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One-dimensional heat conductivity exponent from a random collision model

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We obtain numerically the thermal conductivity of a quasi-one-dimensional classical chain of hard sphere particles as a function of the length of the chain, introducing a fresh model for this problem. The conductivity scales as a power law of the length over two decades, with an exponent very close to the analytical prediction of 1/3.

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Since the surprising result obtained over thirty years ago that the heat current flowing across a one-dimensional chain of harmonic oscillators with a small temperature difference between the two ends is independent of the length L of the chain [1], the conductivity of one-dimensional systems has been studied analytically [2–4] and numerically [4–8] at great length. The standard approach to conductivity would predict that if the temperature gradient ∇T in a material is small, the heat current flowing through should be of the form $j=-\kappa\nabla T$, where κ is a property of the material. On the other hand, the result for the harmonic oscillator chain, that a small temperature difference ΔT results in a current $j\propto\Delta T$ that is independent of L, is equivalent to a conductivity $\kappa \propto L$. In the various models studied thereafter, singular conductivities $\kappa\sim L^{\alpha}$ have been found, with a variety of possible values for α. On the other hand, for some one-dimensional models a conventional L-independent κ has also been obtained.

It is now believed that the singular conductivity of these models has two possible causes. First, if the model is integrable, as in the case of the harmonic oscillator chain, the system does not equilibrate thermally. The behavior of the conductivity then depends on the details of the system. In fact, it has been shown that by changing the coupling of the oscillator chain to the heat reservoirs at the ends, normally a benign procedure, one can tune the exponent α over a range [3]. Second, even if the model is not integrable, if the internal interactions in the system conserve momentum, the conductivity is singular, due to advection of heat in long wavelength modes [6,9,10]. If a model is not integrable and does not conserve momentum, κ should have a well defined limit as L diverges [11]. Analytical studies [6,10] predict that for nonintegrable momentum conserving systems, α should have a universal value of 1/3.

Numerical results for momentum conserving systems have yielded values of α ranging from 0.25 to 0.5. Recent studies of one-dimensional chains of hard point particles with alternating masses have shown unexpectedly large corrections to scaling even for systems of $\sim 10^4$ particles, with α estimated to be 0.25 [7] and 0.33 [6]. Similar results have been obtained for chains of Fermi Pasta Ulam chains, with α estimated to be 0.37 [8]. For the system of hard point particles, the slow convergence to the asymptotic behavior has been justified [6] by noticing that the system is always "close" to an integrable model. Thus, if one considers a chain of particles with equal masses, energy is carried ballistically, the system does not thermalize, and $\alpha=1$. On the other hand, if the ratio of the masses of successive particles in the alternating chain is chosen to be very different from unity, the light particles are almost inconsequential, and the problem again reduces to one of equal mass particles. In Ref. [6], a mass ratio of 2.62 was found to yield the longest power-law scaling range, from which α was estimated.

In this paper, we try to eliminate any residual effect of integrability by considering Sinai's pencase model [12]. In this model, hard sphere particles are confined to a long narrow tube. We consider both periodic and hard-wall boundary conditions in the transverse direction, and apply heat baths to the two ends. 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 get past each other, but allows a large range of incidence angles at the collisions. Thus, the transport of energy along the tube remains quasi-one-dimensional, with the transverse degree of freedom serving as an additional randomizing effect. This model (without heat reservoirs) has been proved to be ergodic in four dimensions and hyperbolic in three [13].

The extra degree of freedom in our model limits the system sizes we simulate. For the range of system sizes that we consider, there is still insufficient universality to obtain the asymptotic value for α with confidence. Therefore, we consider a further modified version of the model: we imagine making the size of the particles extremely small, correspondingly reducing the size of the tube they are confined to. Also, we consider the surface of the particles to be very rough, so that when two neighboring particles collide, they emerge from the collision moving apart in a random direction. In the resultant "random collision model," the transverse coordinate is eliminated as a degree of freedom, but the transverse velocity is retained. Any collision conserves the total energy and the total momentum in both directions. As a result of these changes, probably due to the further randomization introduced by the collision rule, the conductivity fits very well to the form $\kappa\sim L^{\alpha}$, with α close to 1/3. If the masses of all the particles are taken to be equal, the estimated value of α is 0.29 ± 0.01, while when the particle masses alternate with a mass ratio of 2.62, one obtains α to be 0.335 ± 0.01. The small discrepancy from the theoretical prediction of $\alpha=1/3$, although larger than the error bars, is within the range one might expect from corrections to scaling from the leading irrelevant operators.

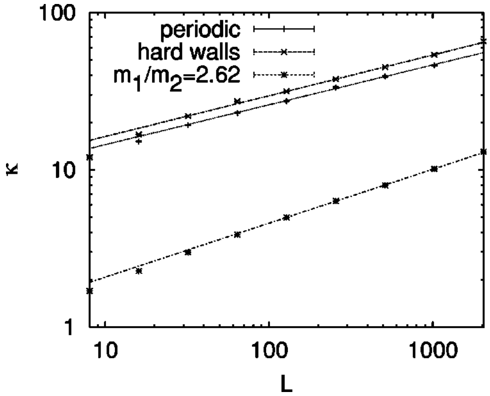

FIG. 1. Log-log plot of the conductivity as a function of the number of particles for Sinai's pencase model [12]. The upper two plots are for periodic and hard-wall boundary conditions in the transverse direction, with the mass of all particles being 1. The slopes of these plots, which should be equal to the conductivity exponent α, are 0.25 ± 0.02 and 0.26 ± 0.01, respectively. The lowest plot is for hard-wall boundary conditions in the transverse direction, with the mass of particles alternating between 2.62 and 1. The slope of the plot is 0.34 ± 0.02. Even though each individual plot fits well to a straight line (apart for deviations at the low L end), the differences between the slopes preclude a good estimate of the asymptotic large L value of α.

One might be concerned whether the analytical derivation of $\alpha=1/3$, which uses the hydrodynamic description of a one-dimensional normal fluid [10] is valid for the models we have considered here. Since the transverse direction is small, it should not affect long wavelength singularities in the dynamics. Of greater concern is, with periodic boundary conditions, the existence of the transverse momentum as another conserved quantity. Even for the random collision model, where the transverse coordinate is eliminated, the transverse momentum is retained. Although this makes the hydrodynamic equations more complicated, and increases their number from 3 to 4, we recall that the analytical calculation relies only on the fact that (without an applied temperature gradient) the system reaches thermal equilibrium, that it satisfies Galilean invariance, and that a finite sound velocity sets a cutoff to the dynamics for any finite system size. None of these conditions is violated by the introduction of the transverse momentum.

Figure 1 shows a log-log plot of the conductivity as a function of the length the system L, for the pencase model. The results for both periodic and hard-wall boundary conditions are shown. All the particles were taken to have the same mass. The diameter of the particles was 0.6, while the cross section of the tube and the average longitudinal separation between centers of neighboring particles were both taken to be 1. The temperatures of the heat reservoirs at the two ends were taken to be 1.0 and 1.2, respectively; it was verified numerically that this temperature difference is sufficiently small for the system to be in the linear response regime. The heat reservoirs at the ends were implemented as follows: whenever an extremal particle collided with the reservoir adjoining it, its velocity was randomized, drawn from the distribution $P(v_x,v_y)\propto v_x\exp[-m(v_x^2+v_y^2)/(2k_BT)]$, where x and y are along the longitudinal and transverse direction, respectively, and T is the temperature of the reservoir. (This is the velocity distribution for particles leaking out of a heat reservoir.) At each such collision, the energy exchanged by the system and the reservoir is kept track of, and used to calculate the time average of the energy current at both ends.

In the same figure, the conductivity as a function of system length is also shown for a different choice of model parameters: alternating particle masses, with a mass ratio of 2.62, a tube cross section of 1.14, and a longitudinal interparticle separation of 0.9. (Only hard-wall transverse boundary conditions are shown for this case.)

The number of particles in the system ranged from 8 to 2048. This is substantially less than the largest system sizes used when simulating the one-dimensional chain of hard point particles. However, introducing the transverse dimension should make the system no longer near integrability, and therefore allow the large L limit to be reached quickly. Unfortunately, as seen in Fig. 1, this is not the case. There is some curvature in all the plots; more importantly, there is substantial disagreement between the slopes obtained when the particles have equal or alternating masses. Note that the plots all curve *downwards*, from which one might be tempted to conclude that the asymptotic slope (i.e., the value of α) would be smaller than obtained from the curves. However, prior experience with the one-dimensional system [6] indicates that it is possible for the curves to turn around at much larger system sizes. Thus, one cannot obtain even an upper bound to α from the figure, and must conclude that the corrections to scaling are large for this model [14].

In order to randomize the dynamics further, enabling faster convergence to the asymptotic scaling form for large L, we modify the model above. First, the diameter of the particles is taken to be negligibly small, while keeping the cross section of the tube as less than twice the diameter. Second, the particles are no longer disk shaped, but irregular. As a result, when two particles collide with each other, in the center of mass frame they can recoil in any direction, unrelated to the direction of impact. For any collision, we take the recoil angle in the center of mass frame to be a random variable [15] respecting detailed balance. The result of both these modifications together is that the transverse coordinate y of the particles becomes redundant and they effectively move along the x axis. However, the transverse velocities v_y are retained. In this "random collision model," each particle has both v_x and v_y, with the latter behaving as an auxiliary variable that is only important in collisions. In any interparticle collision, the total momentum in the x and y directions and the total energy are conserved. Collisions with the reservoirs at the two ends are still implemented as before. In the transverse direction, periodic boundary conditions correspond to v_y for a particle remaining constant between collisions, whereas hard-wall boundary conditions allow v_y to be reversed. In the latter case, since in the zero cross-section limit any particle undergoes a huge number of collisions with the sidewalls between two collisions with its neighbors, one should change the sign of v_y randomly between interparticle collisions.

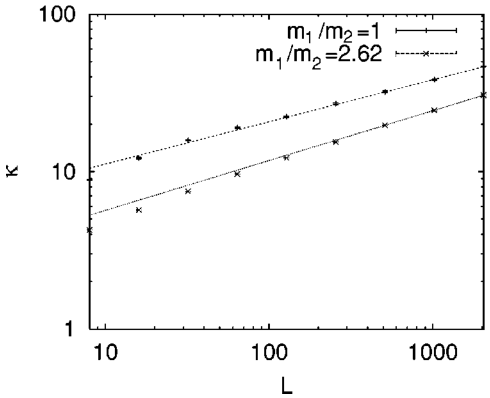

FIG. 2. Log-log plot of the conductivity as a function of the number of particles for the random collision model introduced in this paper. The upper plot is for all the particles with mass 1, while the lower plot is for particles whose masses alternate between 1 and 2.62. The slopes for the two plots are 0.29 ± 0.01 and 0.335 ± 0.01. Both the plots are for periodic boundary conditions in the transverse direction; the results for hard-wall boundary conditions were very similar.

Figure 2 shows a log-log plot of the conductivity as a function of L for the random collision model. The particles are now points, the average interparticle separation is unity, and the temperatures of the reservoirs are 1 and 1.2 as before. In the linear response regime, the dependence of the energy current on the average interparticle separation and the reservoir temperatures can be found trivially, so the only parameters that can be varied (apart from the number of particles) are the masses of the particles. Only the results for periodic boundary conditions in the transverse direction are shown, as the results for the hard-wall case are very similar. As before, plots are shown for the case when all particles have the same mass and the case when the particle masses alternate with a mass ratio of 2.62. Both parameter choices yield plots that rapidly converge to a power-law form, but with slightly different exponents. The estimated exponents are $\alpha=0.29\pm0.01$ and $\alpha=0.335\pm0.01$, respectively, for the two cases. Both of these are very close to the analytical prediction of $\alpha=1/3$. Although the difference between the two estimates for α is larger than the error bars, we expect that this is due to corrections to scaling from irrelevant operators in a renormalization group analysis; an $O(1)$ bare strength for irrelevant operators can produce effective values of α that differ from 1/3 by the desired amount. Thus, the numerical results of Fig. 2 are a strong indication of the validity of the prediction of $\alpha=1/3$.

It is worth noting that earlier work [16] on the one-dimensional Kardar-Parisi-Zhang (KPZ) equation [17] has found it impossible to obtain universal critical exponents from numerical simulations, even with large system sizes. The hydrodynamic description used [10] to obtain α is similar to the KPZ (Burgers) equation, but with three equations instead of one. In fact, α was correctly estimated earlier [6] from the KPZ equation. Thus, the slow convergence that we see for α for the pencase model—and, to a lesser extent, for the random collision model—may be a similar phenomenon to that seen for the KPZ equation.

In this paper, we have introduced a random collision model for studying dynamics of momentum conserving one-dimensional systems, in order to obtain the scaling form of the thermal conductivity κ as a function of system size L. Over a wide range of length scales, we find good agreement with the earlier analytical prediction of $\kappa\sim L^{1/3}$.

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