

Heat conduction and diffusion of hard disks in a narrow channel

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Using molecular dynamics we study heat conduction and diffusion of hard disks in one-dimensional narrow channels. When collisions preserve momentum the heat conduction κ diverges with the number of disks N as $\kappa \sim N^\alpha$ ($\alpha \approx 1/3$). Such a behavior is seen both when the ordering of disks is fixed (“pen-case” model), and when they can exchange their positions. Momentum conservation results also in sound-wave effects that enhance diffusive behavior and on an intermediate time scale (that diverges in the thermodynamic limit) normal diffusion takes place even in the “pen-case” model. When collisions do not preserve momentum, κ remains finite and sound-wave effects are absent.

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According to the Fourier’s law of heat conductivity, when a small temperature difference is applied across a system, in the steady state the heat flux j satisfies the equation

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

where T is a local temperature and κ is the heat conductivity of a given material. Since the heat conductivity κ is one of the most important transport coefficients a lot of effort has been devoted to its calculation. Of particular interest is the case of low-dimensional systems, where κ might diverge and thus Eq. (1) would break down [1]. However, despite intensive efforts the nature of this divergence is not yet fully understood even in one-dimensional systems. Renormalization group calculations [2] show that for one-dimensional fluidlike systems κ should diverge with the number of particles N as $\kappa \sim N^\alpha$ with $\alpha = 1/3$. Although earlier works suggested other values of α , recent simulations for hard-core particle systems agree with this prediction [3]. In the other class of systems, chains of nonlinear oscillators (Fermi-Pasta-Ulam systems), simulations suggest [1,4] a larger value of α (0.37–0.40) and that might be consistent with the predictions of mode-coupling theory $\alpha = 2/5$ [5,6]. However, recently it was suggested that for such chains of oscillators α also should be equal to $1/3$ and numerically observed values of α were attributed to numerical difficulties [7].

It would be desirable to relate the divergence of heat conductivity to other dynamic properties of a given system. For example, it has been shown that chaoticity plays an important role and ensures that κ remains finite [8]. On the other hand, conservation of momentum is known to imply the divergence of κ [2,4]. Some attempts were also made to relate heat conductivity and diffusion. In particular, Li and Wang suggested [9] that the exponent β describing the mean square displacement of diffusing particles

$$\langle x^2(t) \rangle \sim t^\beta \quad (2)$$

should be related with α through the equation

$$\alpha = 2 - 2/\beta. \quad (3)$$

Such an equation implies that the normal diffusion ($\beta = 1$) leads to the normal (nondivergent) heat conductivity ($\alpha = 0$).

Moreover, superdiffusion ($\beta > 1$) and subdiffusion ($\beta < 1$) correspond to divergent ($\alpha > 0$) and vanishing ($\alpha < 0$) heat conductivity, respectively [10]. Although some numerical examples [11] seem to confirm the relation (3), its derivation is based only on qualitative arguments that neglect, for example, interactions between particles and so the suggestions that the relation (3) is of more general validity should be taken with care [12]. In another attempt, studying a class of noninteracting billiard heat channels, Denisov *et al.* [13] obtained a different relation between the exponents α and β , namely

$$\alpha = \beta - 1. \quad (4)$$

The relation (4) was verified numerically for the energy diffusion in a one-dimensional hard-core model [14]. However, it was argued [14] that the Levy walk scenario, that the energy diffusion obeys in this model, might be due to the absence of exponential instability and it is not clear whether this result can be extended to more realistic systems.

Establishing a firm relation between heat conductivity and diffusion could be possibly very influential and shed some light also on other transport phenomena. In the present paper we examine a model of hard disks in a narrow channel. When a fraction of disks is immobile and thus collisions do not conserve momentum, the heat conductivity κ remains finite and normal diffusion takes place. Simulations show that when there are no immobile disks and momentum is conserved, heat conductivity diverges with α close to $1/3$. According to (3) or (4) it should imply a superdiffusion. Although in this case diffusion is enhanced by sound-wave effects, there are no indications of superdiffusivity. Our work suggests that in hard-disk systems in a narrow channel heat conductivity and diffusion might be related but in a more intricate way than relations (3) or (4) would suggest.

In our model N identical hard disks of radius r and unit mass are moving in a channel of size L_x and L_y (see Fig. 1). The channel is narrow ($L_x \gg L_y$) and at both of its ends there are thermal walls that are kept at temperatures T_1 and T_2 [15]. After the collision with the wall kept at temperature T a disk has its normal component sampled from the distribution $p(v_x) = \frac{\Theta(\pm v_x)v_x}{T} \exp\left(-\frac{v_x^2}{2T}\right)$ with the sign in the argument of the

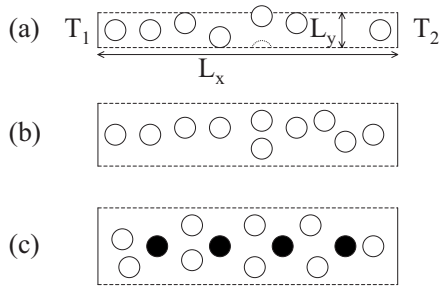


FIG. 1. In our model disks move between thermal walls kept at different temperatures T_1 and T_2 . In the vertical direction periodic boundary conditions are used. In (a) particles cannot pass each other and in (b) such a movement is possible. In (c) a fraction of disks is immobile and placed in the middle of the system (filled circles).

Heaviside function depending on the location of the wall. Its parallel component is sampled from the Gaussian distribution $p(v_y) = \frac{1}{\sqrt{2\pi T}} \exp(-\frac{v_y^2}{2T})$. In the vertical y -direction periodic boundary conditions are used. To calculate the heat conductivity κ we use Eq. (1) with heat flux in the x direction defined as a time average of $j = \sum_i v_{xi}^3/2$ where v_{xi} is the x component of the velocity of the i th particle.

One can note that without heat reservoirs models of this kind are chaotic [16,17]. Such a feature makes this model more realistic than, for example, a frequently examined one-dimensional alternating mass hard-disk model [3,18]. In the simplest setup of our model, known as a “pen-case” model [16,17] [Fig. 1(a)] disks are so large that they cannot exchange their position ($L_y/2 > r > L_y/4$). Heat conduction was already studied in such a case by Deutsch and Narayan [19]. Although their calculations indicate that α is close to $1/3$, reported strong finite size effects and relatively small size of examined systems ($N \leq 2048$) suggest that one must be cautious in the interpretation of these results. When r and L_y become small and the surface of particles is considered as very rough the “pen-case” model becomes the random-collision model. Calculations in such a case also suggest that α is close to $1/3$ [19].

An efficient way to simulate hard-disk systems is to use event-driven molecular dynamics [20–22]. Performance of the algorithm considerably increases upon implementing heap searching and sectorization and such methods have already been applied to a number of problems [23,24]. In our model it is sufficient to use sectorization only in the x direction. With such a technique we examined systems of up to $N = 3 \times 10^4$ hard disks. In the “pen-case” version of the model there is no need to introduce sectorization and simulations are only a little bit more demanding than in a one-dimensional alternating mass model [3].

To allow an exchange of particles we simulated also systems with disks of a smaller radius [Fig. 1(b)] and in such a case the sectorization considerably speeds up simulations. To examine the role of momentum conservation a fraction c of disks are made immobile. These disks are of the same radius and collisions with them conserve energy but not momentum. They are placed along the line $y = L_y/2$ [Fig. 1(c)] but similar (not presented) results are obtained for the random

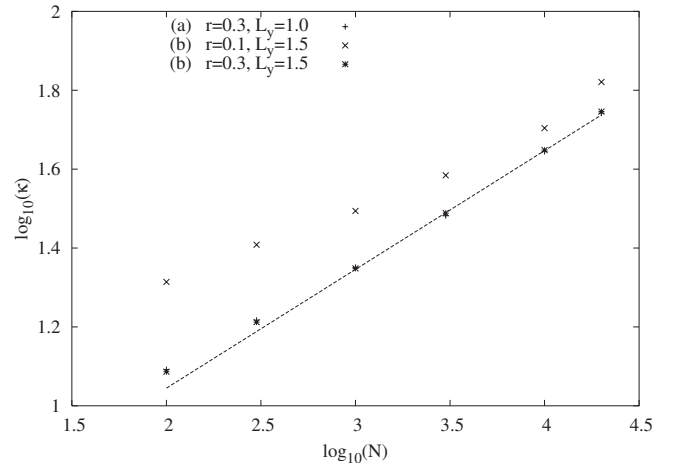


FIG. 2. The size dependence of the heat conductivity κ for the momentum conserving cases (a) and (b). The solid line has a slope corresponding to $\alpha = 1/3$. For $r = 0.3$ our results for $L = 1.0$ and 1.5 are nearly identical.

distribution of immobile disks. In our simulations, the parameters were chosen as follows: $L_x = N$, $L_y = 1.0 - 1.5$, $r = 0.01 - 0.3$, $T_1 = 1$, $T_2 = 2$, and $c = 0 - 0.1$. Initially centers of disks are usually uniformly distributed along the line $y = L_y/2$ (for $c > 0$ they are between immobile disks). Their velocities are sampled from the Boltzmann distribution at temperature interpolating linearly between T_1 at $x = 0$ and T_2 at $x = L$ [25]. Such a system evolves until a stationary state is reached and then computations of some time averages are made.

Numerical simulations in the momentum conserving case show that κ diverges with the number of particles N (Fig. 2) and the exponent α is close to that expected for the one-dimensional systems value $1/3$. In the limit of ideal gas ($r \rightarrow 0$) heat flux is independent on N (note that $L_x = N$ and increasing the number of particles N we also increase the distance they had to travel). This explains the slower convergence seen for $r = 0.1$.

The divergence of κ is an expected feature of momentum conserving systems [2,4], and some arguments suggest that in systems where momentum is not conserved κ should be finite [2]. A simple way to introduce momentum nonconservation into our system is to place some immobile disks. Although we do not present numerical data, our simulations confirm that in such a case κ remains finite in the thermodynamic limit $N \rightarrow \infty$. We noticed that even a small fraction of immobile disks ($c = 0.01$) is sufficient to remove the divergence of κ . It means that the behavior of κ in a very sensitive way depends on the conservation of momentum.

Simulations show that when there are no immobile disks, κ diverges with the same exponent $\alpha (\approx 1/3)$ both when particles cannot exchange their positions [case (a) in Fig. 1] and when they can [case (b)]. If Eq. (3) or Eq. (4) holds, we should observe in both cases the superdiffusive behavior (albeit with different exponents β). To examine diffusive properties we measured the mean square displacement $\langle x^2(t) \rangle$ over disks that at a certain time enter the central part of the system and did not hit a wall before the time t (for the ex-

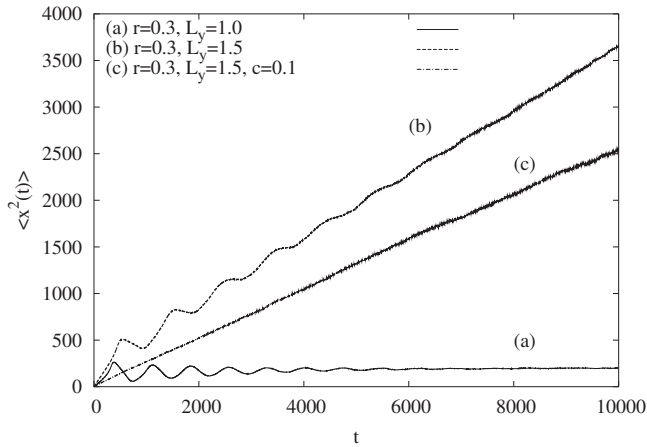


FIG. 3. The time dependence of the mean square displacement $\langle x^2(t) \rangle$ for $N=1000$ and $T_1=T_2=1$.

amined time scale such processes were extremely rare) [26]. To measure $\langle x^2(t) \rangle$ the system is not subjected to the temperature difference ($T_1=T_2=T$).

Numerical results show (Fig. 3) that in the presence of immobile disks $\langle x^2(t) \rangle$ increases linearly in time ($\beta=1$) and since κ remains finite in this case ($\alpha=0$), both (3) and (4) are satisfied. When momentum is conserved, two different behaviors are observed. In the case (a) disks cannot exchange their positions and displacement of particles is severely restricted. As a result $\langle x^2(t) \rangle$ saturates and that is an indication of strong subdiffusion. We will see, however, that this is only a finite size effect and in the thermodynamic limit a different behavior emerges in this case. In the case (b) disks can exchange their positions and asymptotically $\langle x^2(t) \rangle$ increases linearly in time, as in the momentum nonconserving case.

Now, let us examine an interesting similarity in the behavior of $\langle x^2(t) \rangle$ in the cases (a) and (b). Namely, initially $\langle x^2(t) \rangle$ has some oscillatory behavior in these cases and there is no indication of such a behavior in the momentum nonconserving case. To examine the origin of these oscillations we simulated systems of different number of disks and at different temperatures. Simulations show that the time of the first maximum of $\langle x^2(t) \rangle$ is approximately proportional to N (and thus to L_x) and inversely proportional to \sqrt{T} (note that \sqrt{T} is proportional to the typical velocity of disks). Such a behavior indicates that quasiscillations of $\langle x^2(t) \rangle$ are related with sound-wave effects. Size dependence of these quasiscillations for the case (a) is shown in Fig. 4 and a similar behavior was found for the case (b). Let us also notice that in case (b) the short-time growth of $\langle x^2(t) \rangle$ is faster than the long-time growth, although in both cases the growth is linear. Moreover, the saturation value of $\sqrt{\langle x^2(t) \rangle}$ is much smaller than the system length L_x .

Although at the large time scale the behavior of $\langle x^2(t) \rangle$ in cases (a) and (b) is much different (Fig. 3), at the shorter time scale it shows some similarity. Heat conductivity in cases (a) and (b) also behaves similarly. It is thus tempting to suggest that sound-wave effects, that provide a relatively fast transfer of energy but only on a short time scale, are related both with divergence of κ and with quasiscillations of

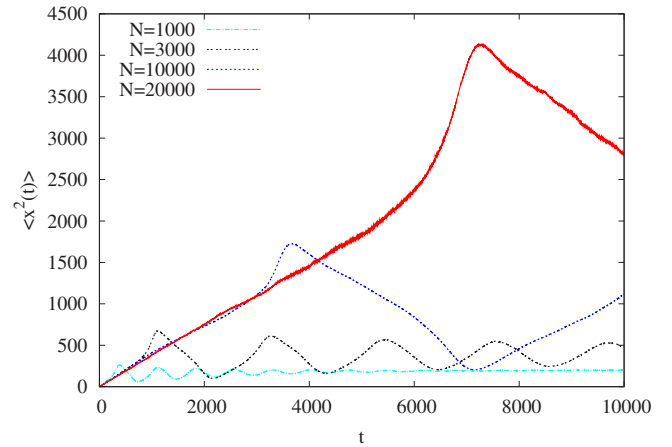


FIG. 4. (Color online) The time dependence of the mean square displacement $\langle x^2(t) \rangle$ for momentum conserving case (a) with different values of N and $T_1=T_2=1.0$.

$\langle x^2(t) \rangle$. In the presence of immobile disks such effects disappear, apparently due to the dissipation of momentum during collisions with immobile disks. As a result κ remains finite and $\langle x^2(t) \rangle$ increases monotonously in time. However, more detailed studies would be needed to substantiate such a claim.

Let us also notice that the time scale set by sound-wave effects diverges in the limit $N \rightarrow \infty$. In that case such effects will dominate diffusive behavior for an arbitrarily long time. As seen in Fig. 4, in such a limit $\langle x^2(t) \rangle$ seems to develop longer and longer linear increase. Thus we expect that in the limit $N \rightarrow \infty$, the diffusion in both cases (a) and (b) (data not shown) is normal, contrary to the predictions of (3) or (4).

That in the case (a) the mean square displacement $\langle x^2(t) \rangle$ increases linearly in time is perhaps interesting on its own. In this case particles cannot exchange their positions and that resembles the molecular diffusion, e.g., in some zeolites [27]. For such, so-called single-file systems, the mean square displacement is known to increase as \sqrt{t} and such a slow increase was derived for some stochastic lattice gas models [28]. As shown in Fig. 4, continuous dynamics and/or momentum conservation considerably modify such a behavior. However, since the thermal motion is usually rather fast, the sound-wave time scale is quite short and it might be difficult to examine such effects experimentally.

In conclusion, our work shows that in momentum-conserving hard disk systems in narrow channels heat conductivity κ diverges with the exponent $\alpha \approx 1/3$ and sound-wave effects enhance diffusion. As a result, in the thermodynamic limit, normal diffusion appears even in the “pen-case” version of our model. When momentum is not conserved, κ remains finite and no enhancement of diffusion was observed. Heat conduction, diffusion, and momentum conservation are terms of fundamental importance in physics. Their intricate relations even in such simple systems like the ones examined in the present paper should warrant further study of these problems.

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