

Nonintegrability and the Fourier heat conduction law

Shunda Chen,^{1,2} Jiao Wang,³ Giulio Casati,^{1,2,4} and Giuliano Benenti^{1,2}

¹*CNISM and Center for Nonlinear and Complex Systems, Università degli Studi dell'Insubria, via Valleggio 11, I-22100 Como, Italy*

²*Istituto Nazionale di Fisica Nucleare, Sezione di Milano, via Celoria 16, I-20133 Milano, Italy*

³*Department of Physics and Institute of Theoretical Physics and Astrophysics, Xiamen University, Xiamen 361005, Fujian, China*

⁴*International Institute of Physics, Federal University of Rio Grande do Norte, Natal, Brasil*

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We study in momentum-conserving systems, how nonintegrable dynamics may affect thermal transport properties. As illustrating examples, two one-dimensional (1D) diatomic chains, representing 1D fluids and lattices, respectively, are numerically investigated. In both models, the two species of atoms are assigned two different masses and are arranged alternatively. The systems are nonintegrable unless the mass ratio is one. We find that when the mass ratio is slightly different from one, the heat conductivity may keep significantly unchanged over a certain range of the system size and as the mass ratio tends to one, this range may expand rapidly. These results establish a new connection between the macroscopic thermal transport properties and the underlying dynamics.

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I. INTRODUCTION

The Fourier heat conduction law is an empirical law that describes how the heat current is sustained by the temperature gradient, i.e.,

$$j = -\kappa \nabla T, \quad (1)$$

where j is the heat current, ∇T is the temperature gradient, and κ is known as the thermal conductivity, which is a finite constant independent of the system size.

However, not all systems obey the Fourier law. It is known that the transport properties are strongly affected by conservation laws [1–4]. In the extreme case that a system is integrable, the heat conductivity is a linear function of the system size. Even in the particular case in which the total momentum is the only conserved quantity, the heat conductivity may diverge as well. In particular, in one-dimensional (1D) and two-dimensional (2D) cases, since 1970 when Alder and Wainwright reported their findings [5], it has been realized that momentum conservation may lead to slow decay of time correlations so that transport is not diffusive and is characterized by diverging transport coefficients. For 1D momentum-conserving systems, the heat conductivity generally depends on the system size N in a power-law manner: $\kappa \sim N^\alpha$. There is no general consensus on the numerical value of α and different theoretical models predict that α is 1/2 if the interparticle interaction is symmetric and 1/3 otherwise [6–8]. It is worth noting that these theoretical predictions equally apply to both fluids and lattices. On the other hand, a recent numerical study [9] suggested that when the interparticle interactions are asymmetric, there is a significant difference between fluids and lattices. To summarize, for 1D systems, the heat conduction properties are believed to depend on integrability, momentum-conservation, interaction symmetry, and the nature of fluids or lattices.

For the particular case of 1D momentum-conserving systems, which is the subject of the present paper, all analytical and numerical results so far available do not allow one to draw definite conclusions yet. This problem was analyzed with various 1D models in a recent study [10], where it was shown that the Fermi-Pasta-Ulam (FPU) chain with symmetric or

asymmetric potential exhibits anomalous heat transport, which is consistent with other recent investigations [11,12]. The plateau in the system size dependence of the heat conductivity found in Ref. [13] for the FPU model with a certain set of parameters turns out to be a finite size effect and, at larger N , the heat conductivity starts increasing again. In particular in Ref. [12] it was surmised that the value 1/3 should be found asymptotically for very large system size, even though, in fact, a value of the exponent $\alpha = 0.15$ was numerically found (up to $N = 65536$). The results of [10] also led to an exponent $\alpha < 1/3$ for the asymmetric FPU chain. In Ref. [11], the value 1/3 was found for the same FPU model but in a different parameter range and for high temperatures. In the same paper, the possibility of a finite temperature phase transition was not ruled out. Finally, in Ref. [10] normal heat conductivity was reported for 1D momentum-conserving systems with the Lennard-Jones, Morse, and Coulomb potential.

The overall picture is therefore far from being clear. *Rebus sic stantibus*, in order to gain a better understanding in such a complex situation, it might be convenient to consider the 1D diatomic hard-point gas. Indeed, this is a clean and simple system of billiard type and, as such, it should reflect general properties since billiards have been found fundamental in understanding both classical and quantum dynamical systems. Moreover, an important feature of billiard-type systems is that their dynamical properties do not depend on the temperature, which makes their analysis even more simplified. By analyzing the hard-point gas, we show that close to the integrable, equal masses limit, the system exhibits normal heat conduction over longer and longer sizes as the integrable limit is approached. Asymptotically, however, the power-law divergence of the thermal conductivity sets in with the power 1/3. To be more precise, we cannot exclude the possibility of a phase transition as the mass ratio is increased; however, our numerical evidence suggests that this possibility should be quite unlikely. The analysis of the diatomic Toda lattice confirms these conclusions. These results lead us to speculate that as one approaches the integrable limit, anomalous behavior is perhaps more general than so far expected [9,10,13] even though it might be hard to detect in numerical simulations.

II. 1D DIATOMIC GAS MODEL

After being initially proposed in 1986 [14], the 1D diatomic gas model has attracted increasing interest for investigating various aspects of 1D transport. The model consists of N hard-core point particles in one dimension with alternative mass M and m (for odd- and even-numbered particles, respectively). We fix the averaged particle number density to be unity so that N refers to the length of the system as well. In order to measure the heat conductivity, two statistical thermal baths with different temperatures T_L and T_R are put into contact with the left and the right end of the system. When the first (last) particle collides with the left (right) side of the system, it is injected back with a new speed $|v|$ determined by the distribution [15],

$$P_{L,R}(v) = \frac{|v|\mu_{1,N}}{k_B T_{L,R}} \exp\left(-\frac{v^2 \mu_{1,N}}{2k_B T_{L,R}}\right). \quad (2)$$

Here μ_1 and μ_N are the masses of the first and the last particle and k_B is the Boltzmann constant which is set to be unity throughout.

In our simulations, each particle is given initially a random position uniformly distributed and a random velocity according to the Boltzmann distribution with temperature $T(x_i) = T_L + x_i(T_R - T_L)/N$ (x_i is the position of the i th particle). Then the system is evolved by using an effective event-driven algorithm [16]. After the system reaches the steady state, we compute the steady heat flux j that crosses the system; i.e., the averaged energy exchanged in the unit time between a boundary particle and the heat bath, or that between any two neighboring particles. The heat conductivity is then measured, by assuming the Fourier law, as $\kappa \approx jN/(T_L - T_R)$. We set $T_L = 6$ and $T_R = 4$ so that the nominal temperature of the system is $T = 5$. The heat conductivity at any other temperature T' can be obtained through the scaling relation $\kappa(T') = \kappa(T)\sqrt{T'/T}$. We will focus on how the heat conductivity κ depends on the system size N and on the mass ratio M/m (hereafter we set $m \equiv 1$). We emphasize that in our simulations, long enough integration times ($>10^8$) have been taken so that the relative errors of all the measured values of κ are less than 1%.

Now let us turn to the simulations results. First of all, if the mass ratio is unity then the system is integrable and, with the heat bath given by Eq. (2), the heat conductivity writes

$$\kappa_{\text{int}} = N \sqrt{\frac{2k_B^3}{m\pi}} \left/ \left(\frac{1}{\sqrt{T_L}} + \frac{1}{\sqrt{T_R}} \right) \right. \quad (3)$$

In Fig. 1(a) this result is compared with our simulations and the agreement is perfect. This can be considered as a numerical test. Now, we change the mass ratio to make it slightly larger than one [see Fig. 1(a)]; it can be seen that for small N ($<10^2$), κ follows its integrable limit case, but as N is increased further, κ tends to saturate and becomes constant for $N > 10^4$. This could be taken as an empirical demonstration that at least for these mass ratios and for large enough system size, heat conduction is governed by the Fourier law, which is in clear contrast with existing theoretical and numerical predictions. (See, for example, Refs. [7,8]).

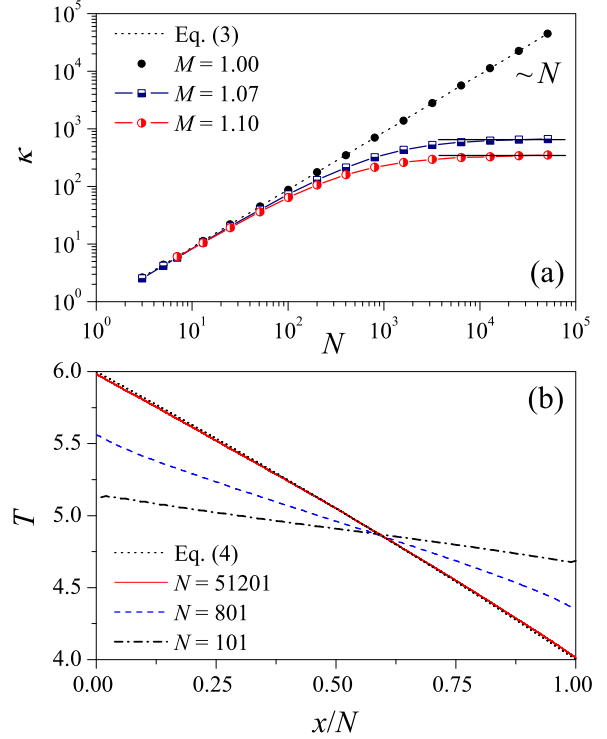


FIG. 1. (Color online) (a) The heat conductivity κ as a function of the system size N in the 1D diatomic gas model. The two horizontal lines denote the saturation value of $\kappa_{\text{GK}}(N)$ [Eq. (5)] at large N , for mass ratios $M = 1.07$ and 1.1 . (b) Comparison between the numerically computed temperature profile and the analytic expression [see Eq. (4)] for $M = 1.07$ at different system sizes.

The validity of the Fourier law also determines the internal temperature profile of the steady state. Indeed by assuming the Fourier law and equating the averaged local heat flux along the system, one obtains [17]

$$T(x) = \left[T_L^{3/2} \left(1 - \frac{x}{N} \right) + T_R^{3/2} \frac{x}{N} \right]^{2/3}. \quad (4)$$

In Fig. 1(b), this prediction is compared with our simulations results for $M = 1.07$. Numerically, the temperature of the i th particle is measured as the time average of its kinetic energy, i.e., $T(x_i) = \langle \mu_i v_i^2 / k_B \rangle$, with $\mu_i \in \{M, m\}$ and v_i being its mass and velocity, respectively. It is seen that numerical results are in very good agreement, for $N > 10^4$, with this theoretical prediction.

We now turn to the linear response theory to check if this approach leads to consistent results thus confirming the validity of the Fourier law for large N . Based on the Green-Kubo formula, which relates transport coefficients to the current time-correlation functions, the heat conductivity of a 1D finite system can be expressed as [18,19]

$$\kappa_{\text{GK}}(N) = \frac{1}{k_B T^2 N} \int_0^{\tau_{\text{tr}}} dt \langle J(0)J(t) \rangle. \quad (5)$$

In this formula, $J \equiv \sum_i \mu_i v_i^3 / 2$ represents the total heat current and $\langle J(0)J(t) \rangle$ is its correlation function measured in the equilibrium state with the periodic boundary condition. The integration is truncated at time τ_{tr} which is suggested to

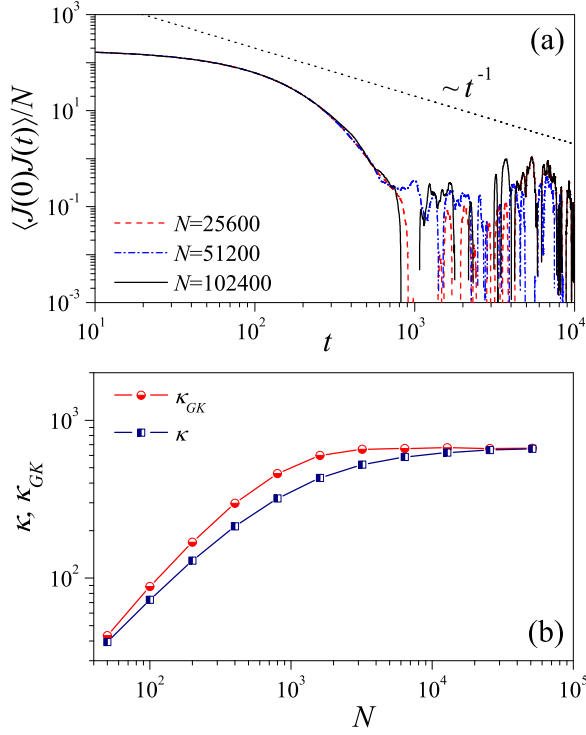


FIG. 2. (Color online) (a) Correlation functions of the total heat current for the 1D diatomic gas model. The dotted line indicates the scaling $\sim t^{-1}$: A faster decay of the correlation function implies convergence of the heat conductivity in the thermodynamic limit. (b) The comparison of the heat conductivity obtained by using the Green-Kubo formula [Eq. (5)] and by using the nonequilibrium setting. In both panels $M = 1.07$.

assume the value of $\tau_{tr} = N/(2v_s)$ (v_s is the sound speed of the system) [20]. To numerically compute $\kappa_{GK}(N)$, we consider isolated systems with periodic boundary conditions. The initial condition is randomly assigned with the constraints that the total momentum is zero and the total energy corresponds to $T = 5$. The system is then evolved and after the equilibrium state is reached, we compute $\langle J(0)J(t) \rangle$ and the integral in Eq. (5).

The results for $M = 1.07$ are presented in Fig. 2. It can be seen from Fig. 2(a) that for a large system ($N > 10^4$), the correlation function changes slowly at short times ($t < 10^2$), which reflects the fact that the system still mimics its integrable limit; however, from $t \sim 10^2$ to 10^3 , the correlation function undergoes a rapid decay and eventually, when $t > 10^3$, it begins to oscillate around zero. (The negative values of $\langle J(0)J(t) \rangle$ are not shown in this log-log scale.) In Fig. 2(b), the dependence of κ_{GK} on the system size is shown. It can be seen that κ_{GK} agrees with κ despite some deviations at small N .

Next we consider the dependence on the mass ratio. By using the same nonequilibrium setting we have extensively investigated the system size dependence of κ for the mass ratio ranging from 1.07 to 64. The results for $1.07 \leq M \leq 3$ are shown in Fig. 3(a). A three-stage process can be recognized: For small system sizes $\kappa \sim N$, similar to the integrable case. For large system sizes, κ shows a tendency to $\sim N^{1/3}$. In between these two regimes, there appears an intermediate, bridging regime, where κ changes at a lower rate (see

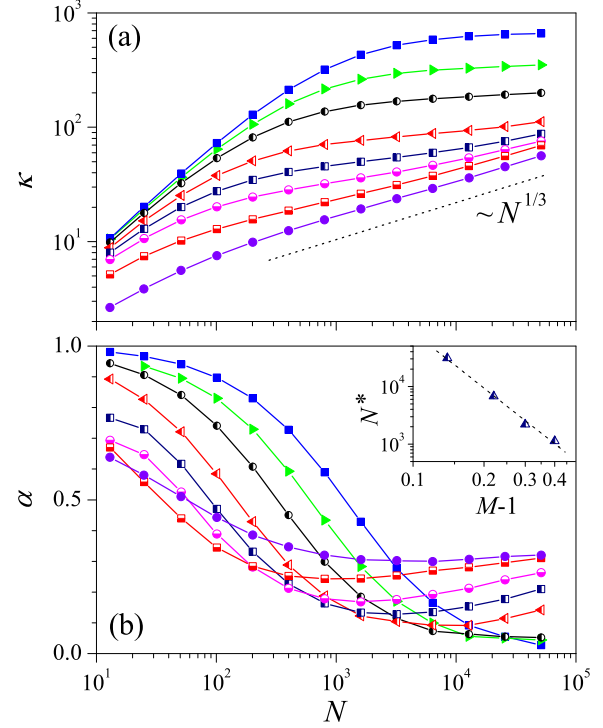


FIG. 3. (Color online) (a) The heat conductivity κ versus the system size N for the 1D diatomic gas model. From top to bottom, the mass ratio M is, respectively, 1.07, 1.10, 1.14, 1.22, 1.30, 1.40, the golden mean (≈ 1.618), and 3. The corresponding tangent α of the κ - N curve is given in (b) with the same symbols. In the inset we plot the turning point N^* , after which α starts growing with N , as a function of $M - 1$. The best fitting (the dotted line) suggests $N^* = 54/(M - 1)^{3.2}$.

particularly the cases of $M = 1.22$ and 1.30). Actually, in this intermediate regime, as M is decreased, the conductivity κ tends to be constant over a larger and larger interval. For $M \geq 3$ instead (data not shown here) the dependence $\kappa \sim N^{1/3}$ appears more and more clearly in agreement with the existing theories [7,8].

In order to better understand the dependence of κ on N , along each curve provided in Fig. 3(a) we computed its tangent $\alpha(N)$ and plot the results in Fig. 3(b). Note that $\alpha(N)$ exhibits a nonmonotonic behavior and reaches a minimum at a certain system size N^* . Interestingly enough, the value of N^* appears to grow very fast with decreasing M [see the inset in Fig. 3(b)]. This result shows that a very small tangent α , i.e., a Fourier-like behavior of thermal conduction, can be observed over an increasingly large system size when the integrable limit is approached. At the same time, for $N > N^*$, anomalous behavior emerges gradually.

The conclusion is that for any mass ratio different from unity the behavior $\kappa \sim N^{1/3}$ seems to always take place even though it cannot be detected numerically when the mass ratio approaches unity since in this limit N^* becomes exceedingly large. On the other hand, based on our available data, the possibility that there is a phase transition around $M \approx 1.3$ cannot be ruled out with certainty.

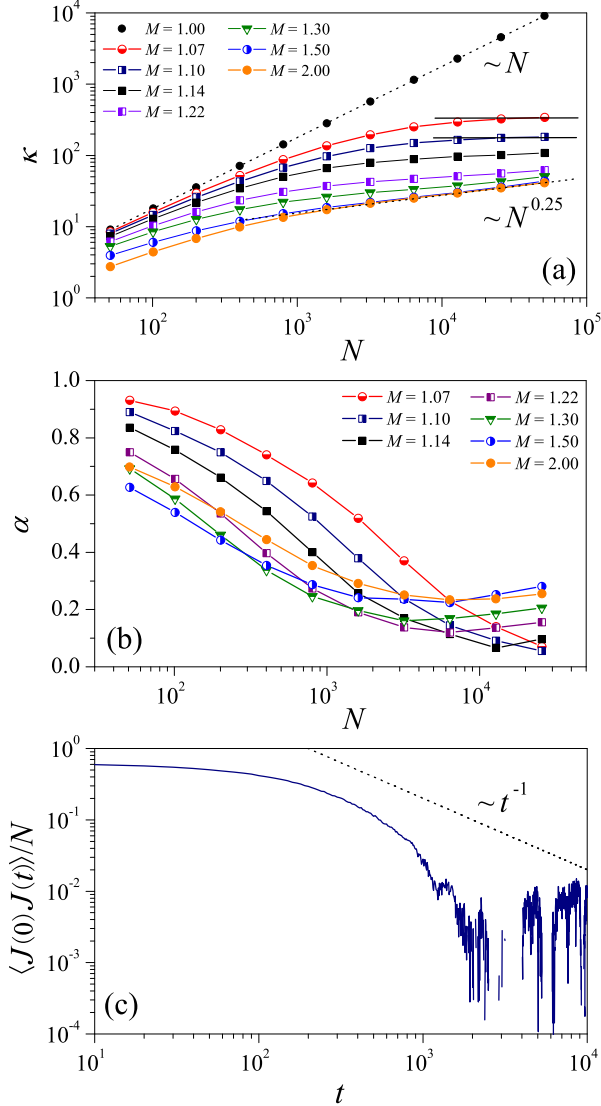


FIG. 4. (Color online) (a) The heat conductivity measured in the nonequilibrium setting for the 1D diatomic Toda lattice with mass $M = 1$ (the integrable case), 1.07, 1.10, 1.14, 1.22, 1.30, 1.50, and 2. The dotted lines indicate, respectively, the ballistic behavior $\kappa \sim N$ and the power law best fitting to the case of $M = 2$, $\kappa \sim N^\alpha$, with $\alpha = 0.25$. The horizontal lines denote the saturated values of $\kappa_{\text{GK}}(N)$ for $M = 1.07$ and 1.10 . (b) The corresponding tangent α of the κ - N curve with the same symbols. (c) The heat current correlation function for $M = 1.10$ with $N = 25\,600$, showing a decay faster than $\sim 1/t$.

III. 1D DIATOMIC TODA CHAIN

The above described scenario in which the Fourier law appears in the “vicinity” of the integrable limit is not exclusive of the gas model. In the following we show that it is also the case for lattices. The model we consider here is a diatomic variant of the Toda lattice [18,21] with the Hamiltonian,

$$H = \sum_i \left[\frac{p_i^2}{2\mu_i} + U(x_i - x_{i-1}) \right], \quad (6)$$

where the potential is $U(x) = \exp(-x) + x$, and the particles take masses M and $m \equiv 1$ alternatively. As for the gas model, this system is integrable when the mass ratio is one. We

measure the heat conductivity in both the nonequilibrium and equilibrium settings again, and find that the results turn out to agree with each other. In the nonequilibrium simulations, we couple the system to two Langevin heat baths [22] with the temperature $T_L = 1.2$ and $T_R = 0.8$. The heat current is defined as $j \equiv \langle j_i \rangle$ with $j_i \equiv v_i \partial U(x_{i+1} - x_i) / \partial x_i$ [23]. In Fig. 4(a) the measured κ for different values of M is given. Again, for mass ratios close to unity, κ is close to the integrable case when the system is small ($N < 10^2$) but tends to a value which agrees with that obtained by using the Green-Kubo formula for the large system’s size ($N > 10^4$). For larger mass ratio (see the case of $M = 2$) the heat conductivity is anomalous. Similarly to the hard-point gas model, the tangent $\alpha(N)$ exhibits a nonmonotonic behavior, with the minimum reached at a system size N^* rapidly growing when the integrable limit $M = 1$ is approached [see Fig. 4(b)]. With regard to the equilibrium simulations, we assume periodic boundary conditions, null total momentum, and total energy corresponding to $T = 1$. The total heat current is $J = \sum_i j_i$ and its correlation function for $M = 1.1$ is shown in Fig. 4(c), where it exhibits a faster than $\sim 1/t$ decay as expected in the case of normal heat conduction. The overall emerging picture is the same as presented above for the gas model. This similarity is unlikely a coincidence due to the contrasting difference in the dynamics of the two systems; rather, it strongly suggests some general mechanisms in the heat conduction properties as one departs from the integrable limit.

IV. SUMMARY AND DISCUSSIONS

We have shown that in two 1D momentum-conserving paradigmatic systems, the heat conductivity can be independent of the system size over a considerably wide range. Such a Fourier-like behavior appears as a quite general feature for lattice or gas models close to the integrable limit. Apart from theoretical implications in transport theory, our finding may have experimental relevance as well, because the system size over which the heat conductivity keeps constant, grows very fast as the system approaches its integrable limit.

Our present understanding of the heat conduction problem is mainly based on numerical empirical evidence while rigorous analytical results are hard to obtain. Numerical analysis consists of steady-state, nonequilibrium simulations or of equilibrium simulations based on linear response theory and the Green-Kubo formula. If both methods give reasonable evidence for the Fourier law and if, moreover, they lead to the same numerical value of the heat conductivity κ , then this has been generally considered as a conclusive evidence that the Fourier law is valid. This conclusion, however, could not be correct. As we have shown in this paper, the agreement between equilibrium and nonequilibrium simulations does not allow, *per se*, to draw any definite conclusion. Indeed this agreement might be a finite size effect and the Fourier law may appear to hold up to some system size N after which anomalous behavior sets in. The main point is that we have no indications at all about the critical value of N after which conductivity becomes anomalous. What we know from the numerical analysis of this paper is that this critical value seems to diverge rapidly as one approaches the integrable limit. This result is quite surprising to us and it is a feature which we

do not understand yet. While it is natural to expect an initial ballistic behavior for larger and larger system sizes as one approaches the integrable limit, it is absolutely not clear why the value of κ appears to saturate to a constant value and why this Fourier-like behavior may persist in an increasingly wide range of the system size before entering the anomalous regime.

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