situation, a steady state is formed where the *pressure* is constant along the system and not the *density*. Typically, in colder regions of the lattice, the density is larger and vice versa. This we call the case of *isobaric* initial state. Then, due to nonuniform density, a gradient of chemical potential is established as well, which drives the heat current in the opposite direction. To leading order in $L$, the contributions to the heat current due to the temperature and chemical potential gradients cancel each other. The difference of the two currents still produces the anomalous transport, since it decreases as $L^{\alpha-1}$. This has been demonstrated in a numerical experiment with high accuracy.[22] The modified Kubo formula referring to the *isobaric* situation[22] reads

$$\kappa = \lim_{T\to\infty} \lim_{L\to\infty} \frac{\beta}{L} \int_{-T}^{T} dt \{ \langle J(t)J \rangle_\beta + \phi \langle V(t)J \rangle_\beta \}, \tag{23}$$

where $V=\Sigma_n v_n$ is the sum of all particles' velocities $v_n$.

Although we have learned that the issue of anomalous transport cannot be resolved easily solely only on the basis of momentum conservation, it is clear from this analysis that the momentum conservation is a key attribute of the problem. It is also interesting to observe that in the case of vanishing pressure $\phi=0$ the isochoric and isobaric situations are described by identical Kubo formulas (17) and (23).

## IV. CHAOS AND NORMAL TRANSPORT: THE BING-BANG MODEL

The relationship between "chaos" and normal transport has been the subject of considerable interest, and it has even been claimed[8] that chaos is both necessary and sufficient the existence of normal transport. We have already shown that there exist models that exhibit both chaotic behavior and anomalous transport, so chaos is clearly not sufficient for normal transport. In this section, we establish the perhaps more surprising result that chaos is also not *necessary* for normal transport. We demonstrate this result using numerical studies of a 1D lattice model which, while exhibiting no chaos at all in the strict mathematical sense, nonetheless exhibits normal conductivity.

We call the particular class of many-body 1D classical lattices we study in this section the *bing-bang* models. As we shall see, they are manifestly nonchaotic in the sense of having Lyapunov exponents that are almost everywhere vanishing, but they are are also nonintegrable. The bing-bang models have infinite hard wall forms for both the *interparticle* potentials $V^{\text{ip}}(q)$, and the on-site potentials $U^{\text{os}}(q)$. If we fix the units such that the average lattice spacing is equal to unity, $a=1$, then the general (homogenous) bing-bang model would depend, apart from the masses $m_n$, on a triple of parameters $b,c,d \in \mathbb{R}^+$ which determine the potentials via

$$V^{\text{ip}}(q) = \begin{cases} 0, & -1 \leqslant q \leqslant b, \\ \infty, & \text{otherwise}, \end{cases} \tag{24}$$

$$U^{\text{os}}(q) = \begin{cases} 0, & -c \leqslant q \leqslant d, \\ \infty, & \text{otherwise}. \end{cases}$$

In fact, for a lattice of $N$ particles, the bing-bang model can be identified with the motion of a point billiard particle inside an $N$-dimensional polytope. Since the boundary consists solely of $(N-1)$-dim. flat hyperplanes—i.e., $-1 \leqslant q_n \leqslant b, -c \leqslant q_{n+1} - q_n \leqslant d$—(almost) any orbit is marginally stable, i.e., *parabolic* with zero asymptotic Lyapunov exponent. However, there is an infinite set (of vanishing Lebesgue measure in the full phase space) of very unstable orbits (which may also be called "diffractive" since they would produce diffraction of quantum mechanical waves) that eventually hit the (hyper)corners, edges, etc., either in the finite future or in the finite past. The simplest singular (infinitely unstable) orbits of this type are those that contain: (i) three particle collisions or (ii) simultaneous collisions of a pair of particles and one of the walls.

Our main goal in studying such physically pathological systems is to gain insight into the extent to which the properties of exponential instability and metric chaos (which our bing-bang models do not possess) are necessary to produce normal transport (or perhaps anomalous transport with a "universal" exponent $\alpha$ if the total momentum is conserved). The insights gained in previous studies of models with pathological, hard wall potentials—such as the "ding-a-ling"[16] and "ding-dong"[17]—provide ample motivation and justification for the current study. On the other hand, our results on decay of correlations (and, hence, perhaps on the mixing property) of nonhyperbolic (nonchaotic) systems with many degrees of freedom should stimulate development of new tools in ergodic theory to deal with such systems in a rigorous way.

With respect to the global dynamical proerties we define two subclasses of bing-bang models.

(i) **Pseudo-integrable bing-bang (PIBB)** models in which the masses of all particles are equal (set to unity) $m_n=1$. The pseudo-integrability of the model is easy to understand as follows. Upon interaction with interparticle potential $V(q_{n+1}-q_n)$ (interparticle collisions) the particles $n$ and $n+1$ just exchange their momenta/velocities, and upon interaction with the on-site potential $U(q_n)$ (collisions with a static hard wall) the momentum/velocity of the particle $n$ just changes sign. Therefore, the dynamics in momentum space acts as a discrete group $(\mathcal{C}_2)^N \times \mathcal{S}_N$, and any symmetric function of the squares of momenta $f(p_1^2,\ldots,p_N^2)$ is an invariant of motion. In fact, $N$ independent analytic invariants of motion $I_k$ can be systematically evaluated; they are the symmetric homogeneous polynomials of $\{p_n^2\}$:

$$I_1 = \sum_{n=1}^{L} p_n^2, \quad I_2 = \sum_{1\leqslant n<m\leqslant L} p_n^2 p_m^2,$$

$$\vdots$$

$$I_k = \sum_{1\leqslant n_1<\ldots<n_k\leqslant L} \prod_{l=1}^{k} p_{n_l}^2. \tag{25}$$

Therefore, any orbit of a PIBB model lies on an invariant surface of dimension $N$ in $2N$-dimensional phase space, and the system is *not ergodic* on the entire energy surface. However, the invariant surface is not a simple $N$ torus as in the case of a completely integrable system, but is an object of (vastly) increasingly complex topology as $N$ increases.

This is precisely the defining property of pseudo-integrable systems: namely, that there should exist a sufficient number of independent conservation laws for integrability but that the topology of invariant surfaces is more complicated than that of $N$-dimensional tori. This can only happen in the cases with singularities in the system: for instance, planar billiards in the shape of a polygon with angles that are rational multiples of $\pi$ are the most commonly studied class of (two-dimensional) pseudo-integrable systems.[41]

In the case of our PIBB models, the dimensionality of the phase space $2N$ can be arbitrarily large and increasing $N$ brings in new aspects and questions on dynamics that to the best of our awareness have not yet been considered in the literature.

Our analysis below suggests that the topology of invariant surfaces can become arbitrarily complex as one approaches the thermodynamic limit $N\to\infty$ and that then such invariant surfaces can more and more densely and uniformly cover the entire energy surface, so that at the end, statistical mechanics cannot distinguish the system from a truly ergodic (and mixing) one. We suggest (but cannot prove) that the topological genus of the invariant surfaces in our PIBB lattices increases faster than any power of $N$. Since it is not essential to our current discussion, we shall leave the rigorous characterization of topology of invariant surfaces of high-dimensional PIBB models as a very interesting open mathematical problem.

(ii) **Ergodic bing-bang (EBB)** models. We have good heuristic arguments (and strong numerical evidence) to support the conjecture that the generic bing-bang model with different masses $m_n$ (which should be generic, perhaps satisfying some irrationality conditions) is *ergodic*, since it corresponds to the motion inside $N$-dimensional polyhedral billiard. For example, it is rigorously known in the mathematical literature (see, e.g., Ref. 41 for a recent review, and references therein) that the set of ergodic polygonal billiards ($N=2$) is (at least) a dense set in the set of all polygonal billiards with a fixed number of vertices. It seems fairly obvious that the same result should apply (even more likely) in higher dimensions $N>2$. An even stronger result has been suggested recently:, namely that the generic polygonal billiard in the plane (e.g., triangular billiard with all angles having *irrational* ratio with $\pi$) is truly a *mixing* dynamical system and therefore exhibits fast decay to statistical equilibrium from (almost) any initial state.[42]

With respect to the key issue of total momentum conservation, we will study both *momentum conserving bing-bang models* (MC–PIBB or MC–EBB) which are characterized by $c,d=\infty$ (or saying that $U^{\mathrm{os}}=0$); and *momentum nonconserving bing-bang models* (MNC–PIBB or MNC–EBB), for which translational invariance is broken and generally at least one of parameters $c,d$ is finite.

### A. Momentum conserving bing-bang models

In this subsection we study two variants of momentum-conserving bing-bang models, one pseudo-integrable (MC–PIBB) and one ergodic (MC–EBB). Although they both behave as anomalous heat conductors, in accordance with the theorem proved in Sec. II, we study both in order to show the subtle but important differences that are a consequence of qualitatively different positions in the *ergodic hierarchy* (pseudo-integrability versus ergodicity).

In our numerical simulations we will study either (i) an open bing-bang lattice between two thermal baths at temperatures $T_L$ and $T_R$, or (ii) a closed bing-bang lattice with

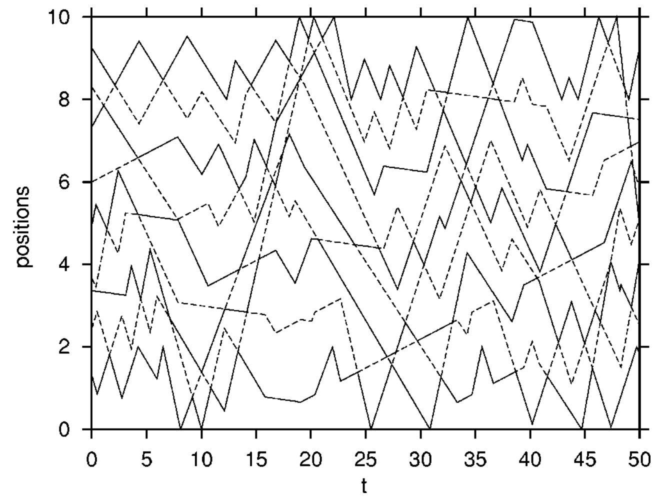


FIG. 3. Typical trajectories of the individual particles in a MC–PIBB model with constant unit masses and size $L=9$. The ordinate shows particle positions $[x_n(t)]$ where for clarity the odd $n$ particle trajectories are plotted with full lines while the even $n$ trajectories are dashed. The walls at $x=0$ and $x=10$ act as thermal baths at temperature $T=1$.

periodic boundary conditions where $N+1\equiv 1$. The thermal bath is realized as a wall (see, e.g., Ref. 43) which works in the following way: when the edge particle (with label 1 or $N$) hits the reservoir, it collides inelastically so that the new momentum (being independent from the old one) is given with the probability distribution

$$d\mathcal{P}/dp_{1,N} \propto p_{1,N}\exp[-p_{1,N}^2/(2m_{1,N}T_{L,R})]. \tag{26}$$

The velocity (momentum) prefactor takes into account the fact that the faster particles collide with the wall more often than the slow ones, so that the resulting velocity (momentum) distribution of the near-bath particles is indeed canonical Maxwellian (Gaussian).

Typical trajectories of the individual particles are shown in Fig. 3 for the MC–PIBB model and in Fig. 4 for the

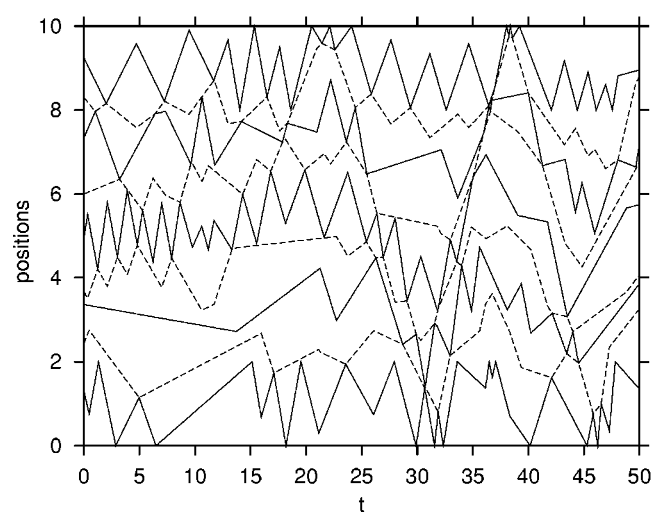


FIG. 4. Typical trajectory of a MC–EBB model with mass ratio $m_2/m_1=0.382$ and size $L=9$. As in Fig. 3, the ordinate shws particle positions $[x_n(t)]$ where for clarity the odd $n$ particle trajectories are plotted with full lines while the even $n$ trajectories are dashed. The walls at $x=0$ and $x=10$ act as thermal baths at temperature $T=1$.

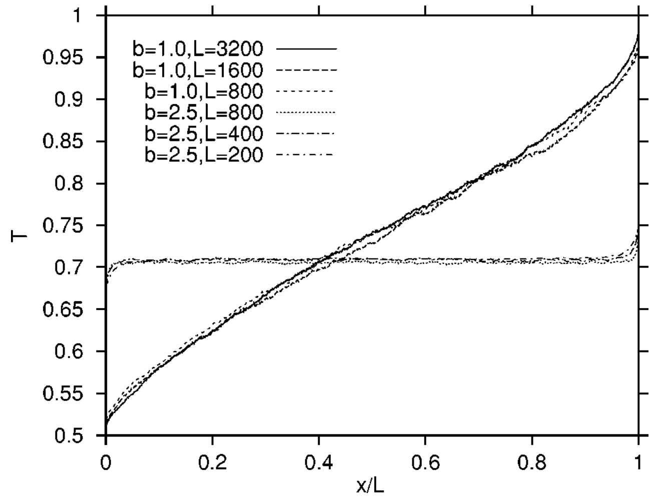


FIG. 5. Scaling of temperature profiles (temperature vs $x/N$ for different system sizes $N$) in a MC–PIBB model with thermal baths at temperatures $T_L=0.5$, $T_R=1.0$. The triple of steep curves refers to a system with symmetric interparicle potential $b=1.0$ (so that the pressure vanishes), while the triple of horizontal curves (at $T=\sqrt{T_L T_R}$, so zero temperature gradient over the bulk of the chain) refers to $b=2.5$ (and a nonvanishing pressure).

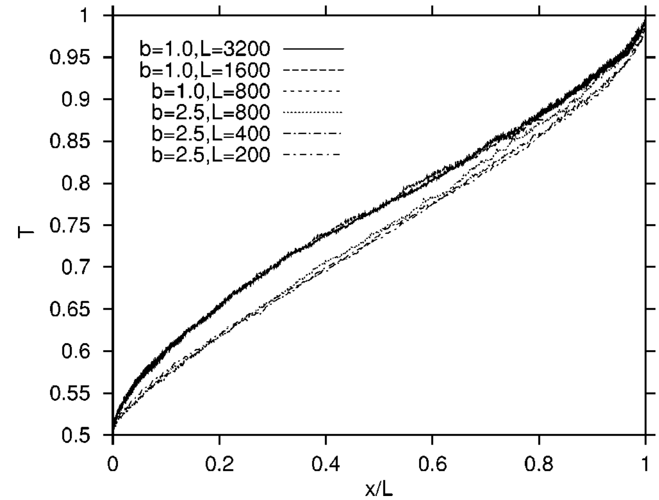


FIG. 6. Scaling of temperature profiles (temperature vs $x/N$ for different system sizes $N$) in a MC–EBB model with mass ratio $m_2/m_1=0.382$. All other parameters are the same as in Fig. 5. Note that here a nonvanishing temperature gradient is established even in the nonsymmetric case $b=2.5$ with nonvanishing pressure.

MC–EBB model, in order to give a reader an impression about the complex geometry of the orbits in bing-bang models despite their manifest nonchaoticity. In both cases, MC–PIBB and MC–EBB, the models are put between two heat reservoirs at the same temperature $T_L=T_R=T=1$. In the following we will present results of numerical simulations of heat conduction in a nonequillibrium stationary state with the bath temperatures $T_L=1$ and $T_R=2$. We measure the average heat flux $J(L)$ through the system as the function of the size $L(=N,$ since $a=1)$ and the kinetic temperature profile

$$T_n = \frac{\langle p_n^2 \rangle}{2m_n}.$$

First, we observe that temperature profile is typically a nonlinear function (non-constant $\nabla T$), although it has a scaling propery: namely, the local temperature for a given system is only a function of the scaled coordinate $n/N$ and reservoir temperatures

$$T_n = \tau(n/N, T_L, T_R). \qquad (27)$$

In Figs. 5 and 6, we show the sets of rescaled temperature profiles (for different lattice sizes) for the two models, MC–PIBB, and MC–EBB, respectively. However, note that in the light of the theorem of the previous section, it may be also important to distinguish the cases, of (i) the symmetric interparticle potential with zero pressure $(b=1, \phi=0)$, and (ii) nonsymmetric case with nonvanishing pressure $(b\neq 1, \phi \neq 0)$. We find that for both models (MC–PIBB and MC–EBB), at zero pressure $\phi=0$, $b=1$, a nonflat but also nonlinear temperature profile is established. However, for nonvanishing pressure, $b=2.5$, the MC–PIBB model exhibits a vanishing temperature gradient, which is consistent with completely ballistic transport (behavior similar to that found for the integrable models), whereas the MC–EBB model, which is "more ergodic," even in the case of nonvanishing pressure, establishes a "nonflat" (and nonlinear) temperature profile.

From our general theorem of Sec. II, we know that all these momentum conserving bing-bang models should exhibit anomalous conductivity. Using our extensive data on lattices of different sizes, we can confirm this by calculating for each of the models the dependence of the thermal conductivity $\kappa(L)$ on the size $L$ of the system. To account for the observed nonlinearity in the temperature gradients across the system, we have determined "average" temperature gradients $\nabla T$ with least squares linear fit of temperature profiles in the range $n=N/4 \ldots 3N/4$. Since the temperature profiles are scaling (27), any other choice would just redefine $\kappa$ by a constant factor (independent of the size $L$). In Fig. 7 we plot $\kappa(L)$ for both lattices (MC–PIBB and MC–EBB) and find significant agreement with the intermediate power-law behavior

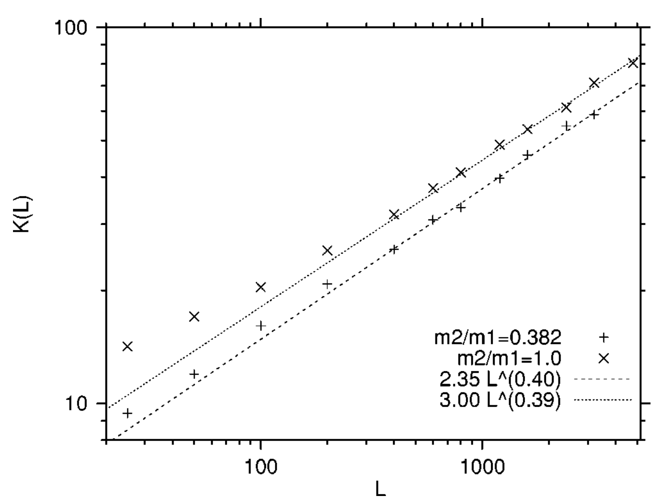


FIG. 7. The finite-size thermal conductivity $\kappa(L)$ vs size $L$ for the MC–EBB $(m_2/m_1=0.382, b=1)$ and MC–PIBB $(m_2/m_1=1, b=1)$ models.

$$\kappa(L) \propto L^{0.4}. \tag{28}$$

This result is in agreement with the existing results on nonintegrable, momentum-conserving lattices in the literature[11,14,18,19,31] and provides further support for the conjecture that there may be some form of universality present in these models.[14,15] Clearly this is an important question worthy of further study.

Our numerical data also permit us to study two other major issues related to the anomalous conductivity and more generally to the applicability of the concepts of statistical mechanics to these systems. First, we can examine the consistency of the above $\kappa(L)$, which we have determined by studying numerically a nonequilibrium steady state, with the behavior of $\kappa$ as determined by applying the Kubo formula to a large but finite system. To perform this consistency check, we have computed the temporal current–current autocorrelation function, $C(t) \equiv \langle J(t)J\rangle_\beta / L$, and spatiotemporal current–current autocorrelation function, $S(x=m,t) = \langle j_m(t) j_0(0)\rangle_\beta$. The homogeneity in space and time imply that all the averages are invariant under the space and time shifts, $\langle F_m(t)\rangle_\beta = \langle F_0(0)\rangle_\beta$, so the temporal correlation function can be writen as the spatial integral of the spatiotemporal one

$$C(t) = \sum_{m=0}^{N-1} S(m,t). \tag{29}$$

We assume that the tails of the current–current autocorrelation function are mainly governed by the acoustic sound wave propagation which moves ballistically with a group sound velocity $c_s = dx/dt$. This will be clearly revealed for the models studied here by inspecting the full spatiotemporal correlation $S(x,t)$ later.

In order to describe $\kappa(L)$ for a finite sistem of size $L$ by the conventional Kubo formula, we need to integrate $C(t)$ up to a finite time $t_0 \sim t_L \equiv L/c_s \propto L$, since for the ultimate asymptotic result, the thermodynamic limit $L \to \infty$ has to be taken prior to the time $t_0 \to \infty$ limit. Therefore, divergence of $\kappa(L) \propto L^\alpha$ is consistent with a slow power-law decay of current–current autocorrelation function

$$C(t) \propto t^{-(1-\alpha)}. \tag{30}$$

In Fig. 8 we show temporal correlation functions $C(t)$ for three different models: (a) for MC–PIBB with vanishing pressure ($b=1$); (b) for MC–EBB with vanishing pressure ($b=1$); and (c) for MC–EBB with nonvanishing pressure ($b=2.5$). Only the case (b) is clearly consistent with the decay $C(t) \propto t^{-0.60}$ whereas for the case (a) (MC–PIBB) the decay of correlations seems to be slightly faster $C(t) \sim t^{-0.78}$ (although the power may approach 0.60 as $N \to \infty$), and the bumps where the sound-wave collides with its symmetric copy after transversing the half of the system are quite remarkable) and for the case (c) (MC–EBB with nonvanishing pressure), we obtain a finite plateau for $C(t)$, in accordance with our theorem of Sec. II.

From these results we conclude that the finite-size relation (30) appears to break down when either (i) the pressure is nonvanishing or (ii) the autonomous dynamics is noner-

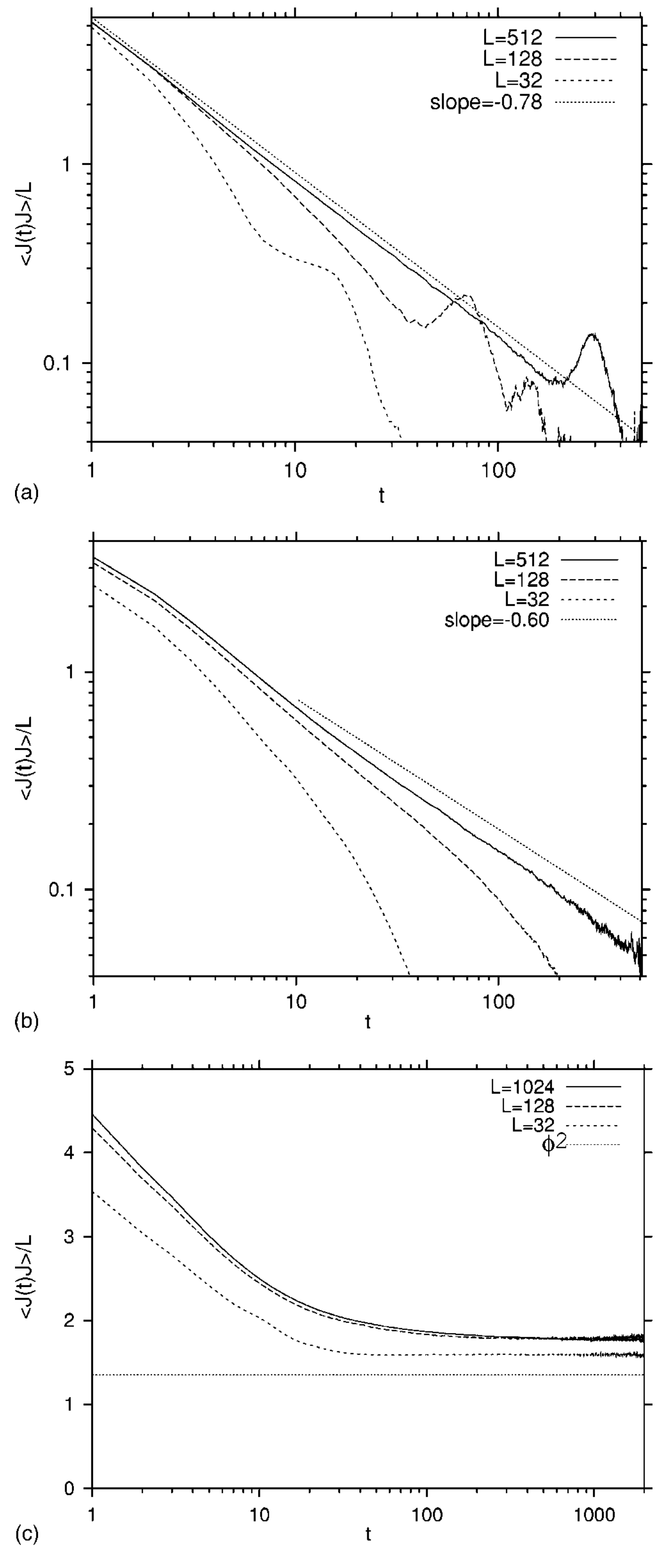


FIG. 8. The current–current temporal autocorrelation function $\langle J(t)J\rangle_\beta / L$ (at temperature $T=1$) for: (a) the pseudointegrable ($m_2/m_1=1$) momentum-conserving bing-bang model with periodic boundary conditions and vanishing pressure, $b=1.0$; (b) the ergodic momentum-conserving bing-bang lattice ($m_2/m_1=0.382$) with vanishing pressure, $b=1.0$; and (c) the ergodic momentum-conserving lattice with nonvanishing pressure $b=2.5$. In each case, three different system sizes are shown. Note that the dotted line in (c) indicates the lower bound from the theorem from Sec. II.

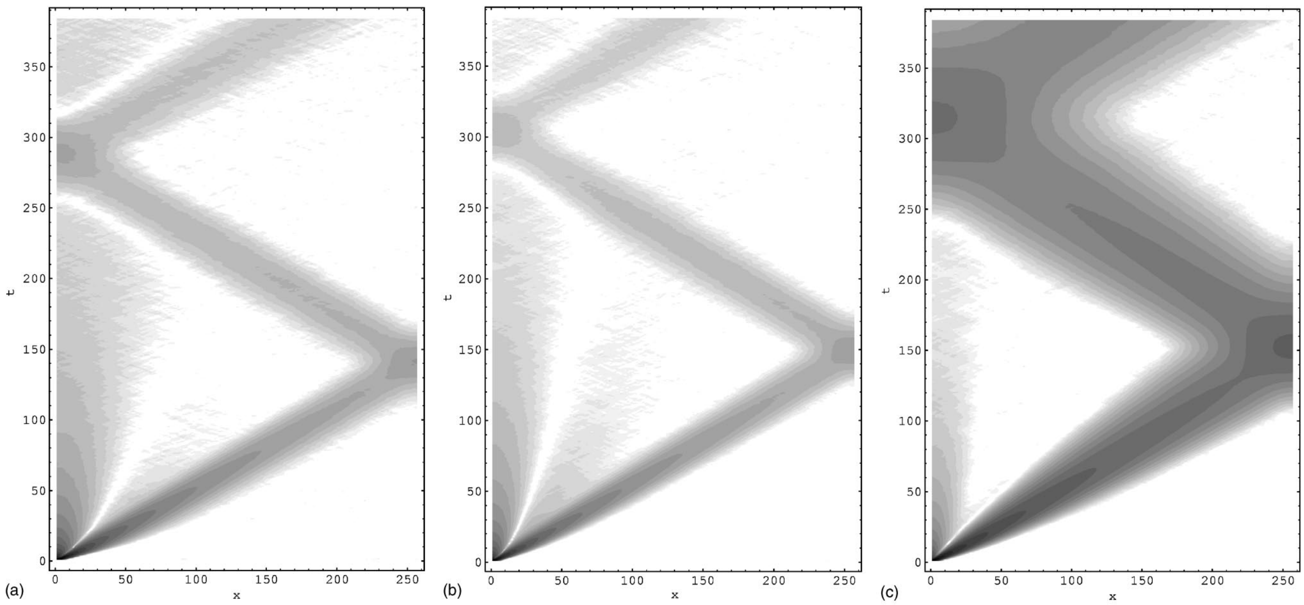


FIG. 9. The spatiotemporal correlation function $S(m,t)=\langle j_m(t) j_0(0)\rangle_\beta$ for the same three cases as in Fig. 8. Note the apparent ballistic propagation. Regions between contours of equidistantly spaced base-$e$ logarithm $\ln S(x=m,t)$ are shaded with 20 different and uniformly increasing levels of greyness in the range $[-10,0]$.

godic (pseudo-integrable or even integrable); however, it appears to hold if the pressure is vanishing and the dynamics is ergodic, and of course even more so if dynamics is ergodic and chaotic, as demonstrated by Refs. 18 and 19. We believe that our results indicate that EBB models are mixing as well, although it is very difficult to make any precise statements about mixing based on numerical results on the decay of time correlations of just one or the few observables, like $C(t)$.

Further insight into the nature of the anomalous conductivity comes from studying the full spatiotemporal correlation function $S(x,t)$. In Fig. 9 we show $S(x,t)$ for the same three cases studied in Fig. 8. Note the clear tongues of ballistic propagation in $S(x,t)$, from which we can easily compute the sound velocity $c_s$. For the earlier three cases the observed sound velocity is: (a) $c_s \approx 1.75$, (b) $c_s \approx 1.67$, and (c) $c_s \approx 1.63$. In addition to the ballistic component, we also observe in all three cases a quite pronounced diffusive component of $S(x,t)$ which is the central enhancement (around $x=0$) inside a band whose width spreads diffusively as $x_{\mathrm{diff}} \propto \sqrt{t}$.

The interpretation of these ballistic modes is clarified by the following simple but instructive observation and numerical experiment. Since there is no on-site potential in our MC models, they behave macroscopically like a liquid or a gas. When such a system (for a large size $L=N$) is confined between hard walls or between heat reservoirs, we expect it to exhibit standing acoustic waves whose frequencies can be computed directly from the size $L$ and the speed of sound $c_s$. Since the displacements of the particles must vanish at the reservoir walls, we also know the appropriate boundary conditions. Thus we should find the same eigenfrequencies as for the acoustic "flute" closed at both ends

$$\nu_l = \frac{l c_s}{2L}, \quad l = 1,2,3 \ldots . \tag{31}$$

Can we excite the long wavelength acoustic eigenmodes by simple thermal excitation of the reservoirs? We explore this question in Fig. 10(a) by plotting the total displacement $q_n$ of the middle particle (in units of unit mean particle spacings) $n=N/2$ of a MC–EBB chain of size $N=400$ which is simply put between the heat reservoirs at unit temperature $T_L=T_R=1$. We observe a nearly periodic signal with a frequency $\nu_1=0.0204$, corresponding to a very clear and pronounced dominant excitation of the longest wave-length mode $l=1$. In the remainder of Fig. 10, we plot the power spectra of the signal, $|\tilde{q}_{N/2}|^2(\omega)$ and $|\tilde{q}_{N/4}(\omega)|^2$, for the four different cases of [see Figs. 10(b)–10(e)]: (b) a MC–EBB chain with vanishing pressure ($b=1$), (c) a MC–EBB chain with nonvanishing pressure ($b=2$), (d) a MC–PIBB chain with vanishing pressure ($b=1$), and (e) a MC–PIBB chain with nonvanishing pressure ($b=2$). In all these cases we observe a dominant excitation of the longest wavelength mode $l=1$ and also clear but weaker excitations of higher eigenmodes ($l>1$) with integer multiple frequencies $\nu_l = l\nu_1$, whose power is a rapidly decreasing function of $l$. The basic acoustic frequencies of the four cases are: (b) $2\pi\nu_1=0.0128$, (c) $2\pi\nu_1=0.0116$, (d) $2\pi\nu_1=0.0135$, and (e) $2\pi\nu_1=0.0116$, from which we can independently calculate the sound velocities: (b) $c_s=1.63$, (c) $c_s=1.48$, (d) $c_s=1.72$, and (e) $c_s=1.48$. Cases (d) and (b) exactly correspond (except for the *different* boundary conditions) to cases (a) and (b) of Figs. 8 and 9, respectively, and indeed the agreement of the sound velocities is very good. Another interesting observation, which we believe is in fact the physical essence of the "proviso" in our theorem of Sec. II, is that the power spectra of the "acoustic" signals of mod-

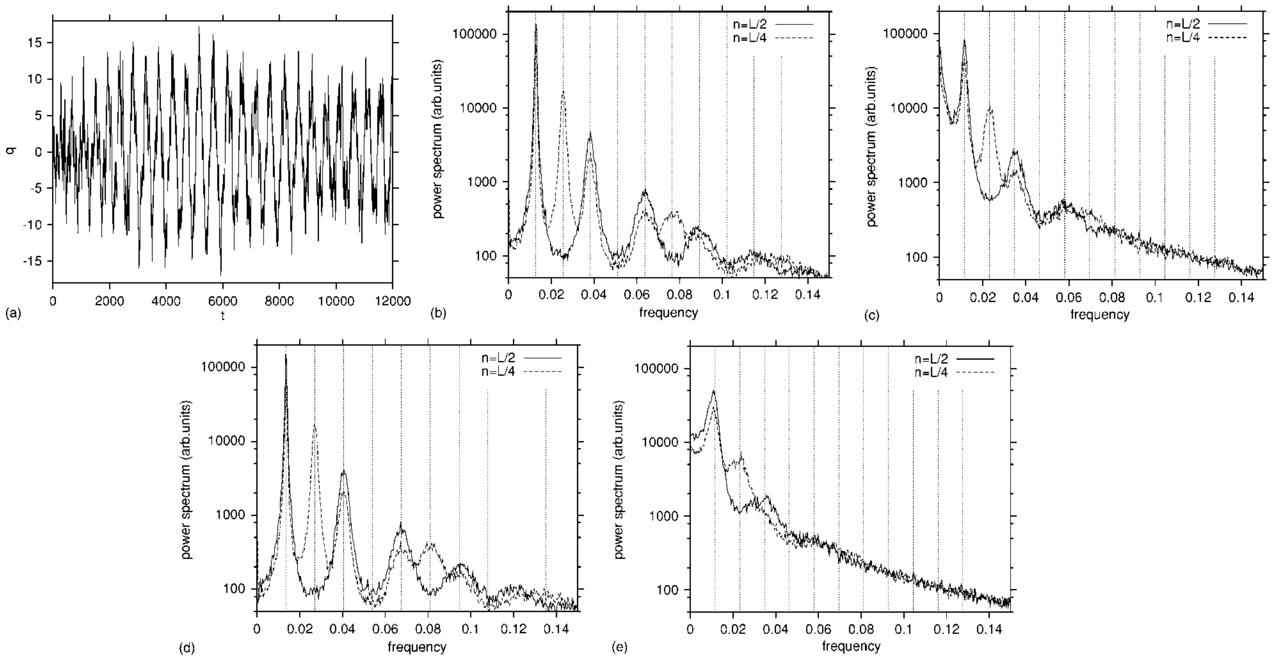

FIG. 10. Thermal excitation of acoustic modes: (a) the time dependence of the displacement $q_n(t)$ of the particle in the middle $n=L/2$ of the diatomic ($m_2/m_1=0.382, b=1.0$) bing-bang lattice of size $L=400$ between thermal reservoirs in equilibrium ($T_L=T_R=1$); (b) the power spectrum of the same signal ( $n=L/2$, full curve) and for the displacements at the one-quarter of the chain ($n=L/4$, dashed curve); dotted vertical lines denote integer multiples of the basic acoustic frequency; (c) the same plot as in (b) but for the MC–EBB with $b=2$ (nonvanishing pressure); (d) the same plot as in (b) but for the MC–PIBB with $b=1$ (vanishing pressure); and (e) the same plot as in (b) but for the MC–PIBB with $b=2$ (nonvanishing pressure).

els with non-vanishing pressure show a peak [as in Fig. 10(c)], or at least relatively large power [as in Fig. 10(d)], at zero frequency, whereas models with vanishing pressure have practically vanishing power at zero frequency. In other words: the zero-frequency mode, which is a rigid displacement of all particles (at least in a large local domain, since a global rigid displacement is prohibited by the boundary conditions), can support energy transport only if the pressure is nonvanishing.

Let us turn now to the second general issue related to the anomalous conductivity and more generally to the applicability of the concepts of statistical mechanics to these systems: namely, is the nonequilibrium state in which we study the heat transport a state of *local thermal equilibrium*? To study the question of the existence of local thermal equilibrium in both PIBB and EBB models in the nonequilibrium stationary state with $T_L=1, T_R=2$, we analyze the velocity/momentum distribution across the system and compare it to the ideal Maxwellian

$$d\mathcal{P}/dp_n \propto \exp[-p_n^2/(2m_nT_n)].$$

To simplify this comparison, we factor out the local temperature by comparing the normalized higher moments

$$M_{2m}(n) = \frac{\langle p_n^{2m}\rangle}{\langle p_n^2\rangle^m} \tag{32}$$

with the Gaussian values $M_{2m}^{\text{gauss}}=(2m-1)!!$.

That we cannot expect to find local thermal equilibrium in a pseudo-integrable (PI) model is shown by the following argument:[44] the momenta of particles in the pseudo-integrable lattice cannot change due to interactions (collisions) with other particles but only due to interactions (collisions) with the reservoirs. Therefore, the velocity distribution at the site $n$ inside the PIBB chain is equal to a linear combination of two Maxwellians with temperatures $T_L$ and $T_R$, the coefficients being just the probabilities that given velocity has been injected from the left/right. Strictly speaking, for this argument[44] to be completely justified, we must assume that the diffusion rate of fixed velocities (or "velocitons") is (at least to some good approximation) independent of the actual value of the velocity. This is indeed the case, for example, if we assume completely uncorrelated random walks for the individual velocities—velocitons. But this assumption may be really justified only for strongly chaotic systems, like the Lorentz gas,[44–48] whereas for PI systems we can consider it just as a qualitative argument that suggests the absence of local thermal equilibrium.

The results of studying the moments of the local velocity distributions in the MC–EBB and MC–PIBB models are shown in Fig. 11. The reader should observe very convincing local thermal equilibrium for the MC–EBB model, while for MC–PIBB model we have notable deviations, as anticipated by the qualitative argument presented earlier.

## B. Momentum nonconserving bing-bang models

The two 1D bing-bang models studied in the previous subsection exhibited both translation invariance (momentum conservation) and the absence of metric chaos. Hence, the result that they also exhibited anomalous transport is not surprising, given previous results and discussion of Sec. II. Nonetheless, our numerics were useful in establishing that the anomalous transport can be viewed as arising from the sound-wave ballistic tongues in spatiotemporal current–current autocorelation function $S(x,t)$. Further, our simula-

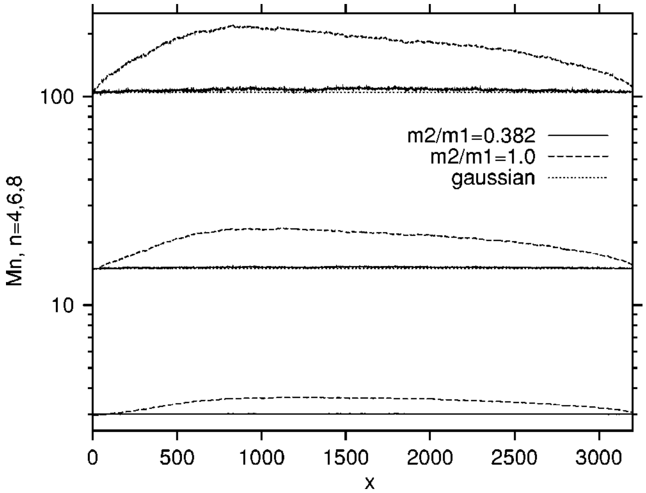


FIG. 11. Moments of the velocity distributions $M_{2n}(m)=\langle p_m^{2n}\rangle_\beta/\langle p_m^2\rangle_\beta^n$ for $n=4$, 6, and 8 for two different momentum conserving bing-bang lattices of size $L=3200$ with $T_L=0.5$, $T_R=1.0$. The results for the EBB model (with $m_2/m_1=0.382$, plotted as solid lines) are essentially indistinguishable from those of the Gaussian model $[M_n=(2n-1)!!]$, plotted as dotted lines), showing that local thermal equilibrium is established in the MC–EBB model, whereas the results for the MC–PIBB model (dashed lines) deviate substantially from the Gaussian model, showing that local thermal equilibrium is *not* established, as anticipated by the heuristic argument presented in the text.

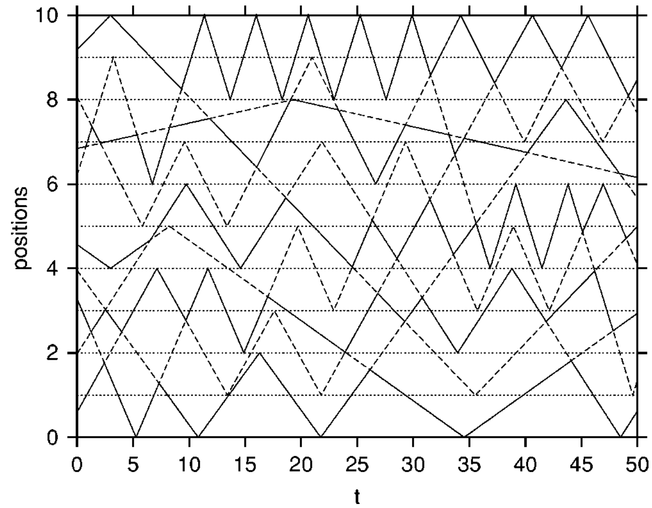


FIG. 12. A typical trajectory of MNC–PIBB chain $(L=9)$. As in Fig. 3, the ordinate shows particle positions $[x_n(t)]$ where for clarity the odd $n$ particle trajectories are plotted with full lines while the even $n$ trajectories are dashed. The walls at $x=0$ and $x=10$ act as thermal baths at temperature $T=1$.

tions also established results—perhaps somewhat surprising, given the complete absence of metric chaos in the bing-bang models—that (i) instead of behaving like integrable systems, the momentum-conserving bing-bang models exhibited the same scaling of $\kappa(L)$ as the generic nonintegrable, and even strongly chaotic, models like the FPU lattice; and (2) that in the MC–EBB model, local thermal equilibrium is established in the conducting stationary steady state. Taken together with previous results (for instance, those on the FPU system) that chaos is not sufficient to produce normal conductivity, our new results show that the relationship between metric chaos (positive Lyapunov exponents, positive Kolmogorov–Sinai entropy) and "statistical mechanical" behavior—including normal transport, local thermal equilibrium, it etc.—is perhaps less direct than previously anticipated.

In this subsection, by studying a momentum nonconserving bing-bang model, we further weaken the link between metric chaos and normal statistical behavior by establishing numerically that a model in which metric chaos is absent (in the strict sense) nonetheless exhibits normal conductivity: that is, we show by a (numerical) counterexample that chaos is also *not necessary* for normal conductivity.

For simplicity and clarity, we focus on a single momentum non-conserving bing-bang model—the "the less ergodic" pseudo-integrable chain (MNC–PIBB) chain—which is defined by the relations (24) with $b=c=d=1$, and $m_n=1$. Physically, this corresponds to a chain of equal mass point particles that collide elastically and are each subject to a hard-wall, confining on-site potential. A typical trajectory of such a model of with nine particles $(N=9)$ is depicted in Fig. 12.

When the MNC–PIBB lattice is placed between heat baths, with temperatures $T_1=1$ and $T_2=2$, a linear temperature profile is established, as shown in Fig. 13, except for the edge particles $n=1$ and $n=N$, which are in contact with the reservoirs. At the reservoirs, we observe a strong drop in temperature arising from manner in which the particles are coupled to the heat bath: in particular, fast particles are more likely than slow ones to collide again with the reservoirs before they "transmit" their velocity to the rest of the chain. Apart from this effect, which can be essentially avoided by defining "renormalized reservoirs" which include one (or a few) particles near to the reservoir, the transport in the MNC–PIBB is completely *normal*: a linear thermal gradient is established and $\kappa(L)$ is independent of $L$. And this normal transport behavior occurs despite the fact that the autonomous MNC–PIBB system has no metric chaos and is not even ergodic! We should note, however, that due to pseudo-integrability of MNC–PIBB, local thermal equilibrium is not

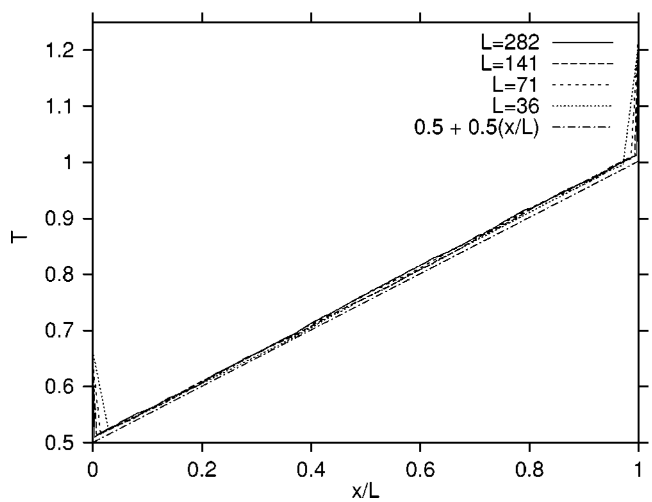


FIG. 13. The scaling of *linear* temperature profiles, $T$ vs $x/L$, for MNC–PIBB chain for different sizes $L$. The dashed-dotted straight line is drawn to guide the eye. The temperatures of stochastic heat baths are $T_L=1$ and $T_R=2$.

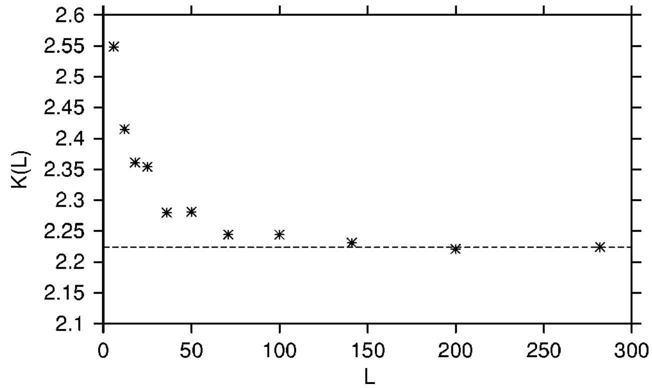


FIG. 14. Convergence of the thermal conductivity $\kappa(L)$ to its $L$-independent asymptotic value for the MNC–PIBB model. In the simulations, $T_L=1$, and $T_R=2$.

established in nonequilibrium heat-flow simulation. Instead, the local velocity distribution has been found to be a linear combination of two Maxwellians at different temperatures.

In Fig. 14 we show the convergence of $\kappa(L)$ to its $L$-independent asymptotic value; the figure shows that the convergence has occurred already for lattice sizes $L\approx 100$.

We have done conducted three additional numerical experiments to confirm and clarify the normal heat transport in this MNC–PIBB model. First, in Fig. 15, we show the magnitude of current–current autocorrelation function $|\langle J(t)J\rangle_\beta|/L$ for MNC–PIBB lattices of several different sizes $N$. We observe a rapid (perhaps exponential) initial decay of the correlations (over three decades) and afterwards a slower, oscillatory decay (so it integrates out and (hopefully) does not produce a divergence in the Kubo formula even if its envelope may not decay exponentially).

Second, and perhaps more conclusive, is the behavior observed for the spatiotemporal correlation function $S(x,t)$ of the MNC–PIBB model, which we show in Fig. 16. In contrast to the behavior observed in the systems with anomalous heat conductivity (see Fig. 9), there are *no* ballistic

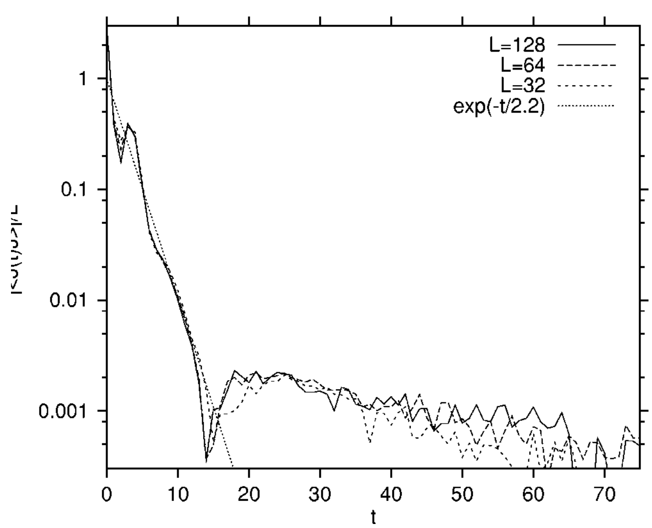


FIG. 15. The magnitude of the current autocorrelation function $|\langle J(t)J\rangle_\beta|/L$ (at temperature $T=1$) for the MNC–PIBB model with periodic boundary conditions for different system sizes.

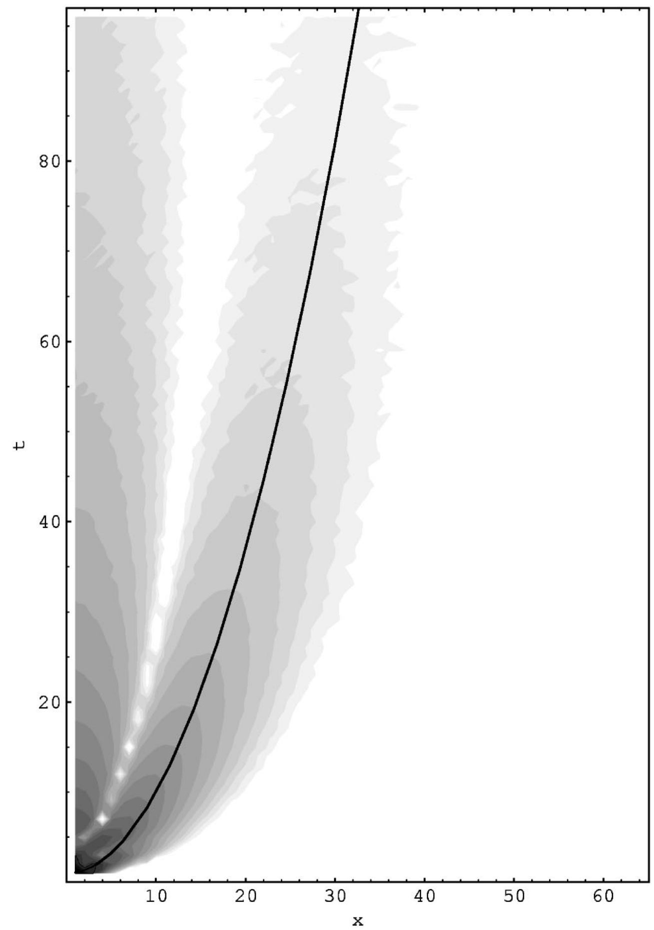


FIG. 16. The spatiotemporal correlation function $S(m,t)=\langle j_m(t)j_0(0)\rangle_\beta$ for the same parameters as in previous Fig. 15 and using the same graphical presentation as in Fig. 9. Note the apparent diffusive propagation. The superimosed full curve is $t=0.09x^2$.

tongues here but instead a clearly diffusive pattern emerges.

Third, we can study the behavior of the imaginary test particles (velocitions) that carry constant (fixed) velocity and which can be clearly defined due to pseudo-integrability of the many-body model: When the velocities $v_n, v_{n+1}$ of a pair of particles $n$ and $n+1$ are exchanged due to the collision, the velociton hops (by definition) from site $n$ to site $n+1$, or vice versa. Choosing the velociton initially to be at the site $n(t=0)=n_0$, clearly determines the evolution $n(t)$ is for all times. If the overall motion of the velociton is diffusive, this provides an indication of the diffusive (normal) nature of energy/heat transport in the system. We start by placing a velociton of velocity $v_0$ somewhere in a large MNC–PIBB lattice (with periodic boundary conditions) and with a canonically thermalized "background," i.e., the momenta of all other particles are distributed according to a Gaussian distributiuon. We then simulate the dynamics, and ask whether the velociton undergoes a normal diffusive proccess. If $n(t)$ labels the real particle that carries a velocity $v_0$ at time $t$, then we check for the linear growth

$$[n(t)-n(0)]^2{}_\beta = D(v_0)t. \tag{33}$$

In Fig. 17 we show $\langle[n(t)-n(0)]^2\rangle_\beta$ as a function of time, for both an intermediate velociton $v_0=1$ (the background tem-

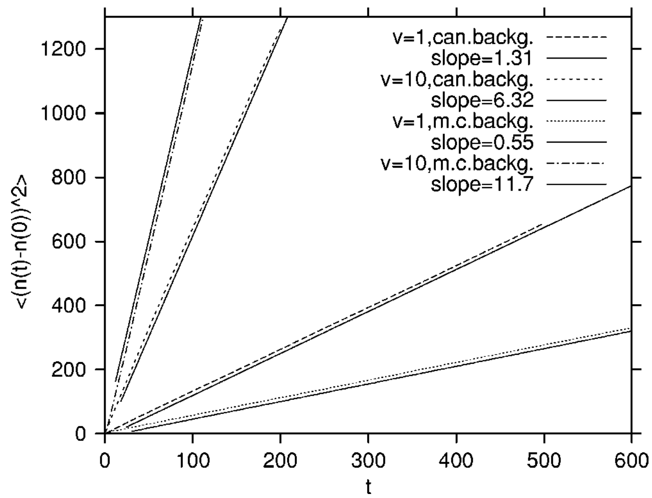


FIG. 17. Diffusion of velocitons in MNC–PIBB lattice. We show root-mean-square displacements vs time for velocitons with $v=1$ and $v=10$, in either canonically thermalized background with temperature $T=1$ or in microcanonically thermalized background (all background particles have equal unit velocities but random signs and initial positions). Full lines give the slopes of best linear fits which support the existence of normal diffusion.

perature is $T=1$) and a fast velociton $v_0=10$. We find normal diffusion in both cases, although the diffusion coefficient $D(v_0)$ is obviously an increasing function of velocity $v_0$. In Fig. 17 we also study velocitons in a "microcanonically thermalized background," by which we mean that momenta/velocities of the real particles all have values $\pm 1$ (with equal probability of both signs). Remarkably, even in this case we find normal diffusive proccesses for both intermediate and fast velocitons.

We believe all these results provide conclusive numerical confirmation of normal diffusive heat transport in the MNC–PIBB lattice, which is neither ergodic nor chaotic but only pseudo-integrable. This strongly supports the result that *metric chaos is not nesseccary to have normal transport*.

This result seems quite surprising and indeed paradoxical, but we believe that the resolution of the seeming paradox lies in the complexity of the $N$-dimensional invariant surfaces in the MNC–PIBB model: namely, these surfaces become more and more dense and uniformly covering of the energy surface as the thermodynamic limit (i.e., as $N\to\infty$), while dynamics on the invariant surface is probably mixing (decay of time correlations of arbitrary observables), which means that any phase-space distribution function on invariant-surface relaxes into statistical equilibrium. Thus, in the thermodynamic limit $N\to\infty$, the macroscopic properties of the dynamics of this complex pseudo-integrable system cannot really be distinguished from those of a truly chaotic system. For example, as we saw in the beginning of this section, the sets of modula of momenta of PIBB lattices are preserved under time evolution. Hence, the invariant surface can be written as a direct product $(\mathcal{C}_2^N\times\mathcal{S}_N)\times[-1,b]^N$. Where $\mathcal{C}_2^N\times\mathcal{S}_N$ is the group of all possible permutations $\mathcal{S}_N$ and sign exchanges $C_2$ on a set of initial momenta $(p_1,p_2,\ldots,p_N)$ and really represents the discrete momentum part of an invariant surface which consists of $2^N N!$ N-dimensional configurational sheets $[-1,b]^N$. When $N$ is large and if initial condition of on the momenta ($\mathbf{p}$) has been chosen with a "canonical measure" for each component $p_n$ (which is the case with probability 1 in thermodynamic limit) then it seems plausible that the dynamics of a single orbit of the PIBB system on its invariant surface can uniformly cover the phase-spaces of small subsystems of size $N'\ll N$ with a canonical measure, just as is the case for a truly ergodic covering system. Obviously, these observations require considerable further mathematical study to be convincing, but we feel that they are well justified as conjectures.

We close this subsection with one final calculation. Since the MNC–PIBB model is equivalent to a (multidimensional) billiard model, we can in this case actually derive the dependence of $\kappa(T)$ on the *temperature* by a simple scaling analysis, either from Kubo formula, or, more directly, from the definition $\kappa=-j/\nabla T$. The heat current is proportional to the average particle energy, i.e., $v^2$ (where $v$ is a typical velocity), times the inverse of the typical time in which a particle scatters with its neighbors and transfers energy: this time is roughly $a/v$, where $a$ is the lattice spacing. Therefore, $j_n \sim v^3$ for billiard-like models. On the other hand, the temperature gradient $\nabla T=T_{n+1}-T_n$ scales as $\sim v^2$, so that $\kappa\propto v$, or

$$\kappa(T)\approx\sqrt{8T}. \tag{34}$$

The factor of $\sqrt{8}$ is an approximation obtained from our numerical simulations, but the scaling with temperature is *exact* since it is a simple consequence of scaling dynamics of billiards. The above result is meaningful, of course, only in the close-to-equilibrium situation where typical (average) temperature has a well-defined value of $T$.

## V. SUMMARY AND DISCUSSION

### A. Summary

The analyses, analytic and numerical, described in the previous sections, have established a several results concerning normal and anomalous heat transport in classical 1D lattices. We have adduced convincing numerical evidence and several theoretical arguments[20–22] to justify the claim that total momentum conservation is sufficient for anomalous heat transport provided the average pressure is nonvanishing. There seem to be momentum-conserving models that have normal conductivity[35,36] but these models cannot sustain pressure, consistent with heuristic arguments that in such a case, the Goldstone modes cannot carry energy.

We have also presented numerical results that convincingly support two other claims:

- total momentum conservation is *not* necessary for anomalous heat transport, as shown by the counterexamples of the linear *optical* chain and the nonlinear integrable IK–SG model; and
- metric chaos, defined in the usual sense of having a set of nonzero measure in phase space in which there are positive Lyapunov exponents and positive Kolmogorov–Sinai entropy, is *neither* sufficient (as shown by the anomalous behavior of the FPU and diatomic Toda models) *nor* necessary (as shown by the momentum non-conerving pseudo-integrable bing-bang (MNC–PIBB) model) for

normal (diffusive) heat transport. Furthermore, even ergodicity is not necessary for normal transport, as shown by our studies of MNC–PIBB models. From our analysis it follows that perhaps even multidimensional pseudo-integrability is sufficient, provided the topology of invariant surfaces becomes sufficiently complex in thermodynamic limit.

As is often the case, these results raise at least as many questions as they answer, so we phrase the remainder of our discussion in terms of several questions.

### B. What is needed for normal transport?

Our results establish that the full set of conditions needed to guarantee normal transport in 1D models is more subtle and less "clean" that previously believed.[8] We know that normal transport for all temperatures requires:

- confining on-site potential,[15] or vanishing pressure with effective means of scattering of long-wavelength Fourier modes;[35,36]
- anharmonicity in either on-site or interparticle potential: this is necessary to exclude the pathological linear systems;
- absence of integrability: integrable models (which can be hard to identify *a priori*) must also clearly be excluded; and
- an *effective* means of achieving dynamical mixing in the thermodynamic limit, although this means can be subtle and perhaps more topological than dynamical, as the results for the pseudo-integrable bing-bang model imply.

### C. What about dimensionality?

Why do we expect our arguments to be limited to on dimension? We could develop a formal analysis of the vector current in two (or higher) dimensions, but intuition gained from thinking of coupled chains is key. The neighboring chains provide an environment for a given chain that leads to an effective on-site potential: this was original motivation for Frenkel–Kontorova model. Based on hydrodynamic or mode-coupling arguments,[32] one would expect $\ln L$ divergence of $\kappa$ in two dimensions and normal conductivity $\kappa L^0$ in three dimensions. The expected logarithmic divergence in 2D has been confirmed in recent numerical experiments.[31] Nonetheless, further studies in explicit lattice models in higher dimensions will certainly provide additional insights.

### D. What are other open issues?

- An outstanding problem in mathematical physics is a rigorous proof of what is really necessary and sufficient for normal conductivity.
- Compelling calculations of the exponents for anomalous transport. Is $\kappa \sim L^{1.0}$ the fastest increase possible? Is $\alpha$ universal, or are there universality classes? Numerical data suggest $\alpha \sim 0.4$ is widespread, but other arguments suggest $\alpha = 1/3$. Is there a systematic "universality theory" that can predict $\alpha$, as was done for the Feigenbaum constants in the period doubling transition to chaos?
- What happens when systems are driven *non*linearly away from equilibrium? What are the corrections to Kubo formula?

Knowledgeable colleagues, many of whom have contributed to this Focus Issue of *Chaos* on the Fermi–Pasta–Ulam problem, can doubtless add still further questions. There is still much to be found in exploring the rich trove of physically relevant and mathematically challenging problems that has been uncovered in seeking to explain FPU's remarkable little discovery.[1]

## ACKNOWLEDGMENTS

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[1] E. Fermi, J. Pasta, and S. Ulam, "Studies of Nonlinear Problems. I," Los Alamos report LA–1940 (1955); reprinted in E. Fermi, *Collected Papers* (University of Chicago Press, Chicago, 1965), Vol. II, p. 978.
[2] M. Toda, "Studies of a Non-Linear Lattice," Phys. Rep. **18C**, 1 (1975).
[3] M. Toda, "Solitons and Heat Conduction," Phys. Scr. **20**, 424 (1979).
[4] E. A. Jackson, "Nonlinearity and Irreversibility in Lattice Dynamics," Rocky Mt. J. Math. **8**, 127 (1978).
[5] R. A. MacDonald and D. H. Tsai, "Molecular Dynamical Calculatiouns of Energy Transport in Crystalline Solids," Phys. Rep. **46**, 1 (1978).
[6] W. M. Visscher, "Computer Studies of Transport Properties of Simple Models of Solids" Methods Comput. Phys. **15**, 371 (1976).
[7] R. Livi, A. Politi, and S. Lepri, "Thermal Conduction in Classical Low-Dimensional Lattices," Phys. Rep. **377**, 1 (2003).
[8] J. Ford, "The Fermi–Pasta–Ulam Problem: Paradox Turns Discovery," Phys. Rep. **213**, 271 (1992).
[9] W. M. Visscher, "Transport Processes in Solids and Linear Response Theory," Phys. Rev. A **10**, 2461 (1974).
[10] Z. Rieder, J. L. Lebowitz, and E. Lieb, "Properties of a Harmonic Crystal in a Stationary Nonequilibrium State," J. Math. Phys. **8**, 1073 (1967).
[11] S. Lepri, R. Livi, and A. Politi, "Heat Conduction in Chains of Nonlinear Oscillators," Phys. Rev. Lett. **78**, 1896 (1997).
[12] H. Kaburaki and M. Machida, "Thermal Conductivity in One-Dimensional Lattices of the Fermi–Pasta–Ulam Type," Phys. Lett. A **181**, 85 (1993).
[13] E. A. Jackson and A. D. Mistriotis, "Thermal Conductivity on One- and Two-Dimensional Lattices," J. Phys.: Condens. Matter **1**, 1223 (1989).
[14] T. Hatano, "Heat Conduction in the Diatomic Toda Lattice Revisited," Phys. Rev. E **59**, R1 (1999).
[15] B. Hu, B. Li, and H. Zhao, "Heat Conduction in One-Dimensional Chains," Phys. Rev. E **57**, 2992 (1998).
[16] G. Casati, J. Ford, F. Vivaldi, and W. H. Visscher, "One-Dimensional Classical Many-Body System Having Normal Thermal Conductivity," Phys. Rev. Lett. **52**, 1861 (1984).
[17] T. Prosen and M. Robnik, "Energy Transport and Detailed Verification of Fourier Heat Law in a Chain of Colliding Harmonic Oscillators," J. Phys. A **25**, 3449 (1992).
[18] S. Lepri, R. Livi, and A. Politi, "Energy Transport in anharmonic lattices close to and far from equilibrium," Physica D **119**, 140 (1998).
[19] S. Lepri, R. Livi, and A. Politi, "On the Anomalous Thermal Conductivity of One-Dimensional Lattices," Europhys. Lett. **43**, 271 (1998).
[20] T. Prosen and D. K. Campbell, "Momentum Conservation Implies Anomalous Transport in Classical 1D Lattices," Phys. Rev. Lett. **84**, 2857 (2000).
[21] O. Narayan and S. Ramaswamy, "Anomalous Heat Conduction in One-Dimensional Momentum-Conserving Systems," Phys. Rev. Lett. **89**,

200601 (2002).
[22] G. Casati and T. Prosen, "Anomalous Heat Conduction in a One-Dimensional Ideal Gas," Phys. Rev. E **67**, 015203(R) (2003).
[23] F. Bonetto, J. L. Lebowitz, and L. Rey-Bellet, "Fourier Law: A Challenge to Theorists," preprint arXiv: math-ph/0002052.
[24] A. Dhar, "Heat Conduction in the Disordered Harmonic Chain Revisited," Phys. Rev. Lett. **86**, 5882 (2001).
[25] M. Toda, "Vibration of a Chain with Nonlinear Interaction," J. Phys. Soc. Jpn. **22**, 431 (1967).
[26] F. Mokross and H. Büttner, J. Phys. C **16**, 4539 (1983).
[27] B. L. Holian, H. Flaschka, and D. W. McLaughlin, "Shock Waves in the Toda Lattice: Analysis," Phys. Rev. A **24**, 2595 (1981); B. L. Holian and G. K. Straub, "Molecular Dynamics of Shock Waves in One-Dimensional Chains," Phys. Rev. B **18**, 1593 (1978); G. K. Straub, B. L. Holian, and R. G. Petschek, "Molecular Dynamics of Shock Waves in One-Dimensional Chains. II: Thermalization," *ibid.* **19**, 4049 (1979).
[28] A. G. Izergin and V. E. Korepin, "A Lattice Sine-Gordon Model," Vestn. Leningr. Univ., Ser. 4: Fiz., Khim. **22**, 88 (1981).
[29] V. O. Tarasov, "A Classical Version of the Lattice Sine-Gordon Model," Zap. Nauchn. Semin. LOMI **120**, 173 (1982).
[30] W. H. Press, B. P. Flannery, S. A. Teukolsky, and W. T. Vetterling, *Numerical Recipes* (Cambridge University Press, Cambridge, 1988).
[31] A. Lippi, Diploma thesis, University of Florence, 1998.
[32] See, e.g., P. G. Wolynes, "Bounds for Convective Contributions to Transport Coefficients," Phys. Rev. A **11**, 1700 (1975); P. G. Wolynes, "Hydrodynamic Boundary Conditions and Mode-Mode Coupling Theory," *ibid.* **13**, 1235 (1976); Y. Pomeau and P. Resibois, "Time Dependent Correlation Functions and Mode-Mode Coupling Theories," Phys. Rep. **19**, 63 (1975); M. H. Ernst, "Mode-Coupling Theory and Tails in CA Fluids," Physica D **47**, 198 (1991).
[33] P. Grassberger, W. Nadler, and L. Yang, "Heat Conduction and Entropy Production in a One-Dimensional Hard-Particle Gas," Phys. Rev. Lett. **89**, 180601 (2002).
[34] A. Dhar, "Heat Conduction in a One-Dimensional Gas of Ellastically Colliding Particles of Unequal Masses," Phys. Rev. Lett. **86**, 3354 (2001).
[35] C. Giardina, R. Livi, A. Politi, and M. Vassalli, "Finite Thermal Conductivity in 1D Lattices," Phys. Rev. Lett. **84**, 2144 (2000).
[36] O. V. Gendelman and A. V. Savin, "Normal Heat Conductivity of the One-Dimensional Lattice with Periodic Potential of Nearest-Neighbor Interaction," Phys. Rev. Lett. **84**, 2381 (2000).
[37] J. M. Deutsch and O. Narayan, "One Dimensional Heat Conductivity Exponent From a Random Collision Model," Phys. Rev. E **68**, 010201(R) (2003).
[38] J. M. Deutsch and O. Narayan, "Correlations and Scaling in One-Dimensional Heat Conduction," Phys. Rev. E **68**, 041203 (2003).
[39] L. Yang and P. Grassberger, "Are There Really Phase Transitions in 1-D Heat Conduction Models?," preprint arXiv: cond-mat/0306173.
[40] R. Kubo, M. Toda, and N. Hashitsume, *Statistical Physics II*, Springer Series in Solid State Sciences Vol. 31 (Springer-Verlag, 1991).
[41] E. Gutkin, "Billiards in Polygons: Survey of Recent Results," J. Stat. Phys. **83**, 7 (1996).
[42] G. Casati and T. Prosen "Mixing Property of Triangular Billiards," Phys. Rev. Lett. **83**, 4729 (1999).
[43] G. Casati, "Energy Transport and the Fourier Heat Law in Classical Systems," Found. Phys. **16**, 51 (1985).
[44] The same argument has been used recently for a one-particle problem, namely the Lorentz gas. See A. Dhar and D. Dhar, "Absence of Local Thermal Equilibrium in Two Models of Heat Conduction," Phys. Rev. Lett. **82**, 480 (1999).
[45] *Transport Phenomena*, Springer Lecture Notes in Physics Vol. 31, edited by G. Kirczenow and J. Marro (Springer-Verlag, 1974).
[46] R. S. Northcote and R. B. Potts, "Energy Sharing and Equilibrium in Nonlinear Systems," J. Math. Phys. **5**, 383 (1964).
[47] P. Mazur, "Non-Ergodicity of Phase Functions in Certain Systems," Physica (Amsterdam) **43**, 533 (1969).
[48] M. Suzuki, "Ergodicity, Constants of Motion, and Bounds for Susceptibilities," Physica (Amsterdam) **51**, 277 (1971).