Heat conduction in two-dimensional momentum-conserving and -nonconserving gases

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Compared to that for two-dimensional (2D) lattices, our understanding of heat conduction in 2D gases is still limited. Here we study heat conduction behavior of 2D gas systems with momentum-conserving and -nonconserving interparticle interactions by using the nonequilibrium and equilibrium molecular dynamics methods. For the momentum-conserving system, we find that when the dimensionality of the system is changed from 2D to quasi-one-dimensional (quasi-1D), the heat conductivity κ diverges with the system size L as $\kappa \sim \ln L$ (the theoretical prediction for 2D systems) for a short L and shows, in the thermodynamic limit, a tendency to $\kappa \sim L^{1/3}$ like that predicted in 1D fluids. This suggests that the dimensional-crossover effect of heat conduction exists in 2D systems with conserved momentum. In contrast, for the momentum-nonconserving system, as L increases, finite heat conductivity independent of L is observed. These findings are in agreement with the predictions given by hydrodynamic theory and thus further confirm the validity of the theory in 2D gases.

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I. INTRODUCTION

A radical understanding of heat conduction is of primary importance for constructing microscopic pictures for macroscopic irreversible heat transfer and provides a theoretical basis for thermal energy control and management [1–7]. Theoretically, the well-known Fourier heat conduction law states

$$j = -\kappa \nabla T, \tag{1}$$

where j and ∇T are, respectively, the heat current and the spatial temperature gradient and κ is the heat conductivity, a finite constant independent of the system size. The transport following this law is usually known as normal heat conduction, and it has been shown that as long as some nonlinearity is present in the interaction, heat conduction is normal in all systems with pinning (on-site potential), and it is expected in three-dimensional systems [1–3].

At variance with the normal picture, more interesting anomalous size-dependent heat conductivity has, however, been observed experimentally in carbon nanotubes and suspended graphene [8–10] as well as numerically in low-dimensional Fermi-Pasta-Ulam-Tsingou systems without pinning (cf. [3], and references therein). Theoretically, it was reported in 2000 that momentum conservation implies anomalous conductivity in one-dimensional (1D) classical lattices [11], and three years later an interesting connection between anomalous heat conduction and anomalous diffusion was established in 1D systems [12]. Actually, the anomalous behavior was first theoretically predicted by the hydrodynamics approach [13] and the mode-coupling theory [1,3]. Both conjectured that for general momentum-conserving systems, the heat conductivity κ would diverge with the system size L as $\kappa \sim L^{\varsigma}$ (with $\varsigma < 1$) in one dimension and in the manner of $\kappa \sim \ln L$ in two dimensions. Later, in 2006 a similar prediction was achieved in an explicitly solvable model of stochastic dynamics [14], which further confirms that in low dimensions, the conservation of momentum is a crucial ingredient for the anomalous heat conduction.

Since the hydrodynamic description is always used in these theories, one may expect that the above theoretical conjecture could apply to both lattice and fluid models. This is indeed the case for 1D momentum-conserving systems, where the power-law divergent heat conductivity has been well verified in 1D lattices [3] and in 1D gas models that represent fluids [13,15–17]. Nevertheless, for the counterpart two-dimensional (2D) systems, to the best of our knowledge, at present only the 2D lattice models have been numerically studied [18–20]. This then raises the question: Can the $\kappa \sim \ln L$ law conjectured by the theories also be observed in 2D momentum-conserving gases?

In addition, the dimensional-crossover behavior of thermal transport from 2D to 1D is another interesting topic for low-dimensional systems [3,6]. Indeed, in 2014 the relevant crossover manner was experimentally observed in suspended single-layer graphene [10]. In this experimental setup, the authors fixed the width of samples and studied how the thermal conductivity changes with the samples' lengths. As the length increases, naturally, a dimensional-crossover behavior from 2D to quasi-1D can be expected. Moreover, in 2015 the 2D lattice model of dissociating particles was used to theoretically explore the dimensional effect [21], and recently, more detailed dimensional-crossover behaviors were revealed from the energy and momentum diffusions [22]. All of these studies greatly enrich our understanding of heat conduction in 2D lattice systems.

In this paper we investigate thermal transport and the relevant dimensional-crossover behavior in 2D gas fluids. Toward

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that end, it might be helpful to consider a 2D gas model of interacting particles in a rectangular box for simulating a fluid. The fluid is modeled by particles whose positions and velocities are treated as continuous variables. Fortunately, the evolution of the particles can be described by a multiparticle collision (MPC) dynamics [23] that correctly captures the hydrodynamic equations [24,25]. In particular, this steady state of a gas of particles, i.e., the MPC fluid, is known to behave with the ideal gas equation of state [26]. The MPC dynamics keeps the total momentum and energy of the system conserved, which thus helps us test the theoretical conjecture $\kappa \sim \ln L$ for 2D momentum-conserving systems. Further, as the usual measurement in heat conduction, we fix the width and increase the length of the rectangular box such that the dimensional-crossover behavior can also be explored. With the molecular dynamics simulations, we show that the prediction of $\kappa \sim \ln L$ for 2D momentum-conserving systems can be verified only for a short L, and in the thermodynamic limit, a tendency to $\kappa \sim L^{1/3}$ for 1D systems can be observed. Furthermore, in order to stress the momentum-conserving importance, we also show that when momentum conservation is broken by stochastic noise, the system exhibits normal heat conduction behavior. These results confirm that the dimensional-crossover behavior of heat conduction exists in low-dimensional momentum-conserving gas systems and further confirm the validity of hydrodynamic theory in gas systems.

This work is organized as follows. We start Sec. II by introducing a 2D gas model and providing the relevant simulation details. Section III is devoted to studying the L-dependent κ and analyzing the dimensionality-crossover property for the system with conserved momentum. In Sec. IV, we give distinct results for systems with broken momentum conservation. This, as mentioned, is achieved by adding certain stochastic noises. Finally, some related issues will be discussed with a brief summary in Sec. V.

II. THE 2D GAS MODEL

We consider a 2D gas system of N interacting particles in a rectangular box of width W (along the y coordinate) and length L (along the x coordinate; see Fig. 1 for a schematic plot). All particles have the same mass $m = 1$. In the y direction the particles are subject to periodic boundary conditions. To study the heat conduction problem, the system is placed in contact with two heat baths at $x = 0$ and $x = L$, through openings of the same size as the width W of the box. The left and right heat baths are modeled as ideal gases and are characterized by two different temperatures, T_L and T_R, respectively. When a particle hits the boundaries of the system, it is reflected back with a new velocity (denoted by v_x and v_y for its x and y components, respectively) chosen from a distribution with probability densities [27]

$$P(v_x) = \frac{|v_x|}{k_B T_\iota} \exp\left(-\frac{v_x^2}{2k_B T_\iota}\right),$$
$$P(v_y) = \sqrt{\frac{1}{2\pi k_B T_\iota}} \exp\left(-\frac{v_y^2}{2k_B T_\iota}\right), \tag{2}$$

where T_ι ($\iota = L, R$) is the temperature of the respective heat bath in dimensionless units and k_B is the Boltzmann constant.

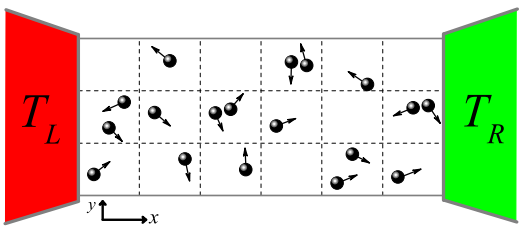

FIG. 1. Schematic plot of the gas model in a rectangular box of width W and length L evolving with the MPC dynamics. The cells with dashed-line boundaries represent the partition of space considered for modeling collisions. The two heat baths with temperatures T_L and T_R are placed on the left- and right-hand sides. The x coordinate goes along the channel, and y is perpendicular to it. See text for more details.

As mentioned, the evolution of this 2D gas system is described by the MPC dynamics. This MPC dynamics was successfully applied to model the steady shear flows in colloids [28], polymers [29], and also the vesicles in shear flow [30] (see also [31] and references therein for a review). More recently, it was adopted to study coupled particle and heat transport [32–34]. The MPC dynamics assumes that the system evolves in discrete time steps, consisting of free propagation during a time τ followed by collision events. During the free propagation period, a particle keeps its velocity $\mathbf{v}_i$ unchanged and updates its position as

$$\mathbf{r}_i \to \mathbf{r}_i + \tau \mathbf{v}_i. \tag{3}$$

For each collision event, the system's volume is partitioned into identical square cells of size $a \times a$ (see Fig. 1), and then the velocities of all particles found in the same cell are rotated with respect to their center of mass velocity $\mathbf{V}_{CM}$ by an angle, α or $-\alpha$, randomly chosen with equal probability. The velocity of a particle in a cell is thus updated as

$$\mathbf{v}_i \to \mathbf{V}_{CM} + \hat{\mathcal{R}}^{\pm\alpha}(\mathbf{v}_i - \mathbf{V}_{CM}), \tag{4}$$

where $\hat{\mathcal{R}}^{\pm\alpha}$ is the 2D rotation operator of the angle. The time interval between successive collisions τ and the collision angle α tune the strength of the interactions and, consequently, affect the transport of the gas particles. Note that the angle $\alpha = \pi/2$ corresponds to the most efficient mixing of the particle momenta, and such MPC dynamics preserve the total momentum and energy of the gas system.

In our simulations, each particle is initially given by a random position uniform distribution and a random velocity generated from the Maxwellian distribution at an average temperature $T = (T_L + T_R)/2$. Then the system is evolved for a long enough time ($>10^7$) to ensure that it has relaxed to the stationary state. After the system reaches the steady state, we compute the temperature profile $T(x)$, where x is the space variable. To calculate $T(x)$, we divide the space of the system into $N_a = \frac{L}{a}$ bins of equal size a. The total kinetic energy observed in the ith bin in a unit time is denoted by $\mathcal{E}_i$; thus, $T(ia)$ is defined as $T(ia) = \langle \mathcal{E}_i/a \rangle$, where $\langle\cdot\rangle$ represents the time average. In addition, the heat current j that crosses the system is measured, which is equal to the averaged energy exchanged in the unit time and area between the particles and the heat

bath. The heat conductivity is finally obtained by assuming Fourier's law, as $\kappa \approx jL/(T_L - T_R)$, where we have checked that in the linear response regime, the temperature jump between the heat bath and simulated system is not sensitive to the choice of L and thus can be neglected (as shown in Fig. 4 below). In the simulations, we set $T_L = T + \Delta T/2$ and $T_R = T - \Delta T/2$ so that the nominal temperature of the system is T and the main parameters adopted throughout are as follows: $k_B = 1$, $T = 1$, $\Delta T = 0.2$, $a = 0.1$, $\alpha = \pi/2$, $\tau = 0.25$, and the averaged particle number density $\rho = N/(WL) = 22.75$. In this work, long enough integration times ($>10^8$) are utilized to ensure the relative errors of all numerical results are smaller than 0.5%.

III. MOMENTUM CONSERVATION

Now let us turn to the simulation results. First of all, it is interesting to see the extreme case of no collisions. That means particles do not interact but propagate ballistically from one heat bath to the other as they cross the system. Under this consideration and with the heat baths given by Eq. (2), we can derive an analytical expression for the heat conductivity:

$$\kappa = 3\rho L\sqrt{\frac{k_B^3}{2\pi}}\Big/\left(\frac{1}{\sqrt{T_L}} + \frac{1}{\sqrt{T_R}}\right). \tag{5}$$

In Fig. 2 we plot the result for this extremely integrable system. As can be seen, κ diverges linearly with L, which is indeed verified by our numerical simulation (see the black circles). In contrast, for the interacting systems with collisions, we clearly show evidence of the nonballistic, superdiffusive thermal conduction behavior; that is, κ perfectly diverges with L as $\kappa \sim \ln L$ for a small range of L. This quite fast convergence to the prediction of the $\kappa \sim \ln L$ law suggests that the 2D gas system is a more ideal platform than lattices to check the validity of existing theories [3,14]. This is not strange

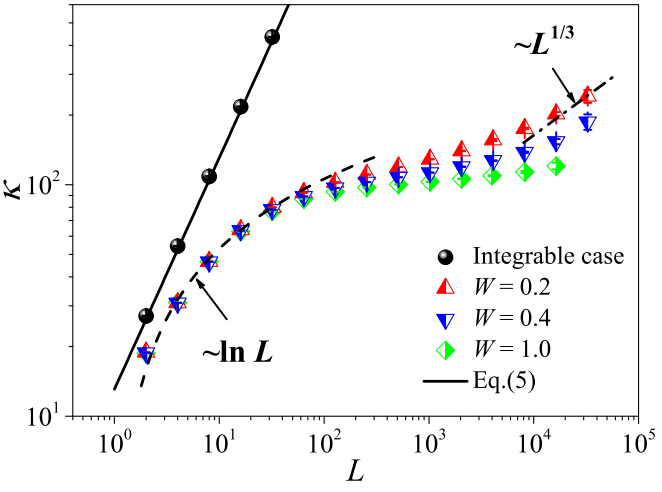

FIG. 2. Dependence of the heat conductivity on the system length, obtained from nonequilibrium simulations with different W. The symbols are for the numerical results, and the black line is the analytical result given by Eq. (5). The two curves correspond to the scalings $\sim \ln L$ (dashed) and $\sim L^{1/3}$ (dot-dashed), respectively.

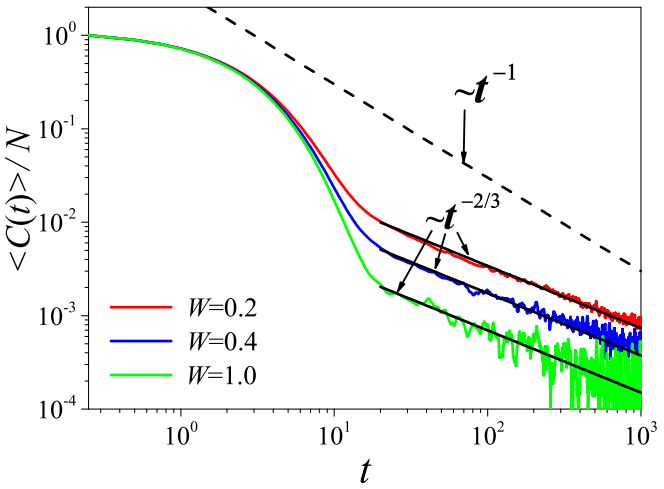

FIG. 3. The total heat current autocorrelation function for the 2D momentum-conserving gas system. The black dashed line and the black solid lines indicate the decay with t as $\sim t^{-1}$ and $\sim t^{-2/3}$, respectively. Here we fix $L = 4096$.

since most of the existing theories rely on the hydrodynamic description, which is for fluids.

For each fixed W, by further increasing L we see that the dimensionality-crossover effects play a role, and therefore, κ eventually shows a tendency to $\kappa \sim L^{1/3}$ for large L. This is consistent with the prediction for 1D momentum-conserving fluids [13,17] and also recent experimental observations in 2D materials [10]. This result thus suggests that such dimensionality-crossover effects would be ubiquitous in 2D systems and essentially root in the underlying hydrodynamics.

The underlying hydrodynamics over a long time can be revealed in more detail by studying the time decay of the total heat current autocorrelation function defined by $C(t) \equiv \langle J(0)J(t)\rangle$, where $J \equiv \frac{1}{2}\Sigma_i^N(v_{x,i}^2 + v_{y,i}^2)v_{x,i}$ is the total heat current along the x coordinate. With $C(t)$ and based on the celebrated Green-Kubo formula [1], one then obtains the heat conductivity as

$$\kappa_{GK} = \frac{1}{k_B T^2 d}\lim_{t_c\to\infty}\lim_{V\to\infty}\frac{1}{V}\int_0^{t_c} C(t)dt, \tag{6}$$

where d and V are the dimension and the volume of the system, respectively. In practice, as only a finite system with periodic boundary conditions can be dealt with, to calculate the heat conductivity, the integral is usually truncated up to $t_c = L/c_s$ (c_s is the sound speed) [1,35]. This results in the superdiffusive heat transport $\kappa \sim L^{1-\lambda}$ as long as $C(t)$ decays as $\sim t^{-\lambda}$.

To compute $C(t)$, we consider isolated systems with periodic boundary conditions. In the simulations, the initial condition is randomly assigned with the constraints that the total momentum is zero and the total energy corresponds to $T = 1$. The system is then evolved for a long enough time, and after the equilibrium state is reached, we use the following time to gain the time average. The results of $C(t)$ versus t for different system widths are presented in Fig. 3. As can be seen, after a rapid decay for a short time ($t < 10^1$), $C(t)$ finally decays in a power law $C(t) \sim t^{-2/3}$, showing a long, slowly decaying hydrodynamic tail. This result, combined

with the Green-Kubo formula, leads to $\kappa_{GK} \sim L^{1/3}$, which is consistent with $\kappa \sim L^{1/3}$ in the above result obtained with the nonequilibrium setting. Finally, we note that the rapid decay of $C(t)$ for a short time that deviates from the t^{-1} decay is usually due to a strong kinetic effect [36].

IV. MOMENTUM NONCONSERVATION

The momentum-nonconserving lattice systems are more common than the counterpart gas systems. For the lattice systems, one can add the pinning, i.e., the on-site potentials, into the systems to break the momentum conservation and obtain the normal heat conduction [37]. The underlying mechanism of this normal behavior is mainly related to the strong phonon-lattice interactions. However, in gas systems, one does not have such a way to destroy the momentum conservation, and further the mechanism is certainly distinct from the phonon-lattice interactions. Therefore, the thermal conduction in 2D momentum-nonconserving gas systems is actually an open issue.

With this open issue in mind, we now consider a 2D gas system with a source of stochastic noise. From a physical point of view, the noise source may model the interactions of the gas particles with the boundaries of the system or the inelastic scattering from impurities in the material. Following [32] to study the robustness of thermoelectric efficiency by noise, the stochastic noise in our model is added by modifying the MPC dynamics as follows: After a collision of the particles in a given cell has already taken place, with a probability p the velocities of all particles in the cell are reflected, namely, $\mathbf{v}_i \to -\mathbf{v}_i$. For any $p > 0$, the total momentum is thus no longer conserved, and we will study how the heat conduction behavior depends on the strength p of the perturbation.

First of all, we verify that when the system is in contact with the heat baths, the validity of Fourier's law determines the internal temperature profile of the steady state. Indeed, by assuming Fourier's law and equating the averaged local heat current along the system, we can obtain a temperature profile [15]:

$$T(x) = \left[T_L^{3/2}\left(1 - \frac{x}{L}\right) + T_R^{3/2}\frac{x}{L}\right]^{2/3}. \tag{7}$$

In Fig. 4 we compare our simulation results with this prediction. It can be seen that a very good agreement occurs for a relatively large system size. The small deviations for a small L are usually a result of the boundary (Kapitza) resistance. As expected, these boundary effects can be neglected by increasing the system size.

Figure 5 shows κ versus L for the nonequilibrium molecular dynamics measurement for different p. Here the counterpart momentum-conserving system of $p = 0$ is used as a reference system. In Fig. 5, the momentum-nonconserving systems of $p > 0$ is compared to the reference system (the momentum-conserving system of $p = 0$), it is clear that a small enough $p = 0.05$ can make the system's κ finite for a relatively large L. Moreover, the finite heat conductivity of this system can also be well inferred from the decay of the total heat current autocorrelation function with t (see Fig. 6) from an equilibrium measurement, where $C(t)$ undergoes an exponential decay, and eventually, it begins to oscillate around zero (the negative values are not shown in the logarithmic axis), showing a decay, as expected in the case of normal heat conduction. These results again somewhat demonstrate distinctions between lattice and gas systems, as in a lattice system with a relatively weak strength pinning, usually, it is hard to observe the true normal heat conduction [38]. However, despite this difference, our results further confirm that breaking the momentum conservation would generally lead to normal heat conduction in 2D systems. Finally, we also note that the value of finite heat conductivity decreases with an increase of p, as expected since the stronger the perturbation p is, the greater the heat resistance is.

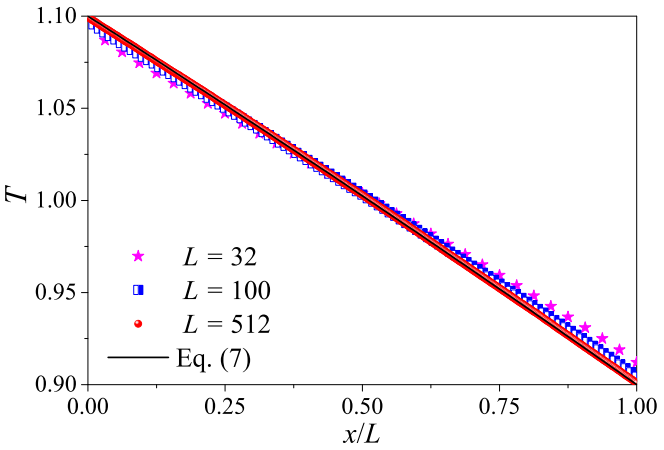

FIG. 4. Typical temperature profile for the 2D gas system with $p = 0.05$ and different L. Here our numerical results are compared with the analytical expression [see Eq. (7)]. Here and in the following figures, we fix $W = 1$.

V. SUMMARY AND DISCUSSION

In summary, with the advantage of MPC dynamics we have presented results of heat conduction in 2D gas systems. We

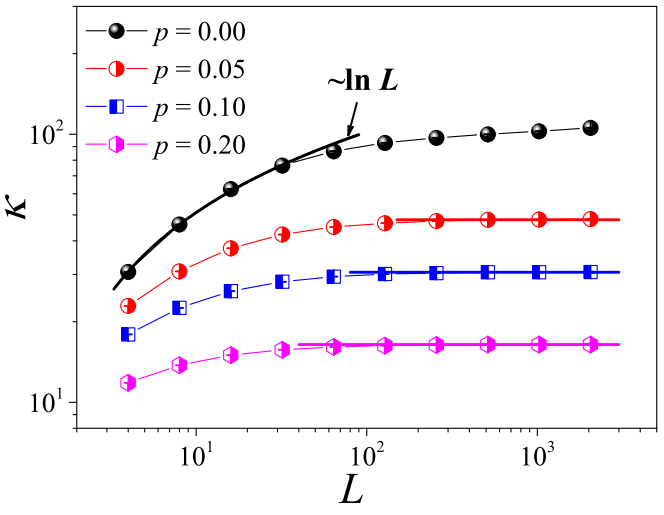

FIG. 5. The heat conductivity as a function of the system size for the momentum-nonconserving system with different p values. For reference the black line is the best logarithmic fit, $\kappa \sim \ln L$, and the three horizontal lines denote the saturation value of κ at large L.

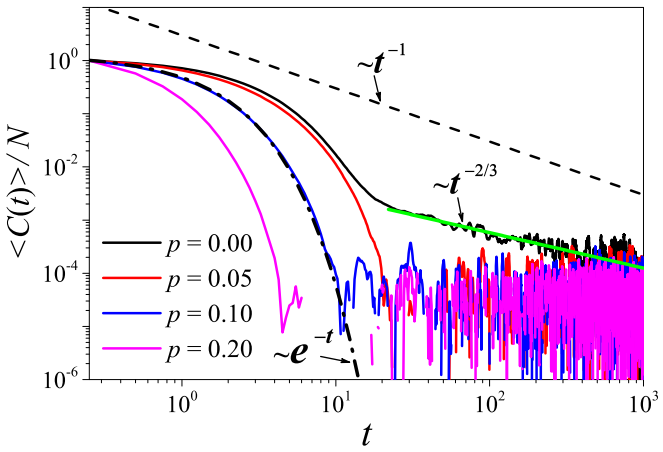

FIG. 6. The total heat current autocorrelation function for $L = 1024$ with $p = 0, 0.05, 0.10, 0.20$, showing a decay faster than $\sim 1/t$. The black dashed line, the green solid line, and the black dot-dashed lines indicate the scalings $\sim t^{-1}$, $\sim t^{-2/3}$, and $\sim e^{-t}$, respectively.

have shown that in the momentum-conserving gas system, the heat conductivity diverges in a logarithmic law for small system sizes as conjectured by the existing theories for 2D systems but tends to diverge in a power law for large system sizes such as that predicted in the 1D case. This suggests that the dimensionality-crossover behavior of heat conduction in both 2D lattices and 2D materials can also take place in 2D gas systems. In addition, we have included stochastic noise to study a 2D gas system with broken momentum conservation and observed the finite thermal conductivity independent of the system size that follows Fourier's law. This observation demonstrates qualitatively the same conclusion for the lattice and gas systems and further supports the general well-accepted viewpoint of the important role of momentum conservation in anomalous heat conduction.

Despite these observations being qualitatively the same, our results also reveal some distinctions between lattices and gases. The convergence to the logarithmic law for 2D gases is quite fast, and this seems unaffected by the width of the system. This indicates that the gases are more ideal than lattices for checking the validity of theory. However, this fast convergence still is not able to avoid the issue of dimensionality-crossover behavior. To solve this, a disk gas system similar to that proposed in lattices [20] would be helpful. Moreover, only a weak violation of momentum conservation in gases can already induce normal heat conduction. This implies that in addition to the mechanism of phonon-lattice interactions [37] in lattice systems, the inelastic interactions which break the momentum conservation are crucial for the validity of Fourier's law in gas systems.

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