HEAT CONDUCTION IN HOMOGENEOUS AND HETEROGENEOUS BILLIARD SYSTEMS

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We investigate the heat conduction in a modified Lorentz gas with freely rotating disks periodically placed along one-dimensional channel. The heat conductivity is dependent on the moment of inertia $\eta$ of the disks, with a power-law decay when $\eta > 1$. By plotting the Poincaré surface of the section, we observe a contraction of phase space over the range of $\eta > 1$, which is sensitive to the initial condition. We find that the power-law decay of the heat conductivity is relevant to the mixing phase space. As a possible application, we model the heterostructure by connecting the segments of different $\eta$, and predict the analytical results of the temperature profiles and the heat conductivity, which are in good agreement with the numerical ones.

Keywords: Heat conduction; billiard; rotating scatterer.

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1. Introduction

Rapid progress in device miniaturization evokes a better understanding of heat conduction in low dimensional systems. Since the pioneering work of Casati et al., where a finite heat conductivity is obtained in one-dimensional system, a number of attempts have been made to determine the exponent $\alpha$ in heat conductivity $\kappa \sim L^\alpha$, where $L$ is the system size, and to identify the corresponding system characteristics which are indispensable to normal ($\alpha = 0$) and anomalous heat conduction, respectively. The finite heat conductivity has been so far obtained in nonintegrable systems, such as the so-called “ding-a-ling” and “ding-dong” models, complete chaotic models, the system with on-site potential, disordered systems, mixing systems, and the systems where momentum conservation is broken. Despite these efforts, there is still no generally accepted conclusion on common requirement to ensure Fourier’s law.

For the case of $\alpha > 0$, where the heat conductivity diverges with the system size, a universal scaling of divergent exponent $\alpha$ is expected. It has been proved
analytically\textsuperscript{11} and numerically\textsuperscript{12-14} that momentum conservation results in anomalous heat conduction in one-dimensional lattice models. However, the determination of $\alpha$ is still a controversial problem. The mode-coupling analysis gives a divergent exponent $\alpha = 2/5,\textsuperscript{15,16}$ while the renormalization group theory suggests $\alpha = 1/3.\textsuperscript{12}$ To clarify the crossover of the divergent exponent from $2/5$ to $1/3$, Wang \textit{et al.}\textsuperscript{17,18} studied a one-dimensional chain by introducing transverse motions. In terms of a high precision numerical calculation and a detailed mode-coupling analysis, they argued that the $1/3$ power-law comes from the mode coupling between the longitudinal modes and transverse modes, and the $2/5$ is ascribed to the absence of coupling.

When $\alpha < 0$, 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\textsuperscript{9} giving $\kappa \sim L^{-0.63}$, and the other is the model with on-site potential\textsuperscript{19} showing an exponential decay $\kappa \sim \exp(-bL)$ over the range of large system size.

Recently, modified Lorentz models have been introduced in heat problems\textsuperscript{20-23} since the classical Lorentz model does not satisfy local thermal equilibrium (LTE). In these models, the additional degree of freedom of the freely rotating disks allows the energy exchange between the noninteracting particles through the rotating disks, and therefore LTE is established in this modified Lorentz system.\textsuperscript{22,23}

In this paper, we investigate the influence of the rotating disks on heat conduction in a modified Lorentz model in which noninteracting particles fly freely between collisions with the rotating scatterers. In Sec. 2, we describe the model including the configuration of the channel and the collision rules of the particles and rotating scatterers. In Sec. 3, we obtain the significant dependence of heat conductivity on the moment of inertia $\eta$ of the disks, which possesses totally distinct characteristics in two areas divided by $\eta = 1$. When $\eta < 1$, the heat conductivity has a stable value which is almost the same compared to that of classical Lorentz model, while a power-law decrease occurs when $\eta > 1$, at least within the range of our simulations. In Sec. 4, we calculate the mean square displacement of the particles in time over a wide range of $\eta$, which indicates normal diffusion with a robust exponent. Particularly, we find the existence of a contraction in phase space when $\eta > 1$ by plotting Poincaré surface of the section. In Sec. 5, we calculate analytically and numerically the temperature profiles and the heat conductivity for heterogeneous systems. Finally, the conclusion and discussions are given in Sec. 6.

2. The Model
We consider a quasi one-dimensional channel including two horizontal walls at a distance $h$ and a series of freely rotating disks of radius $R$ placed periodically. The centers of these scatterers are fixed on the upper and the bottom boundaries, and two adjacent scatterers are at a distance of $2R$ in the horizontal direction. Each
unit cell includes two disks with one up and the other on the bottom. The channel is constructed by $N$ replica cells in the horizontal direction, as shown in Fig. 1 (the shaded area). Point particles fly freely in the quasi one-dimensional channel, frequently making collisions with the boundaries and the scatterers. To avoid a long flying distance for a particle without undergoing a collision, the geometry should satisfy $h \leq 2R/\sqrt{3}$. So we take $h = 1.0$ and $R = 0.9$ in our simulations unless otherwise stated.

In the channel, noninteracting particles of mass $m$ collide with the rotational scatterers under the conditions of local conservation of energy and angular momentum, while making mirror-like collisions with the two horizontal walls. Therefore, during each collision, the energy and the momentum are repartitioned between the point-like particle and the rotating disk. We have the normal $v_n (v'_n)$ and tangential velocities $v_t (v'_t)$ of a particle and the angular velocity $\omega (\omega')$ of a disk before (after) the collision as follows:

\begin{align*}
  v'_n &= -v_n, \\
  v'_t &= v_t - \frac{2\eta}{1 + \eta} (v_t - R\omega), \\
  R\omega' &= R\omega + \frac{2}{1 + \eta} (v_t - R\omega),
\end{align*}

where $\eta = I/mR^2$ is a dimensionless parameter characterizing the magnitude of the moment of inertia of the rotating disk. From the above equations, we obtain

\begin{equation}
  \eta = \frac{v'_t - v_t}{R\omega - R\omega'},
\end{equation}

which determines the momentum and energy exchange between the particle and the disk during a collision.

At the two ends of the channel, we impose two heat baths with temperature $T_L$ and $T_R$, respectively. After colliding with either of the heat baths, a particle in the
channel acquires a velocity chosen from the stochastic boundary conditions,

\[ P(v_x) = \frac{m|v_x|}{k_B T} \exp \left( -\frac{mv_x^2}{2k_BT} \right), \]

\[ P(v_y) = \sqrt{\frac{m}{2\pi k_BT}} \exp \left( -\frac{mv_y^2}{2k_BT} \right), \]

where \( v_x \) and \( v_y \) denote the horizontal and vertical components of the velocity respectively, \( T \) represents \( T_L \) or \( T_R \), and \( k_B \) is Boltzmann’s constant. In our simulations, \( m \) and \( k_B \) are set to unity.

3. Heat Conduction in the Homogeneous Billiard Channel

After a long time simulation, the system reaches the steady state. The temperature of the particles in the \( i \)th cell is defined by averaging the kinetic energy over all visits into the cell\(^4\)

\[ T_i = \langle E \rangle_i = \frac{\sum_{j=1}^{P} (\sum_{k=1}^{M} t_{jk} E_{jk})}{\sum_{j=1}^{P} (\sum_{k=1}^{M} t_{jk})}, \]

where \( E_{jk} \) is the kinetic energy of the particle for \( k \)th collision of \( j \)th visit in \( i \)th cell, and \( t_{jk} \) is time spent for \( k \)th collision of \( j \)th visit. Here \( P \) is the total number of visits and \( M \) the number of collisions during \( j \)th visit.

It is known that the classical Lorentz model will not arrive at the local thermal equilibrium (LTE) state, since no energy is transferred between the particles and the disks during the collisions.\(^2^4\) The modified Lorentz models with rotating scatterers\(^2^2,2^3\) have been used to characterize the thermodynamical equilibrium. In our simulations, we extensively investigate the temperature fields and have obtained linear temperature profiles over a wide range of \( \eta \). The rotating scatterers allow the energy exchange between particles, thus the unique LTE is established. Particularly, we find that the moment of inertia \( \eta \) of the rotating disks affects the realization time of the steady state. One can see from the time evolution of particle temperature shown in Fig. 2 that it takes much more time to achieve a steady state for the system with larger \( \eta \).

We now turn to investigate the heat flow along the channel. For a single particle, the heat flow \( J_1 \) can be calculated by the time average of energy exchange \( (\Delta E)_j \) after and before the \( j \)th collision with a heat bath,\(^1,7\)

\[ J_1 = \frac{1}{t_M} \sum_{j=1}^{M} (\Delta E)_j = \frac{1}{t_M} \sum_{j=1}^{M} (E' - E)_j, \]

where \( E' \) and \( E \) are the energies of a particle after and before colliding with the heat bath, and \( t_M \) is the time spent for \( M \) such collisions. In our model, each cell
Heat Conduction in Billiard Systems

Fig. 2. Time evolution of \((T(t) - T_{\text{asp}})^2\). \(T(t)\) is the temperature at the 5th cell. Here the system size is \(N = 11\) with two heat baths at fixed temperature \(T_L = T_R = 1\), and \(T_{\text{asp}} = 1\) is the asymptotic temperature of the system at the steady state.

is assumed to contribute one heat carrier. For a channel with \(N\) cells of the unit length \(L\), it follows that the heat conductivity can be expressed as

\[
\kappa = \frac{J_1 N^2 L}{\Delta T},
\]

where \(\Delta T\) is the temperature difference of two heat baths. The unique LTE is established at the steady state, similar to those in Refs. 22 and 23, thus Eqs. (4)–(6) are proved to be valid. The collisions between particles and scatterers guarantee the realization of interaction between particles involved.

After a long simulation time (totally \(2 \times 10^9\) visits in the cells in our simulations), the system reaches the steady state. We extensively investigate the heat conductivity \(\kappa\) of the system for a series of finite \(\eta\). For the system of \(R = 0.9\) and \(h = 1.0\), the geometry of the model is closed. The heat conductivity \(\kappa\) we obtained are independent on the system size, which means the heat transport is normal. Remarkably, two areas with totally different characteristics are divided by the dashed line at \(\eta = 1\). When \(\eta \leq 1\), the heat conductivity almost has an unchanged value. While in the area where \(\eta > 1\), the heat conductivity has a power-law dependence on the parameter \(\eta\) with \(\kappa \sim \eta^{-0.44}\), as shown in Fig. 3(a). It indicates that the heat conduction is affected significantly by the moment of inertia \(\eta\) of the scatterers. Further investigations show the existence of the power-law dependence even in the systems with open horizon, for example, for the cases of \(R = 0.8\) and 0.6, where infinitely long flying distances may exist. Therefore, the significant influence on heat conduction is prevalent due to the introduction of the rotational degree of freedom.
Fig. 3. Heat conductivity in the system of $N = 11$ cells. The temperature difference $\Delta T / T$ is fixed at 0.2 for various temperatures. (a) Heat conductivity as a function of parameter $\eta$ in the channel ($\square$). The temperatures of left and right heat baths are $T_L = 1.1$ and $T_R = 0.9$, respectively. The heat conductivity in open horizon channels with $R = 0.8$ ($\bullet$) and $R = 0.6$ ($\blacktriangle$) is also displayed. (b) Heat conductivity as a function of average temperature $T$ for $\eta = 0.1$ ($\bullet$), $\eta = 10^3$ ($\blacktriangle$) and the case of classical Lorentz model ($\square$).

Contrastively, we calculate the heat conductivity in the classical Lorentz gas model with fixed scatterers. The heat conductivity for various cases are displayed in Fig. 3(b), from which we have two results: one is the temperature dependence $\kappa \sim T^{1/2}$ which is in accordance with the kinetic theory; the other is that there is almost no difference on the heat conduction between the systems for $\eta \leq 1$ and the classical Lorentz model. Therefore, the heat conduction in modified Lorentz model with rotating scatterers is affected rigorously only when $\eta > 1$.
4. The Dynamics of the System

It has been found that heat transport in one-dimensional dynamic system is related closely to the diffusion behavior of heat carriers (phonons in lattice models and particles in gas channels).\textsuperscript{25,26} It is not strange that the billiard models\textsuperscript{4,7–9,27,28} connect heat transfer to the diffusion of heat carriers due to the absence of interaction between the particles. We will see in the following that normal transport behaviors are related even in the systems with interacting particles. To study the

\begin{figure}[h]
\centering
\includegraphics[width=0.8\textwidth]{figure4a.png}
\caption{(a) Mean square displacement $\langle \Delta x^2 \rangle$ for different $\eta$ and classical Lorentz model ($\ast$). An ensemble of $2 \times 10^5$ particles whose initial velocity is in Gaussian velocity distribution at average temperature $T = 1$ is used. (b) Diffusion coefficient $D$ for different $\eta$ at temperatures $T = 1$ and 10, respectively.}
\end{figure}
diffusion property in our model, we put an ensemble of $2 \times 10^5$ particles at the center of the channel ($x = 0$) at initial time $t = 0$, and calculate the time evolution of the mean square displacement $\langle \Delta x^2 \rangle$ by averaging the ensemble. In our simulations, the particle acquires the velocity chosen from Gaussian velocity distribution at average temperature $T = 1$ at the starting point, and moves freely along the channel. The initial rotational velocity of the disks are set to 0, and the first $10^3$ particles are excluded from the statistical average. We obtain the relation of $\langle \Delta x^2 \rangle = 2Dt$, as shown in Fig. 4(a). The curves with a linear increase with exponent $\beta \sim 1$ over a wide range of $\eta$ imply a normal diffusion which is robust to changes of $\eta$. When $\eta \to 0$, for example, $\eta = 0.001$, the curve is asymptotically close to that of classical Lorentz model, as one might expect. Furthermore, the diffusion coefficient $D$ for different $\eta$ has similar characteristic compared to the heat conductivity, namely, a stable value for $\eta \leq 1$ and power-law decay when $\eta > 1$ [Fig. 4(b)].

It is surprising that the introduction of new collision rules almost has no influence on the dynamics of the systems unless $\eta > 1$. The natural question is: what property of the systems results in the different dynamics between small and large $\eta$?

We start from analyzing the time evolution of the dynamics of one moving particle. When $\eta = 1$, the particle and the disk simply exchange velocities during the collision.

$$v'_t = R\omega,$$
$$R\omega' = v_t.$$  \hspace{1cm} (7)

If $\eta \to 0$, the tangential velocity of the particle is unaffected by the collision. Therefore, the particle makes a mirror-like collision with the scatterer, recovering the dynamics in classical Lorentz gas model as follows\textsuperscript{23}

$$v'_t = v_t,$$
$$R\omega' = 2v_t - R\omega.$$  \hspace{1cm} (8)

For $\eta \to \infty$, the velocities reduced to

$$v'_t = -v_t + 2R\omega,$$
$$R\omega' = R\omega.$$  \hspace{1cm} (9)

In this case, the rotation of the disk is unaffected during the collisions and the particle almost turns backward when colliding with these scatterers of infinitely large $\eta$. As a result, the overlapping trajectories bring about the existence of localization of the particles.

It is much more complicated to analyze the particle dynamics for the cases of $0 < \eta < 1$ and $1 < \eta < \infty$. Only numerical results are available. Our extensive simulations show that the particles are unbounded when $0 < \eta < 1$. The analytic solution in Ref. 29 presents a similar conclusion in one-dimensional Lorentz gas with rotating scatterers.
Fig. 5. (a) The trajectory of the particle in a unit cell. (b) The Poincaré section of \((s, v_t)\) for \(\eta = 10.0\) corresponding to (a).

It is helpful to illustrate the dynamical characteristics determined by the dimensionless moment of inertia \(\eta\) by plotting the Poincaré surface of the section. To this end, we take a unit cell and close it by two vertical walls with which the particle makes elastic collisions. The particle starts from the center of a vertical wall at a certain velocity, e.g., the value of unity. The initial rotational velocity of the disks is set to 0. We calculate extensively the phase space \((s, v_t)\) for various injection angles at different values of \(\eta\), where \(s\) is the distance at the collision site along the boundary from the starting point, and \(v_t\) denotes the tangential velocity with respect to the boundary after the collision. For the case of \(\eta \leq 1\), a smooth phase space density is obtained, as the case in Ref. 28. The system is ergodic and the difference of \(\eta\) does not bring about essential distinctness of the dynamics. Surprisingly, when \(\eta > 1\), the phase space of the system is sensitively dependent on the initial condition. The surface of section in Fig. 5(a) shows a contraction of the phase space to the isolated islands.\(^{21}\) This indicates the existence of quasi-periodic trajectory which may localize the particle in a certain area for a period of time,
thus slowing down the propagation of the particle. With the increase of $\eta$, the localization becomes prevailing for various initial conditions. It is much harder for a particle to escape from a certain area. If $\eta \to \infty$, the particle will be completely bounded, thus no energy can be transferred.

Despite of the dependence on the initial condition of the trajectory, the randomness of the boundary condition at the two heat baths in the model guarantees the success of the particle propagation when we take the value of $\eta$ between 1 and $10^5$. The mixed phase space leads to a power-law decay which is observed in Figs. 3 and 4.

5. Heat Conduction Across Heterojunction

Since the increasing application of the materials with multilayer structure on a length scale of several nanometers, such as polymer nanocomposites, superlattices, multilayer coatings, and microelectroic devices, the heat control of the heterogeneous systems becomes an interesting problem. In the following, we discuss the heat conduction across a single heterojunction. If two different materials are contacted, the propagation of the heat carriers will be determined by the properties of the material. We extensively calculate the temperature profiles of the system where two segments of different properties $\eta_L$ and $\eta_R$ are combined. The temperature of the left heat bath is set at $T_L = 1.1$ and the right at $T_R = 0.9$ in order to fulfill the linear response theory at the nonequilibrium steady state. The results are shown in the inset of Fig. 6.

Now we discuss the temperature profiles through kinetic theory, which predicts the relation of $\kappa = \alpha T^{1/2}$ for one-dimensional gas system. Our numerical results have confirmed the temperature dependence of heat conductivity, as shown in Fig. 3(b). Under the fixed boundary conditions, the temperature field can be expressed as

$$T(x) = [T_L^{3/2} + (T_R^{3/2} - T_L^{3/2})x]^{2/3}. \quad (10)$$

Thus, the heat conductivity can be written as

$$\kappa = \frac{2}{3} \alpha \frac{T_R^{3/2} - T_L^{3/2}}{T_R - T_L}. \quad (11)$$

For the heterogeneous system where the heat conductivity of left and right segments has the relation of $\kappa_L = \alpha_L T_L^{1/2}$ and $\kappa_R = \alpha_R T_R^{1/2}$ respectively, we predict the temperature field as

$$T(x) = \begin{cases} [T_L^{3/2} + (T_R^{3/2} - T_L^{3/2})2x]^{2/3}, & 0 \leq x \leq 0.5, \\
{T_L^{3/2} + (T_R^{3/2} - T_L^{3/2})(2x - 1)]^{2/3}, & 0.5 \leq x \leq 1, \end{cases} \quad (12)$$

and the heat conductivity

$$\kappa^{-1} = \frac{3}{4\alpha_L} \frac{T_{in} - T_L}{T_L^{3/2} - T_L^{3/2}} + \frac{3}{4\alpha_R} \frac{T_R - T_{in}}{T_R^{3/2} - T_R^{3/2}}, \quad (13)$$
where the temperature of the interface $T_{in}$ is defined as

$$T_{in} = \left( \frac{\alpha_L T_{in}^{3/2} + \alpha_R T_{in}^{3/2}}{\alpha_L + \alpha_R} \right)^{2/3}.$$ 

The analytical results of Eqs. (12) and (13) are shown in Fig. 6, which is in accordance with the numerical results. This indicates that the whole heat resistance is the sum of the resistance of each segment without contact resistance.

As the properties of the segments determine the temperature and the heat flow across the system, the existence of temperature jump is expected when two segments of $\eta_L$ and $\eta_R$ are coupled by a joint cell of $\eta_M$, which acts as a contact resistance. The temperature profiles with the sharp discontinuity are displayed in Fig. 7. These jumps are a consequence of the fact that the system dynamically adjusts the local temperatures to make a smooth heat current. Furthermore, we study the jump $(\Delta T)_{int}$ as a function of $\eta_M$ in the inset of Fig. 7. The results show that the jump increases with increasing $\eta$. Thus, the contact resistance in this case plays a crucial role when $\eta_M > 1$, which rigorously dominates the heat conductivity of the whole channel. When $\eta_M \rightarrow \infty$, the system becomes an insulator asymptotically.
3912  J.-W. Mao, Y.-Q. Li & L.-Y. Deng

Fig. 7. Temperature profiles of the heterogeneous system with two segments of $\eta_L = \eta_R = 0.1$ contacted through a joint cell of $\eta_M$. The temperatures at two heat baths are $T_L = 1.1$ and $T_R = 0.9$. Here $N_L = N_R = 5$ and $N_M = 1$. Inset: the temperature jump $\Delta T_{\text{int}}$ as a function of $\eta_M$.

6. Conclusion

We have demonstrated the influence of the rotating disks on heat conduction through a modified Lorentz gas model. The remarkable dependence of the heat conductivity on moment of inertia $\eta$ of rotating disks is observed. When $\eta \leq 1$, the heat conductivity for the system stays at a stable value, which shows almost no difference compared to the classical Lorentz gas model with fixed scatterers, while a remarkable power-law decay appears in the area of $\eta > 1$. The numerical results show that the system with larger $\eta$ requires much more time to achieve the steady state.

The mean square displacement grows linearly in time over a wide range of $\eta$, and therefore the transport is diffusive, which is robust to changes of $\eta$. The obtained diffusion coefficient $D$ displays a similar power-law dependence on $\eta$, as the heat transport behavior. The heat and mass transport behaviors are closely related even in systems with interacting particles. We have found a smooth phase space which is independent of the initial condition when $\eta \leq 1$ through dynamical studies, while a contraction in phase space is observed when $\eta > 1$, which is sensitive to the initial condition. Consequently, the existence of the mixed phased space is considered to be responsible for the power-law decay in transport behavior. However, what causes the robustness of the diffusive transport to the changes of $\eta$ is still not clear.

In recent years, the heat conduction in dissimilar materials have attracted more and more interest, and the thermal rectification phenomenon in the lattice\textsuperscript{32} and
billiard system\textsuperscript{33} has been studied intensely. As a possible application in controlling the heat flow, we have modeled the heterostructure by linking the segments of different $\eta$. We have predicted the analytical temperature profiles and heat conductivity, which are in good agreement with the numerical results of the heterogeneous systems. Differing from previous atomic-level simulations on heat problem in heterogeneous systems,\textsuperscript{34} our models have simple microscopic dynamics but abundant statistical properties. Nevertheless, further studies are needed to better understand the heat problem in the systems of an array of superlattice other than a merely ideal interface belonging to two semi-infinite systems.

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