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# Current progress on heat conduction in one-dimensional gas channels

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**Abstract** We give a brief review of the past development of model studies on one-dimensional heat conduction. Particularly, we describe recent achievements on the study of heat conduction in one-dimensional gas models including the hard-point gas model and billiard gas channel. For a one-dimensional gas of elastically colliding particles of unequal masses, heat conduction is anomalous due to momentum conservation, and the divergence exponent of heat conductivity is estimated as  $\alpha \approx 0.33$  in  $\kappa \sim L^\alpha$ . Moreover, in billiard gas models, it is found that exponent instability is not necessary for normal heat conduction. The connection between heat conductivity and diffusion is investigated. Some new progress is reported. A recently proposed model with a quantized degree of freedom to study the heat transport in quasi-one dimensional systems is illustrated in which three distinct temperature regimes of heat conductivity are manifested. The establishment of local thermal equilibrium (LTE) in homogeneous and heterogeneous systems is also discussed. Finally, we give a summary with an outlook for further study about the problem of heat conduction.

**Keywords** heat conductivity, hard-point gas, billiard, anomalous, local thermal equilibrium

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## 1 Introduction

We have known that heat is transported along the direction of a temperature gradient. The macroscopic transport rate is described by the Fourier law:

$$J = -\kappa \nabla T \quad (1)$$

Under the assumption of local thermal equilibrium, the heat flow  $J$  is linearly dependent on the temperature gradient  $\nabla T$  in the steady state, with the coefficient  $\kappa$  being the heat conductivity. In spite of the ubiquity of the phenomena in our daily life, there are still many open problems that puzzle theoretical physicists. One of the central issues is the problem of describing the macroscopic phenomenological law of irreversible thermodynamics in terms of the reversible microscopic dynamics [1].

### 1.1 Early results

From a microscopic point of view, energy is transported by the movements of heat carriers including electrons, phonons, photons, and molecules. The heat conductivity can be elementarily estimated by the kinetic theory of diluted gases:

$$\kappa = \frac{1}{3} C v \Lambda \quad (2)$$

where  $C$  is the volumetric specific heat,  $v$  and  $\Lambda$  are the mean velocity and mean free path of heat carriers. For heat carriers such as electrons and phonons, the heat conductivity can be expressed as [2]:

$$\kappa = \frac{\pi^2 k_B^2 n_e T}{m v_F} \Lambda \quad (3)$$
$$\kappa = \frac{\Lambda}{3} \int_0^{\omega_{\max}} C_\omega v_\omega d\omega$$

where  $m$  is electron mass,  $n_e$  is the electron number density, and  $v_F$  is the electron velocity at the Fermi surface. Correspondingly,  $C_\omega$  and  $v_\omega$  are the volumetric specific heat and the velocity at each frequency.

More systematic theory arising from nonequilibrium transport is the Boltzmann transport equation (BTE), proposed in 1872 by Boltzmann. For diluted particles such as gaseous molecules, electrons, and phonons, the well-known equation can be expressed as [3, 4]:

$$\frac{\partial f}{\partial t} = D\{f\} + S\{f\} \quad (4)$$

The left term describes time evolution of the distribution function  $f(\mathbf{p}, \mathbf{r}, t)$  of an ensemble of heat carriers. The first term of the rhs is the drift term, which is responsible for the change of the distribution function resulting from the inertial motion of the particles and their acceleration in external fields:

$$D\{f\} = -\mathbf{v} \cdot \nabla_{\mathbf{r}} f + \mathbf{F} \cdot \nabla_{\mathbf{p}} f \quad (5)$$

where  $\mathbf{r}$ ,  $\mathbf{p}$  and  $\mathbf{F}$  are position vector, momentum vector, and external force, respectively. The second term of the rhs is the scattering term, which is crucial to the BTE. If the system is not far from the equilibrium, one can take the relaxation time approximation:

$$S\{f\} = \left( \frac{\partial f}{\partial t} \right)_c = \frac{f_0 - f}{\tau(\mathbf{r}, \mathbf{p})} \quad (6)$$

where  $f_0$  is the equilibrium distribution and  $\tau(\mathbf{r}, \mathbf{p})$  is the relaxation time, which is often assumed as a function of  $\mathbf{r}$  and  $\mathbf{p}$ . The BTE has successfully explained the temperature, impurity, isotope scattering, and quantum confinement dependence of the electrical and thermal conductivity [5]. However, when the relaxation time approximation does not apply it is not possible to present a solution of the Boltzmann equation in closed form, which includes all possible external fields [3]. In this case it is difficult to deal with the equation mathematically.

In 1929, Peierls developed a theory on the basis of Boltzmann equation for the phonons [6]. Peierls theory states that the mean free path of an insulating solid is infinite without *Umklapp* processes, thus the heat conductivity becomes divergent. That is to say, the *Umklapp* scattering can drastically modify the results based on momentum conservation. Peierls theory successfully describes the temperature dependence of the thermal conductivity. Furthermore, according to this theory, one does not anticipate a finite thermal conductivity in one-dimensional mono-atomic lattices with pair interactions. This seems so far to be a correct prediction, at least in the numerous numerical results performed on existing models [7].

Another mostly adopted approach on transport process is Green-Kubo formula proposed in 1952, which is based on linear response theory [1, 8–11]. The heat conductivity is calculated in terms of time-correlation functions by:

$$\kappa = \frac{1}{k_B T^2} \lim_{t \rightarrow \infty} \int_0^t d\tau \lim_{V \rightarrow \infty} V^{-1} \langle \mathbf{J}(\tau) \mathbf{J}(0) \rangle \quad (7)$$

where  $\mathbf{J}$  is total heat flux,  $V$  the volume of the system under

consideration, and the bracket denotes ensemble averaging. It is worth noticing that  $\langle \mathbf{J}(\tau) \mathbf{J}(0) \rangle$  is the correlation function in thermal equilibrium. The Green-Kubo method relates the transport coefficient in nonequilibrium to the correlation function in thermal equilibrium state, independent of whether a particular system can actually reach this state.

## 1.2 Lattice models

Due to the drastic achievement in computer capacity, a large number of studies, especially numerical simulations, have been devoted to the problem of heat conduction in the past several decades, which is expected to link the irreversibility of macroscopic law with the time reversible microscopic dynamics. The pioneering computer simulation was performed by Fermi, Pasta, and Ulam [12, 13] at the begin of the 1950s. They integrated the dynamical equations, the cited FPU model that describes a chain of classical oscillators coupled by nonlinear forces, to test how equilibrium is approached by an isolated set of nonlinearly coupled oscillators.

It has been known that the dimensionality of a system has a great influence on its characteristics of heat transport. In low-dimensional systems ( $d \leq 2$ ), the heat conductivity is no longer the property of a material. Narayan and Ramaswamy [14] justified the dimension effect on the heat conductivity and found that the thermal conductivity diverges as the length of a one-dimensional system increases, following a power law. Furthermore, modern experimental techniques allow to directly probe the heat conductivity of one-dimensional micro-devices such as single-walled nanotubes [15] and nanostructures [16–18]. It is believed that the studies of heat conduction in one-dimensional systems would help in understanding these experimental results on heat conduction in one-dimensional and quasi-one-dimensional devices.

The anomalous heat conductivity in classical one-dimensional system arouses more and more attention to the old problem of identifying the minimal requirements for a dynamical system to fulfil the Fourier law [1]. The heat conductivity  $\kappa$  in one-dimensional systems has a size dependence with the relation of  $\kappa \sim L^\alpha$ . The case of  $\alpha = 0$  is called “normal” heat conduction, indicating that the Fourier law holds in the system. When  $\alpha > 0$ , “anomalous” heat transport occurs, implying that heat conductivity diverges with the system size  $L$ .

A general model describing the heat conduction in crystals is one-dimensional classical lattice, whose Hamiltonian reads [19]:

$$H = \sum_{i=1}^N \left[ \frac{p_i^2}{2m_i} + U(q_i) + V(q_{i+1} - q_i) \right] \quad (8)$$

where  $q_i$  denotes the particle displacement from its equilibrium position. Here,  $U(q_i)$  is called the *On-site potential*, which represents a phonon-fixed lattice interaction; and

$V(q_{i+1}-q_i)$  is *interparticle* potential, which denotes phonon-phonon interaction. Only the nearest-neighbor interaction is considered for simplicity.

Rieder, Lebowitz, and Lieb [20] studied a linear chain of  $N$  harmonically coupled (with uniform strength) particles, namely,

$$U(q) = 0, \quad V(q) = \frac{1}{2} \omega^2 q^2 \quad (9)$$

The harmonic oscillator model showed that the transport is ballistic with  $\kappa \sim L^1$ , and the temperature profile is asymptotically flat at the value of the average temperature.

The model becomes a discretized Klein-Gordon system [19] if on-site potential is harmonic,

$$U(q) = \frac{1}{2} \Omega^2 q^2, \quad V(q) = \frac{1}{2} \omega^2 q^2 \quad (10)$$

The presence of the quadratic potential breaks the momentum conservation of the model but retaining its linearity. The momentum non-conserving linear optical chain also exhibits ballistic heat transport. Actually, this optical model behaves essentially in the same way as the acoustic chain does. It is found that anomalous transport does not imply momentum conservation. Thus, momentum conservation is not a necessary condition for anomalous transport.

The celebrated Toda lattice [21, 22] with

$$U(q) = 0, \quad V(q) = e^{-q} \quad (11)$$

is an example of a nonlinear but integrable and momentum conserving model. The numerical simulation obtained by Mokross and Büttner [23] showed a flat temperature profile and a ballistic heat transport. Hence, heat transport in this *integrable* and *momentum conserving* but *nonlinear* chain is found to be the same way as in linear system, which is explained by the freely propagating of independent solitons [24, 25].

What happens to a nonlinear but integrable chain that does not conserve momentum, i.e., with  $U(q) \neq 0$ . One of such models has been proposed by Izergin and Korepin [26]. They introduced a spatially discrete version of the famous  $\sin(h)$ -Gordon model [19], which preserves the integrability of the continuum limit and has an on-site potential. The result strongly suggests that integrability alone is sufficient to lead to anomalous (ballistic) heat transport, irrespective of the presence of on-site potential. This provides another illustration of the result that momentum conservation is not necessary for anomalous transport, even in a nonlinear chain.

Since the pioneering work of Fermi, Pasta, and Ulam (FPU) [12], a series of recent studies have been involved in the celebrated FPU- $\beta$  chain, which has

$$U(q) = 0, \quad V(q) = \frac{1}{2} q^2 + \frac{1}{4} \beta q^4 \quad (12)$$

Careful numerical simulations by different groups [27, 28] showed that the model exhibits power-law divergence of thermal conductivity in the thermodynamic limit  $\kappa \sim L^\alpha$ ,

with  $\alpha = 2/5$ , despite strongly chaotic behavior which is characterized by almost everywhere positive Lyapunov exponents. Whereas, Casati *et al.* [29] always conjectured that chaos might be the essential condition under which heat transfer obeys the Fourier law by numerical computing one-dimensional many-body system, the “ding-a-ling” model. It is considered that the anomalous heat behavior in FPU- $\beta$  chain is due to the solitary wave propagation along the chain [30]. Hatano [31] has shown that for the diatomic Toda chain with dimerized masses, where  $m_{2n} = m_2 \neq m_{2n+1} = m_1$ , there exists practically the same scaling with  $\alpha \approx 0.4$  as for FPU models. More recently, a similar scaling has been obtained where  $V(q)$  has the form of Lennard-Jones or Morse potentials [32]. These results suggest possible universality of the scaling exponent  $\alpha \approx 2/5$  of the divergence of heat conductivity for strongly chaotic, momentum conserving lattices. Furthermore, the universality of scaling has been analytically explained by self-consistent mode-coupling theory from Lepri [27, 33, 34] and Boltzmann equation by Perezenev [35].

However, Narayan and Ramaswamy [14] recently predicted the universal exponent  $\alpha = 1/3$  for the divergence of heat conductivity using a hydrodynamic description for momentum conserving system. Numerical results of hard-point gas [36] and random collision model [37, 38] confirm the prediction. Furthermore, Cipriani *et al.* [39] presented evidently that energy diffusion is anomalous in the hard-point particles from a Levy walk description, and proved definitely the divergence rate of heat conductivity which turns out to be  $0.333 \pm 0.004$ , in good agreement with the renormalization-group prediction  $1/3$  [14].

To study the crossover of the divergent exponent from  $2/5$  to  $1/3$ , Wang and Li [40, 41] introduced a polymer-like chain. The chain consists of  $N$  point particles with mass  $m$  on a 1D lattice. The particles have both longitudinal and transverse motions. Only the neighboring particles interact is considered. The Hamiltonian is written as:

$$H(\mathbf{p}, \mathbf{r}) = \sum_i \frac{p_i^2}{2m} + \frac{1}{2} K_r \sum_i (|\mathbf{r}_{i+1} - \mathbf{r}_i - a|^2) + K_\phi \sum_i \cos \phi_i \quad (13)$$

where the position vector  $\mathbf{r} = (x, y)$  and momentum vector  $\mathbf{p} = (p_x, p_y)$  are two-dimensional;  $a$  is a lattice constant. They found that the thermal conductivity diverges with system size  $L$  as  $\sim L^{1/3}$  at high temperature, while at the low temperature regime, the thermal conductivity diverges with power  $2/5$ . A detailed mode-coupling theory analysis argued that the  $1/3$  power law comes from the mode coupling between the longitudinal modes and transverse modes. When the coupling is absent, for example, in the 1D FPU model, the  $2/5$  is recovered.

The FPU model discussed above is a typical example of lattice model without on-site potential. The Frenkel-Kontorova model, on the other hand, is representative of a general one-dimensional lattice with on-site potential. It describes a chain of particles connected by springs with

strength constant  $\lambda$ , and put on the substrate with periodical potential [19, 42]. The average particle distance is  $l$ , and the periodicity of on-site potential is  $2a$ . This potential is given by:

$$U(q_i) = \frac{\beta}{2} \left( 1 - \cos \frac{\pi}{a} q_i \right), \quad V(q_i) = \frac{\lambda}{2} (q_{i+1} - q_i - l_0)^2 \quad (14)$$

The FK model was first proposed by Frenkel and Kontorova [43] in 1938 to study surface phenomena. Since then it has found applications in a wide variety of physical systems, such as adsorbed monolayers, Josephson junctions, charge density waves, magnetic spirals, and DNA denaturation. The numerical results of Hu, Li, and Zhao [44] have rigorously convinced that this nonintegrable model exhibits normal heat transport. A more detailed review can be found in Ref. [42].

The strength [45] and the periodicity [46] of the external potential affect the thermal conductivity significantly. This characteristic can be used to design a controllable thermal conductor. For potential applications, various designs of thermal conductors by controlling the periodicity of the external potential have been presented [19]. The thermal conductivity can change nearly 10 000 times. Accordingly, one can control the system from a good thermal conductor to a thermal insulator to meet the requirement of the devices. More appealingly, the thermal diode and thermal rectifier can be designed by coupling two or three FK chains with different parameters [19, 47].

Although great progress has been made, many issues need to be ascertained both from an analytical and numerical point of view. Although lattice models are the very idealization of a real crystal, there are other gas models including the hard-point gas and billiard gas channels that play a crucial role in understanding the dynamic behavior of complex systems consisting of a large number of particles. In Section 2, we present a line of development of gas models. In Section 3, we provide current progress on billiard gas channels, especially discussing the role of chaos in heat conduction and the influence of the quantized degree of freedom on heat transport in the billiard channel. Furthermore, in Section 4, we provide a clue of the studies on the basic problem of local thermal equilibrium. Finally, we give a summary with discussions.

## 2 One-dimensional hard-point gas models

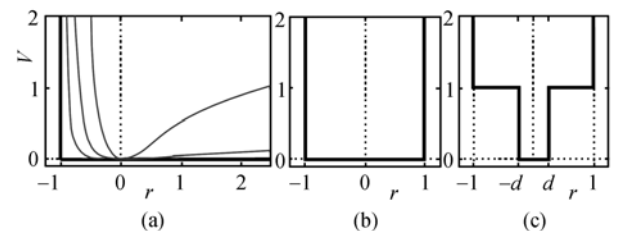
Understanding the dynamical origin for the validity of the Fourier law of heat conduction in deterministic one-dimensional particle chains is one of the oldest and most frustrating problems in nonequilibrium statistical physics. An alternative and useful model is of hard-point gases where a chain of  $N$  point particles labelled by  $i = 1, \dots, N$  moving on a line and undergoing perfectly elastic collisions when neighboring particles contact. In this model, the interaction merely occurs between the nearest-neighbor particles through a hard-point potential  $V(r)$ . When an elastic collision between particle  $i$  and  $i+1$  happens, the new velocities are determined by momentum and energy conservation:

$$\begin{aligned} u'_i &= \frac{m_i - m_{i+1}}{m_i + m_{i+1}} u_i + \frac{2m_{i+1}}{m_i + m_{i+1}} u_{i+1} \\ u'_{i+1} &= \frac{2m_i}{m_i + m_{i+1}} u_i - \frac{m_i - m_{i+1}}{m_i + m_{i+1}} u_{i+1} \end{aligned} \quad (15)$$

where the mass, position, and velocity of the  $i$  th particle are denoted by  $m_i$ ,  $x_i$ , and  $u_i$ , respectively. During the period between two successive collisions, the particles travel freely with constant velocity. The chain is coupled to heat baths with Maxwell boundary conditions. Namely, whenever a particle of mass  $m$  collides with a wall at temperature  $T$ , it is rebounded with a velocity chosen from the distribution  $P(u) = (m|u|T) \exp[-mu^2/(2T)]$ .

When all the masses are equal, the system becomes integrable and the heat current is independent of the size of the system, the same behavior as observed in harmonic chains [48]. However, as soon as the masses are different, the system is non-integrable. Thus, it becomes a possible candidate for checking the validity of Fourier law. But the known results are quite controversial: for the case of alternate masses, which was considered by Casati [28],  $m_{2i} = 1$ ;  $m_{2i+1} = 1 + \delta$ , it was not possible to draw any definite conclusion about the scaling behavior of the conductivity. More recently, numerical simulations performed by Dhar [48] showed a slow divergence of  $\kappa$  ( $\sim L^\alpha$  with  $\alpha < 0.2$ ), while equilibrium simulations on a 1D gas of elastically colliding particles of unequal masses discussed by Garrido *et al.* [49] have led to a normal behavior. However, Prosen and Campbell [50] have proved a theorem according to which any 1D system with momentum conserving dynamics has infinite (anomalous) thermal conductivity.

To shed light upon these controversial results for thermal conductivity in one-dimensional systems, a series of studies [36, 51, 52] have been made into the conducting problem of the alternating mass hard-point gas recently. Savin *et al.* [51] presented an extensive and accurate numerical study of the 1D gas with different interparticle hard-point interactions, as shown in Fig. 1. When the particles interact through elastic hard-point collisions (and therefore their total momentum equal to zero on average), the system is shown to have infinite (anomalous) thermal conductivity always, independent of the ratio of the masses. In



**Fig. 1** Three types of interparticle hard-point potentials. (a) Asymmetric potential with one reflection wall (thick lines) and the sequence of Lennard-Jones potentials (thin curves) converging to the hard-point one. (b) Symmetric potential with two reflection walls. (c) Symmetric potential with metastable states.

the systems with symmetric interparticle interactions of the types shown in Fig. 1 (b) or (c), Prosen-Campbell theorem does not apply.

Theoretically, one would expect a universal value of divergence exponent  $\alpha$  for different one-dimensional models. It seems reasonable to hypothesize that the uncertainty of the divergence exponent is due to strong finite-size effects that slow down the convergence to the expected asymptotic behavior. Grassberger *et al.* [36] presented large scale simulations for a one-dimensional chain of hard-point particles with alternating masses to make simulations more efficient by following Dhar's work [48]. A fast simulation algorithm allowed them to make much larger simulations than in previous works. They gave a compelling evidence that heat conduction in the 1D hard-point gas shows the anomalous divergence with a universal power law  $\kappa \sim N^\alpha$  with  $\alpha \approx 0.33$ , in spite of strong finite-size and finite-time effects. Casati *et al.* [52] provided firm convincing evidence that the energy transport in a one-dimensional gas of elastically colliding free particles of unequal masses is anomalous by a theoretical and numerical analysis based on a Green-Kubo-type approach specialized to momentum-conserving lattices. The numerical results demonstrated  $\kappa \propto N^\alpha$  with  $\alpha \approx 0.25$  over a very large range in  $N$ , instead of a different power-law behavior. And the scaling exponent  $\alpha$  does not change appreciably with the mass ratio  $r = m_1/m_2$ .

In order to obtain a universal scaling form of the thermal conductivity  $\kappa$  as a function of system size  $L$ , Deutsch *et al.* [37] introduced a "random collision model" for studying dynamics of momentum conserving one-dimensional systems. In this model, hard sphere particles with rough surface are confined to a long narrow tube. Any collision keeps the total energy being conserved and the total momentum in both directions being conserved. The extent in the transverse direction is taken to be slightly less than twice the diameter of the particles. This ensures that the particles cannot pass through each other, but allows a large range of incidence angles at the collisions. Thus, the energy transport along the tube remains quasi-one-dimensional, with the transverse degree of freedom serving as an additional randomizing effect.

The heat reservoirs at two ends were implemented through the velocity distribution of particles leaking out of a heat reservoir: whenever an extremal particle collided with the reservoir adjoining it, its velocity was chosen from the distribution:

$$P(v_x, v_y) \propto v_x \exp[-m(v_x^2 + v_y^2)/(2k_B T)] \quad (16)$$

where  $x$  and  $y$  are along the longitudinal and transverse direction, respectively, and  $T$  is the temperature of the reservoir.

By introducing a model, Deutsch *et al.* [37] obtained the thermal conductivity of a quasi one-dimensional classical chain of hard sphere particles as a function of the length of the chain, in good agreement with the earlier analytical

prediction of  $\kappa \sim L^{1/3}$  [14] over a wide range of length scales for such momentum conserving systems. Subsequently, they examined numerically the full spatiotemporal correlation functions for all hydrodynamic quantities for the random collision model [38]. The autocorrelation function of the heat current, through the Kubo formula, gives a thermal conductivity exponent of 1/3 in agreement with the analytical prediction and previous numerical work. By the way, this result depends crucially on the choice of boundary conditions: the exponent turns to 1/2 for periodic boundary conditions, in comparison to 1/3 for open boundary conditions.

Recently, a Levy walk description, which is so far invoked to explain anomalous heat conductivity in the context of noninteracting particles, was introduced in a one-dimensional chain of diatomic hard-point particles [39]. The results provided a firm evidence that energy diffusion is anomalous in the diatomic gas, and estimated the divergence rate of heat conductivity as  $0.333 \pm 0.004$ . Furthermore, they concluded that the anomalous behavior is due to the long-range correlations between collisions by comparing the collision pattern in their model with a set of completely uncorrelated events.

After several decades of intensive investigations, it seems that overall momentum conservation in a Hamiltonian system is a key factor for divergence of heat conductivity  $\kappa$  as a function of the system size  $L$  [14, 31, 33, 34, 50, 52]. Therefore, Li *et al.* [53] constructed a one-dimensional model of elastically colliding particles with alternate masses  $m$  and  $M$  without total momentum conservation by confining the motion of particles of mass  $M$  (bars) inside unit cells. Schematically, the model is shown in Fig. 2. As one might expect, the results presented convincing numerical evidence for the validity of Fourier law of heat conduction in spite of the lack of exponential dynamical instability. It has been shown that breaking the total momentum conservation is crucial for the validity of the Fourier law.

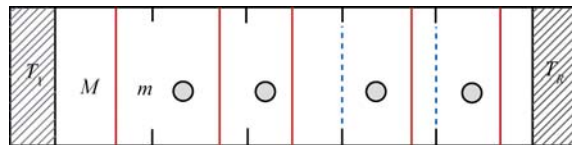


Fig. 2 The geometry of the model. The elementary cell is indicated by two dotted lines.

### 3 Quasi-one-dimensional billiard channels

#### 3.1 Heat transport

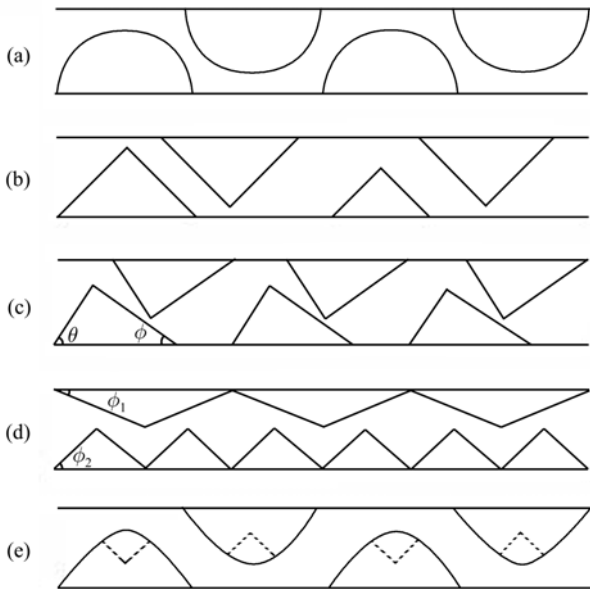
In recent years, a class of model with noninteracting particles moving along a periodic array of convex scatterers (billiard gas channels) has been applied to the problem of heat conductivity in low-dimensional systems. The absence of interactions allows one, on one side, to trace back heat con-

ductivity properties to the diffusion of single particles in equilibrium; on the other side, simplifies the task of understanding heat conductivity.

To study heat conduction, the two ends of the billiard gas channel (see Fig. 3) are put into contact with heat baths. The heat baths can be modelled by  $\delta$  function, implying a uniform velocity obtained by particles from the heat bath [54, 55]. More usually, the heat bath with stochastic kernels of Gaussian-type is applied [56–58]. In this case, the probability distribution of velocities for particles coming out from the baths is

$$P(v_x) = \frac{v_x}{T} \exp\left(-\frac{v_x^2}{2T}\right)$$

$$P(v_y) = \frac{1}{\sqrt{2\pi T}} \exp\left(-\frac{v_y^2}{2T}\right) \quad (17)$$



**Fig. 3** The geometrical configuration of billiard gas channels. (a) The Lorentz gas channel (Ref. [57]). (b) The Ehrenfest channel (Ref. [54]). (c) The triangle gas channel (Ref. [56]). (d) The polygonal gas channel (Refs. [58, 59]). (e) The channel with different degree of chaos (Ref. [55]).

for  $v_x$  and  $v_y$ , respectively. By dividing the configuration space into a set of boxes  $C_i$ , the temperature field at a stationary state is calculated by time averages,

$$T_{C_i} = \langle E \rangle_{C_i} = \frac{\sum_j^M t_j E_j(C_i)}{\sum_j^M t_j} \quad (18)$$

The time spent within a box in the  $j$ th visit is denoted by  $t_j$  and the total number of crossings of a box  $C_j$  during the simulation is  $M$ . Here  $E_j(C_i)$  is the kinetic energy of the particle at its  $j$ th crossing of the  $C_i$  box. The heat flux is calculated by the change of energy carried through to the left and right ends by the particles,

$$J = \frac{1}{t_M} \sum_{j=1}^M \Delta E_j \quad (19)$$

where  $\Delta E_j = (E_{\text{in}} - E_{\text{out}})_j$  is the energy change at the  $j$ th collision with a heat bath,  $t_M$  is the total time spent for  $M$  such collisions.

As mentioned above, Casati *et al.* suggested that the exponential instability might be essential to the normal heat transport [29] in 1984. This conjecture has been further confirmed by the study of heat conduction in a quasi-one-dimensional Lorenz gas channel [57] in 1999. It has been demonstrated that the heat conduction in this model obeys the Fourier law. As shown in Fig. 3 (a), the model consists of two parallel lines at a certain distance, and a series of semi-circles of radius  $R$  placed in a triangular lattice along the channel. The dynamics in the Lorenz gas is chaotic, namely, the nearby trajectories are separated exponentially. It has been demonstrated that the heat conduction in this model obeys the Fourier law.

However, is chaos a sufficient factor to normal heat conduction? The results from the FPU- $\beta$  model [27, 60] indicated anomalous transport behavior in spite of the existence of chaos. To clarify whether the exponential instability is indispensable to normal heat conduction, Li *et al.* introduced a so-called Ehrenfest gas channel [54]. Instead of the semi-circles of radius  $R$ , they placed right triangles periodically along the chain, shown in Fig. 3 (b). Due to the existence of free path, this model demonstrates a superdiffusive motion, the heat conductivity diverges with the system size as  $k \sim N^\beta$  ( $\beta > 0$ ). But the astonishing result occurs if the triangles are placed randomly, either in position or in height. They found the heat conduction obeys the Fourier law due to the normal diffusion induced by the disorder, despite the linear instability (not exponent instability) in this case.

A triangle gas model [56] which consists of two parallel lines of length  $L$  at distance  $H$  and a series of triangular scatterers is proposed by Li *et al.*, as shown in Fig. 3 (c). In this channel, no particle can move between the two reservoirs without suffering elastic collisions with the triangles. Therefore, this model is similar to the one studied in the Lorenz gas channel, with triangles replacing discs. The essential difference between them is that in the triangular model the dynamical instability is linear and, therefore, the Lyapunov exponent is zero. The numerical results from this model depend sensitively on whether the ratio  $\theta/\pi$  and  $\phi/\pi$  are rational or irrational numbers. In the case of irrational ratios, the motion of heat carriers is mixing and diffusive, thus the heat conduction obeys the Fourier law; while in the case of rational ratios, the system shows a superdiffusive behavior.

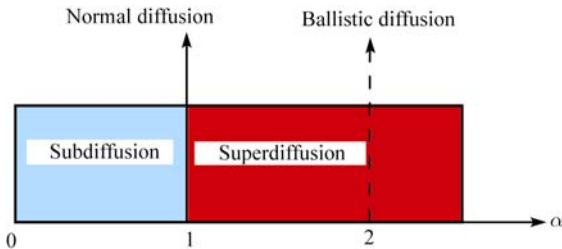
Another interesting billiard gas channel was proposed by Alonso *et al.* [58, 59]. The geometry of this model is shown in Fig. 3 (d). By fixing  $\phi_1 = (\sqrt{5}-1)\pi/8$ , and adjusting the angle  $\phi_2 = \pi/q$  with  $q = 3, 4, 5, 6, 7, 8, 9$ , this model displays a very interesting transition from a superdiffusive motion ( $q$

=3, 5, 6, 7), to a subdiffusive motion ( $q = 4$ ), and normal diffusion at  $q = 8$  and 9. This subdiffusive behavior,  $\alpha < 1$  in this case, is quite interesting for heat conductivity. It means that the thermal conductivity of such a subdiffusive system is an insulator in the thermodynamic limit.

Therefore, chaos is neither essential nor necessary to normal heat conduction. Despite that the heat conduction in a quasi-one-dimensional Lorenz gas channel [57] is normal, however, the subsequent studies on disordered Ehrenfest gas channel [54], triangle gas channel [56], and polygonal gas channel [58, 59], and an alternate mass hard-core potential chain [53] show that a system with zero Lyapunov exponent can also display a normal diffusion and the heat conduction obeys the Fourier law.

### 3.2 Connection between heat transport and its diffusion

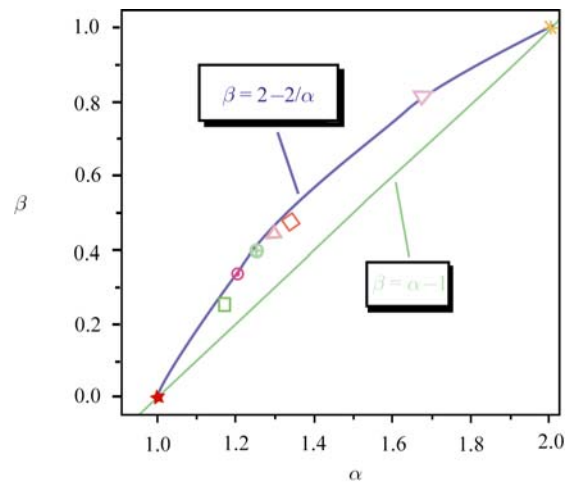
Li and Wang [61] proposed a relationship to link the heat transport and mass transport. Four types of diffusion in one-dimensional are illustrated in Fig. 4. If the mean square of the displacement of the particle is  $\langle \Delta x^2 \rangle = 2Dt^\alpha$ , and the thermal conductivity can be expressed in terms of the system size  $L$  as  $\kappa \sim L^\beta$ , then the relation  $\beta = 2 - 2/\alpha$  holds. Existing numerical data support the results, which are summarized and represented in Fig. 5.



**Fig. 4** Different domains of diffusion, defined by  $\alpha$  in the mean square displacement  $\langle \Delta x^2 \rangle = 2Dt^\alpha$ .

In the absence of resistance and umklapp processes, the phonons transport ballistically in a harmonic lattice model ( $\alpha = 2$ ), while the thermal conductivity in the 1D harmonic lattice diverges as  $L^\beta$  with  $\beta = 1$ , this is exactly what was shown by Lebowitz *et al.* [20]. Moreover, with this relation, normal diffusion ( $\alpha = 1$ ) indicates normal heat conduction obeying the Fourier law ( $\beta = 0$ ). A number of one-dimensional models have been found to be of normal diffusion and normal thermal conduction. For instance, the 1D Frenkel-Kontorova model [44], the 1D Lorentz gas channel [57], the 1D disordered Ehrenfest gas channel [54], the 1D irrational triangle channel [56], the alternate mass hard-core potential model [53], and some 1D polygonal billiard channels with irrational  $\phi_1$  and certain rational triangles  $\phi_2$  [58]. And 1D disordered lattice model under certain boundary conditions is also included [64, 65]. Between these two cases is superdiffusion ( $\alpha > 1$ ), which implies anomalous heat conduction with a divergent thermal conductivity. In this case, the ex-

ponent  $\beta$  ranges between 0 and 1, and differs from model to model. The exploration of universal scaling is under discussion. Some billiard gas models like Ehrenfest gas channel [54], the rational triangles model [56], the FPU-like model mentioned above and the nanotube are belong to this category. When  $\alpha < 1$ , the heat conductivity diminishes with the system size. Unfortunately there have not been so many systems working in this range, though it may attract more interest as the systems in this case act as a thermal insulator in the thermodynamic limit. One example is the polygonal gas channel [59] giving  $\kappa \sim L^{-0.63}$  and the other is the model with on-site potential [66] showing a exponential decay  $\kappa \sim \exp(-bL)$  in the range of large system size.



**Fig. 5** The divergence exponent of heat conductivity  $\beta$  versus the diffusion exponent  $\alpha$ .  $\star$ : Normal diffusion;  $*$ : The ballistic transport;  $\nabla$ : 1D Ehrenfest gas channel (Ref. [54]);  $\square$ : The rational triangle channel (Ref. [56]);  $\triangle$ : The polygonal billiard channel with  $\phi_1 = (\sqrt{5}-1)\pi/4$  and  $\phi_2 = \pi/3$  (Refs. [58, 59]);  $\circ$ : The FPU lattice model at high temperature regime, and  $\oplus$ : The single walled nanotubes at room temperature. For comparison, the relation of  $\beta = \alpha - 1$  from Denisov *et al.* (Ref. [62], lower line), and the result of  $\beta = 2 - 2/\alpha$  obtained by Li *et al.* (Ref. [62], upper line) are plotted. (Source: from Ref. [63])

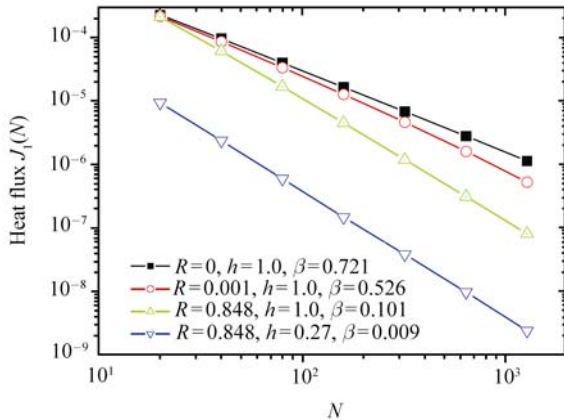
It is worth mentioning that another scaling relation between the anomalous diffusion and the anomalous heat conduction was proposed also by Denisov *et al.* [62] for the dynamic channel. According to their scaling, if the particle moves in a superdiffusive way, then the thermal conductivity of the channel diverges as the system size as  $L^\beta$ , with  $\beta = \alpha - 1$ . However, Li *et al.* [67] argued that this relation might be useful for some unknown models, but not valid for the low-dimensional models of the heat conduction, as there is a fundamental difference in probability distribution function of the first passage time for the Levy walk model and the billiard gas channels.

### 3.3 The role of chaos

There are still some questions, i.e., the role of chaos, in heat conduction deserving further investigation. It has been

shown by the chaotic FPU model that chaos is clearly not sufficient for ensuring the Fourier law [27, 28]. Further studies exhibit that chaos is also not necessary for normal heat conduction. A series of lattice models [19] and billiard gas channels [54, 56, 58] of no chaos exhibit normal conductivity. To study the role of chaos from the microscopic point of view, Mao, Li and Ji constructed a billiard gas channel of various degree of chaos [55]. In this model, the mass and heat transport is significantly related to the degree of dynamical chaos of a channel. The numerical results of two exponents  $\beta$  and  $\alpha$  for both non-chaotic and chaotic cases satisfy the formula  $\beta = 2 - 2/\alpha$  when  $\alpha \geq 1$  [61]. Furthermore, The numerical results showed that the aperiodicity of trajectory plays an important role in diffusion behavior, and the finite-size effect is more crucial for chaotic chaos.

The scatterers in the channel are the isosceles right triangle with a segment of circle substituting for the right angle. Such a channel is of chaos, indicating various degree of exponential instability of microscopic dynamics at different radius. After a sufficient long period of simulation time, the heat flux approaches to a constant value. For different radius  $R$  of the top arc of the scatterers, the heat flux of a single particle versus system size was shown in Fig. 6. Clearly, the value of heat flux decreases with increasing  $R$  for the same size.

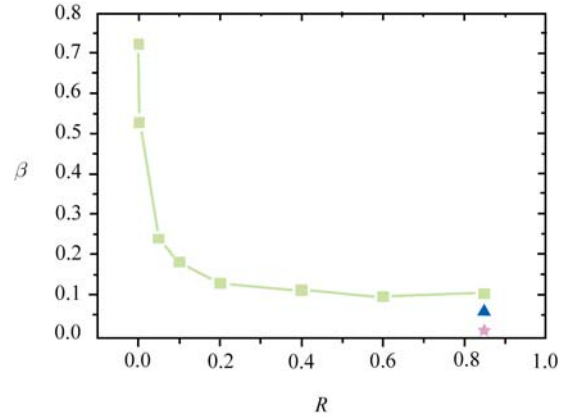


**Fig. 6** The heat flux of a single particle versus system size ( $N = 20, 40, 80, 160, 320, 640$  and  $1280$ ) with the divergence exponent of heat conductivity  $\beta = 0.721, 0.526, 0.101, 0.009$  for four typical cases respectively.

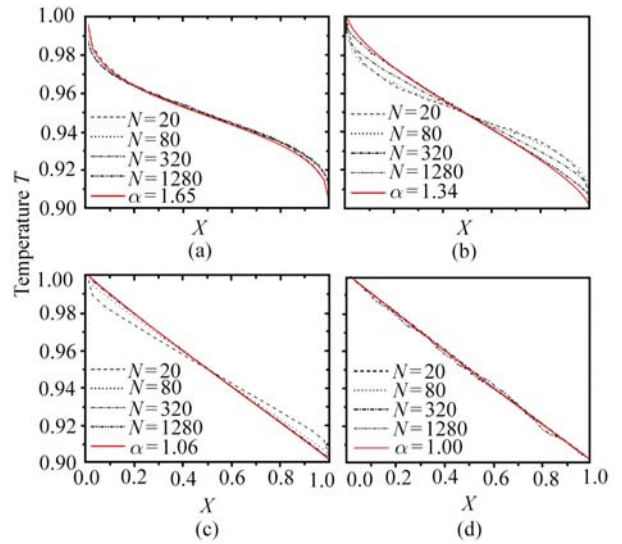
Mao, Li and Ji [55] calculated  $\beta$  versus  $R$  for various radius  $R$  plotted in Fig. 7. The rapid descending of  $\beta$  illustrates that the chaos suppresses the divergent exponent  $\beta$  drastically. The  $\kappa$  appears to be independent of system size and the Fourier law holds in case of  $h = 0.27$  and  $R = 0.848528$ . The relation between divergent exponent  $\beta$  and diffusion exponent  $\alpha$  fits the relation of  $\beta = 2 - 2/\alpha$  proposed by Li and Wang in Ref. [61].

Further, the temperature profiles are estimated from the statistic point of view (Fig. 8) [55]. The temperature is given by:

$$T(x) = \frac{T_L n_L(x) + T_R n_R(x)}{n_L(x) + n_R(x)}$$



**Fig. 7** Conductivity divergence exponent  $\beta$  versus circular radius  $R$ . The  $\blacksquare$ , refers to the magnitude of  $\beta$  for  $h = 1.0, R = 0, 0.001, 0.05, 0.1, 0.2, 0.4, 0.6,$  and  $0.848528$ ; the  $\blacktriangle$  for  $h = 0.5$  and  $R = 0.848528$ ; the  $\star$  for  $h = 0.27$  and  $R = 0.848528$  has the value of  $0.009$ .



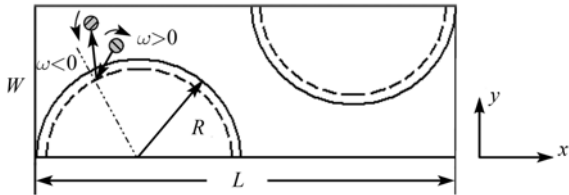
**Fig. 8** Numerical results of temperature profiles for  $T_L = 1.0, T_R = 0.9$  and sizes  $N = 20$  (dash),  $80$  (dot),  $320$  (dash dot), and  $1280$  (dash dot dot), respectively. The four panels refer to (a)  $R = 0, h = 1.0$ ; (b)  $R = 0.001, h = 1.0$ ; (c)  $R = 0.848528, h = 1.0$ , and (d)  $R = 0.848528, h = 0.27$ . The solid lines correspond to the best fits for the numerical temperature profile at  $N = 1280$  with Eq. (20), giving the analytical values  $\alpha$  with  $1.65, 1.34, 1.06$  and  $1.00$  for above four cases respectively.

$$= \frac{T_L T_R^{\alpha/2} (1-x)^\gamma + T_L^{\alpha/2} T_R x^\gamma}{T_L^{\alpha/2} x^\gamma + T_R^{\alpha/2} (1-x)^\gamma} \quad (20)$$

where  $\gamma = (2/\alpha - 1) \alpha^{3/2}$ . Additionally, both  $\delta$ -function velocity distribution and Gaussian type for the heat bath are used in numerical calculations. It is found that the heat-transport behavior is not affected by the heat baths. The intensive calculations bridged two research lines of exponent instability [57] and linear instability [54], which were so far disconnected from each other. They concluded that strong chaos results in normal diffusion of heat carriers, hence, the normal heat transport.

### 3.4 A proposal for the introduction of quantized degree of freedom

Along with the dramatic achievements in nanotechnology, the control of heat transport for nanoscopic devices becomes increasingly important. Thus, it is crucial to understand the temperature dependence of heat conductivity in low dimensional system. Mao and Li proposed a model in which the heat carriers possess an additional quantized degree of freedom (rotational velocity) beyond two translational ones to study the heat transport in quasi-one dimensional system [68]. In general, this kind of degree of freedom can come from the composite nature of the carriers, or from the confinement in a third dimension. The inelastic collisions with the rough surfaces make the occurrence of energy transfer between the translational and the rotational degrees of freedom, as shown in Fig. 9.



**Fig. 9** Schematic of the collision of a particle of radius  $r$  with a scatterer in a unit cell of the channel. The surface of the semicircle scatterers are plotted by dashed lines, near which the solid lines are the surrounding tracks of the center of particles when colliding with the scatterers.

The particle with radius  $r$  has a rotational velocity  $\omega$  in addition to the conventional velocities  $v_x$  and  $v_y$ , describing particles' translational movement. Since each unit cell contributes only one heat carrier whose radius is small compared with the scale of the channel, the interaction between the particles is not taken into account for simplicity. Under the assumption of  $v'_\perp = -v_\perp$ , the conservation of energy and angular momentum is

$$\frac{1}{2}mv_{//}^2 + \frac{1}{2}I\omega^2 = \frac{1}{2}mv_{//}^2 + \frac{1}{2}I\omega^2 \quad (21)$$

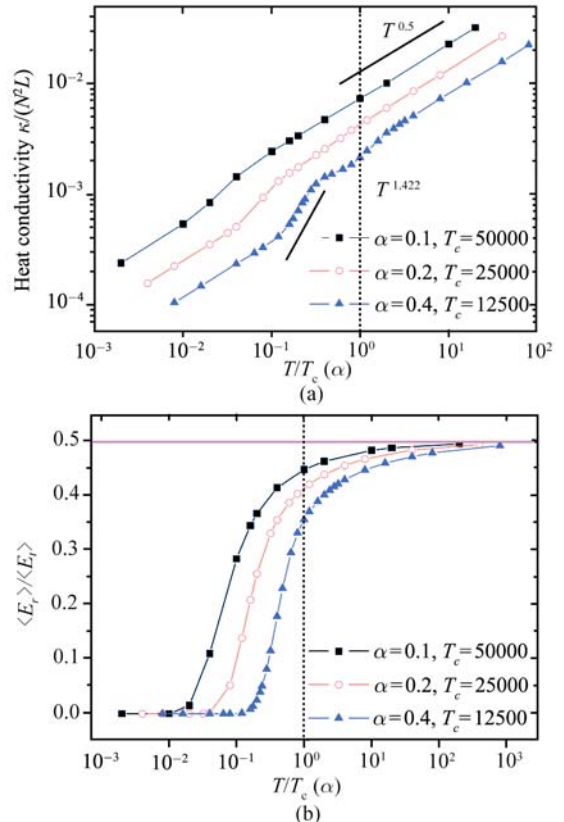
$$mv'_// + I\omega' = mv_{//} + I\omega \quad (22)$$

where the primed and unprimed ones represent the quantities after and before a collision; the  $v_{//}$  and  $v_\perp$  refer to the components tangential and perpendicular to the scatterer surface, respectively. The moment of inertia around an axis through the center of a particle of mass  $m$  is  $I = cmr^2$ . Note that in this model  $\alpha$  from 0 to 1 measures the moment of inertia, which is relevant to the mass distribution of the disk particle, i.e.,  $\alpha = 0$  for point particles,  $1/2$  for uniform distributed mass.

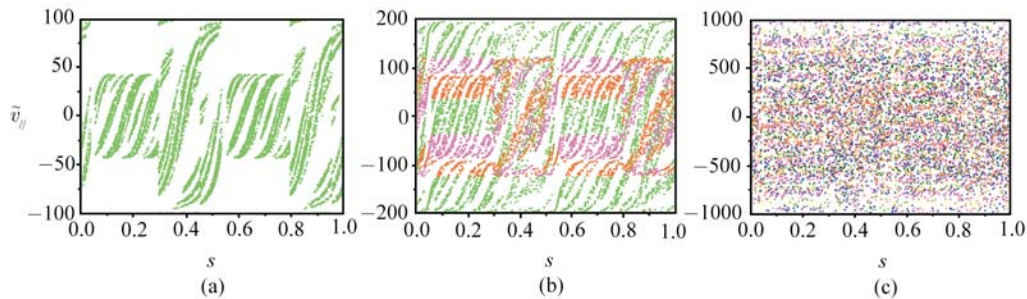
The quantization condition  $I\omega_l = l\hbar$ ,  $l = 0, \pm 1, \pm 2, \dots$  is naturally introduced in this model. Clearly, the moment of inertia determines the spacing of the quantized angular velocity  $\Delta\omega = \hbar/I = \hbar/cmr^2$ , and the energy spacing  $\hbar^2/(cmr^2)$  between the ground state and the first excited state defines a

characteristic temperature  $T_c = \hbar^2/(cmr^2)k_B$ . If the energy for such excitation is much less than  $k_B T_c$ , the internal degree of freedom is frozen. In the simulations, the particle's  $\tilde{\omega}$  takes an allowed discrete value near the  $\omega'$ . Under this assumption, the conservation of angular momentum is broken down, for the tangential component of velocity  $\tilde{v}_{//}$  is the same as  $\tilde{v}'_{//}$ , while the perpendicular component  $\tilde{v}_\perp$  is determined by the energy conservation.

Figure 10(a) shows the heat conductivity-temperature curves for a channel. Here  $T_c = 5000/\alpha$  (in units of  $\hbar^2/mk_B a^2$ ). For simplicity, an average value of temperature  $T = (T_L + T_R)/2$  is assumed under small temperature gradient. One can clearly see that the curves have larger slope at temperatures near and less than  $T_c$ . Accordingly, there are three regimes due to the temperature exponent  $\gamma$  in the heat conductivity  $\kappa \sim T^\gamma$ . The transition from high temperature regime to intermediate temperature regime occurs close to a characteristic temperature  $T_c$ , below which the translational velocity distribution deviates from the Boltzmann distribution while energy is distributed unequally among the three degrees of freedom. In addition, by projecting the points in phase space to the  $s-\tilde{v}_{//}$  plane, one can see the clear emergence of strange attractor accompanying the frozen of rotation degree of freedom at low temperatures.



**Fig. 10** (a) Temperature dependence of heat conductivity. (b) The ratio of average rotational energy over average translational energy at different temperatures.



**Fig. 11** Poincaré surface of section projected to  $s$ - $\tilde{v}_{\parallel}$  plane, by following the first  $10^4$  bounces with zero initial angular velocity. The particle of velocity  $v$  and  $\alpha = 0.4$  starts from the center of the left boundary of the cell with an incident angle of 0.9. **(a)**  $v = 100$ , and the allowed  $\tilde{\omega} = 0$ ; **(b)**  $v = 200$ , and the allowed  $\tilde{\omega} = -25\,000, 0$ , and  $25\,000$ ; **(c)**  $v = 1000$ , and more values of  $\tilde{\omega}$  are allowed.

The characteristic three regimes showed that the temperature-dependent interplay between the translational and rotational degrees of freedom plays a crucial role in heat conduction. The non-equipartition of energy between the translational and rotational degrees of freedom is explicitly shown except in the high temperature limit, and strange attractor occurs remarkably in the low temperature limit.

#### 4 Modelling heat conduction in local thermal equilibrium

In nonequilibrium steady state, the heat conduction describes the response of a system to a temperature gradient. The presence of driving potential induces the flow of heat, which tends to homogenize the medium. However, there is no equivalent procedure for going from the microscopic to the hydrodynamic picture and two phenomenological assumptions are needed to calculate the heat conductivity: Local Thermal Equilibrium (LTE) and Linear Response. That is to say, if the macroscopic quantities vary very slowly over a mean-free path, the collisions quickly produce a state that is as close as possible to the equilibrium state, but only locally; and the local equilibrium function reduces to the true equilibrium distribution if the small temperature gradient holds. It follows that one can define thermodynamical quantities such as local temperature, which determines all other local properties in the system.

A great number of studies on heat conduction are performed by the “direct method”, by adding a temperature gradient on the system to mimic the experiments in nonequilibrium. After a long simulation time, the systems arrive at the nonequilibrium steady states (NSS), based on which the thermodynamical quantities such as temperature, heat flow are calculated. However, the uniqueness of the steady state is still under discussion [66], and even NSS is obtained, it does not guarantee the realization of the local thermal Equilibrium (LTE) which really allows the definition of the temperature, etc. While most of the studies focus on heat conduction for obtaining a normal heat behavior or the universal divergent exponent, the more fundamental problem that the

existence of local thermal equilibrium (LTE) in the steady state has not been investigated much so far, even though it is quite crucial for stating Fourier law and using results of linear response theory.

To clarify the necessary (or sufficient) conditions for the fast establishment or nonestablishment of LTE, A. Dhar and D. Dhar [69] studied two simple models. The first is a linear chain of  $L$  planar spins. The spin at site  $i$  ( $1 \leq i \leq L$ ) of the lattice is specified by the angle  $\theta_i$ ,  $0 \leq \theta \leq 2\pi$ . The spins interact with nearest neighbors by ferromagnetic coupling  $K$ . The Hamiltonian of the system is given by:

$$\mathcal{H} = -K \sum_{\langle i,j \rangle} \cos(\theta_i - \theta_j) \quad (23)$$

where the sum is over all nearest neighbors. The dynamics of the spin model evolves with a Markovian stochastic dynamics. They found that local thermal equilibrium is not achieved in the nonequilibrium steady state in this model even in the limit of system size  $L \rightarrow \infty$ .

The second model is a  $d$ -dimensional ( $d > 1$ ) Lorentz gas of noninteracting particles scattering elastically with a series of randomly placed obstacles (e.g., spheres) of finite density. In this model, all collisions with the obstacles are elastic, and the energy is conserved. But collisions between the particles and the two walls (at  $x = 0$  and  $x = L$ ) are inelastic and lead to the energy after collision being thermalized corresponding to the temperature of the wall. The average density of particles  $\rho(E, x)$  with energy between  $E$  and  $E + dE$  in a small volume centered at point  $x$  is given by:

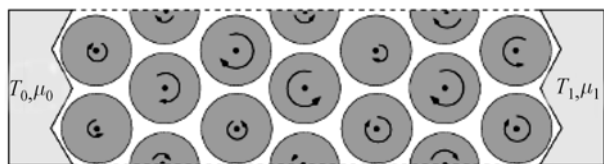
$$\rho(E, x) = P(x)\rho(E, x = 0) + [1 - P(x)]\rho(E, x = L) \quad (24)$$

where  $P(x)$  is the probability that a randomly chosen particle in the small volume near  $x$  was introduced at the left end. As the linear combination of two Maxwellians is not a Maxwellian, and the distribution must be a Maxwellian in thermal equilibrium, it follows that there is no thermal equilibrium in the Lorentz model.

Motivated by a proper understanding of the LTE in nonequilibrium steady state, A. Dhar [48] studied the heat conduction in simple (but nontrivial) models in the nonequilibrium state: the hard sphere system. The steady states for the case of equal masses and the case with arbitrarily small mass

differences are completely different. When all particles have equal masses, the system is integrable and the temperature profile is flat (with  $T(x) = \sqrt{T_+ T_-}$ ), and heat current is independent of system size, and there is no LTE in the steady state. For the case of diatomic gas where the masses of the two atoms are different, the system becomes nonintegrable, and LTE is established and the acquired temperature profile is in accordance to the predictions of kinetic theory.

As both the models without LTE have an infinity of locally conserved quantities, A. Dhar and D. Dhar argued that the breakdown of the infinity of conservation laws would lead to LTE in nonequilibrium system. Subsequently, local thermal equilibrium in steady state is well realized in a modified Lorentz gas model with fixed freely rotating scatterers and noninteracting point particles colliding with them inelastically [70]. The modified Lorentz gas is illustrated in Fig. 12. The centers of the scatterers are fixed on a triangular lattice, along a narrow channel with periodic boundary conditions in the vertical direction. At the ends, the walls are used to fix both the temperature  $T$  and the quantity  $\mu/T$ , where  $\mu$  is the chemical potential.

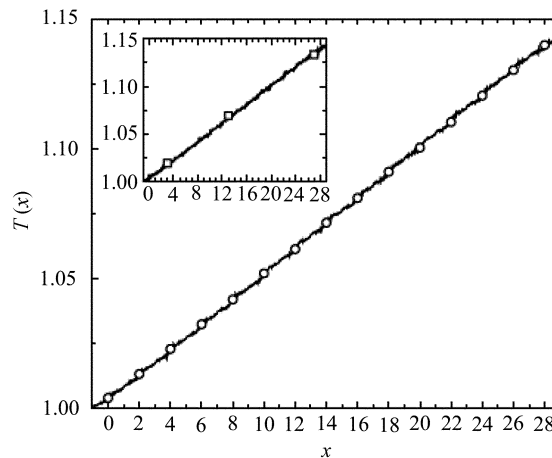


**Fig. 12** Schematic illustration of the scatterer geometry. (Source: from Ref. [70])

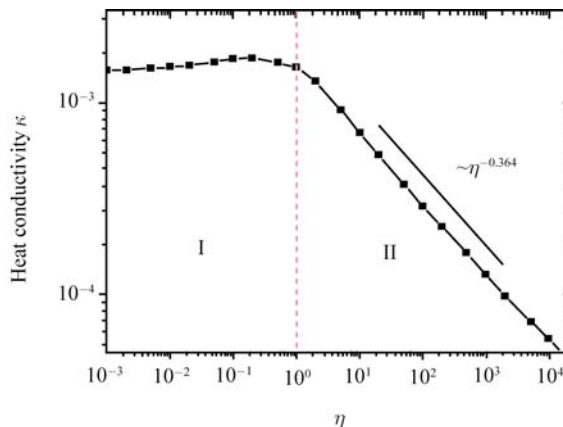
The collisions with the rotating disks occur according to the conservation of energy and angular momentum. In Fig. 13, the temperature profiles of both particles and disks are displayed, which are found to be linear. The coincidence between them indicates that disks equilibrate with the particles locally along the channel. Furthermore, the agreement of the temperatures obtained from the fits to Boltzmann distribution in the inset reinforces the conclusion that the system establishes a LTE in its steady state.

To explore heat transport in low-dimensional systems in local thermal equilibrium, Mao and Li [71] investigated a billiard gas channel in which noninteracting particles fly freely between inelastic collisions with the freely rotating scatterers placed periodically along the channel, by following Ref. [70]. They have demonstrated the realization of LTE in homogeneous system in a wide range of parameter  $\eta$ , the moment of inertia of the rotating disk. The calculations exhibited a significant dependence of heat conductivity on  $\eta$ : totally distinct characteristics in two areas divided by  $\eta = 1$ . The heat conductivity saturates when  $\eta < 1$ , and a power-law decrease occurs when  $\eta > 1$ , at least with the range of their simulations [71], as shown in Fig. 14. Furthermore, they have modelled the heterostructure [71] by linking two segments of different materials with a joint cell whose parameter characterizes the property of the interface. Their results showed the establishment of LTE in the inhomoge-

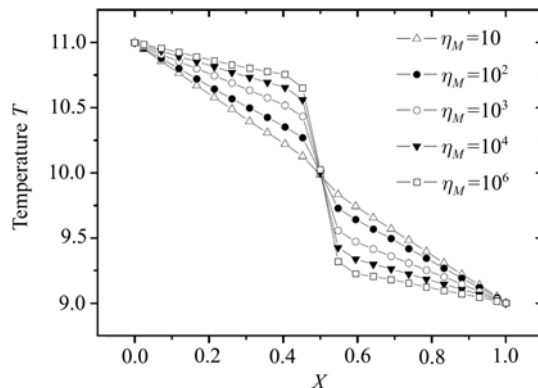
neous system with multilayer structure, and a clear temperature discontinuity at the interface (see Fig. 15).



**Fig. 13** Temperature profile for the simulation. The solid line corresponds to the particle temperature along the channel while the open circles are the temperature of the disks. In the inset the particle temperature profile (solid line) is compared with the temperatures obtained from the fits to the Boltzmann distribution (open squares). (Source: from Ref. [70])



**Fig. 14** Heat flow as a function of parameter  $\eta$  in the channel with  $N=11$  unit cells. The average temperatures of high and low heat baths are  $T = 10$ . The temperature difference  $\Delta T/T$  is fixed at 0.2.



**Fig. 15** Temperature profile in inhomogeneous system. The two segments with  $\eta_L = \eta_R = 0.01$  contacted through the cell of  $\eta_M$ . The temperatures at two heat baths are  $T_+ = 11$  and  $T_- = 9$ .  $N_L = N_R = 10$  and  $N_M = 1$ .

## 5 Summary and remarks

Several decades have witnessed the progress to the problem of the heat conduction in low-dimensional systems, yet there are still many questions unresolved. We have reviewed previous studies on the problem of heat conduction, especially hard-point gas models and billiard gas channels which have simple microscopic dynamic but abundant statistical properties. These works have been primarily involved in the determination of sufficient and necessary ingredient for normal heat transport in a one-dimensional dynamical system, and a universal divergent exponent  $\alpha$  in heat conductivity  $\kappa \sim L^\alpha$  expected for systems with anomalous heat conduction. We also discussed the realization of local thermal equilibrium (LTE) in low-dimensional systems, even in heterogeneous systems. Some important results are contributed to the problem of heat conduction:

- The finite heat conductivity has been so far obtained in noninterable systems which are called “ding-a-ling” model [29] and “ding-dong” model [72], in complete chaotic models [29, 57], in the system with on-site potential [44], in disordered systems [54, 64], in mixing systems [58, 61], and in the systems where momentum conservation is broken [53].
- Chaos is neither sufficient nor necessary for a system to obey Fourier law [19, 53, 54, 56].
- Overall momentum conservation in a Hamiltonian system appears to be a key factor for divergence of heat conductivity  $\kappa$  as a function of the system size  $L$  [14, 31, 33, 34, 50, 52]. Thus, the introduction of on-site potential in one-dimensional lattice model results in normal heat transport, since the conservation of momentum is broken down in this case [44, 73].
- For a chain of elastical particles with equal masses, energy is carried ballistically, showing that the heat conductivity  $\kappa \sim L^\alpha$  with  $\alpha = 1$ , as in the harmonic oscillator chain. For a 1D gas of elastically colliding particles of unequal masses, the divergence exponent of thermal conductivity is  $\alpha \approx 0.33$  [36–39], in good agreement with the result of renormalization group [14]. However, the results from mode-coupling theory [27] and the Boltzmann equation [35] show that  $\alpha = 2/5$ .
- A connection between divergent heat conductivity and anomalous diffusion is obtained from recent study [61] which is supported by existing numerical data. Whereas another scaling based on Levy walk assumption was provided by Denisov *et al.* [62] and confirmed by Zhao [74] in terms of solitons and phonons.

While progress has been made, some questions still lie in, e.g., whether LTE can be really established, even in inhomogeneous systems? If yes, how is the temperature profile? This problem is of significance for the increasing application of the materials with multilayer structure on a length scale of several nanometers, such as polymer nanocomposites, superlattices, multiplayer coatings, and microelectronic devices,

etc. A more interesting question is the shape of the temperature profile for different kind of models [48, 55, 57]. The constant temperature gradient inside systems determines the heat conductivity correctly. Another issue is the temperature dependence of heat conductivity in different models. We have proposed a method to introduce the quantized degree of freedom for the first time and demonstrated three characteristic regimes for heat conductivity [68]. As numerical results sometimes contribute different conclusions due to the delicate nature of the questions under discussion, longer simulation and analytical results are needed for further investigating the problem of heat conduction in low-dimensional systems.

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