One dimensional heat conductivity exponent from random collision model

J. M. Deutsch and Onuttom Narayan

Department of Physics, University of California, Santa Cruz, CA 95064.

(Dated: November 16, 2018)

We study numerically the thermal conductivity coefficient \( \kappa \) as a function of system length \( L \) for several different quasi one dimensional models: classical gases of hard spheres with both longitudinal and transverse degrees of freedom. We introduce a model that is ergodic and highly chaotic but also conserves energy and momentum, and is very useful because it shows scaling even at small system sizes. We find that \( \kappa \sim L^\alpha \) over more than two decades, with \( \alpha \) very close to the analytical prediction of 1/3.

PACS numbers: 05.10.Ln, 75.40.Mg

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, 3, 4, 5] and numerically [6, 7, 8, 9, 10] at great length. The standard approach to conductivity would predict that if the temperature gradient \( \nabla T \) in a material is small, the heat current flowing through should be of the form \( j = -\kappa \nabla T \), where \( \kappa \) is a property of the material. On the other hand, the result for the harmonic oscillator chain, that a small temperature difference \( \Delta T \) 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 \( \alpha \). On the other hand, for some one-dimensional models a conventional \( L \)-independent \( \kappa \) has also been obtained.

It is now believed that the singular conductivity of these models has two possible causes. Firstly, 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 \( \alpha \) over a range [3]. Secondly, 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 [3, 4, 5]. If a model is not integrable and does not conserve momentum, \( \kappa \) should have a well defined limit as \( L \) diverges [11]. Analytical studies [3, 4, 5] predict that for non-integrable momentum conserving systems, \( \alpha \) should have a universal value of 1/3.

Numerical results for momentum conserving systems have yielded values of \( \alpha \) 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 \( \alpha \) estimated to be 0.25 [6] and 0.33 [7]. Similar results have been obtained for chains of Fermi Pasta Ulam chains, with \( \alpha \) estimated to be 0.37 [8]. For the system of hard point particles, the slow convergence to the asymptotic behavior has been justified [8] 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. [9], a mass ratio of 2.62 was found to yield the longest power-law scaling range, from which \( \alpha \) was estimated.

In this paper, we study how to eliminate residual effects of integrability by considering non-integrable and highly chaotic models. We start with Sinai and Chernov’s pencease model [12] that was initially introduced by them to study one dimensional hydrodynamics. 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 \( \alpha \) with confidence. Therefore, we have devised a novel 1d model that we call the “random collision” (RC) model, discussed in detail below, that is extremely chaotic, yet still satisfies energy and momentum conservation.

Probably due to the further randomization introduced by our new dynamics, the conductivity fits very well to the form \( \kappa \sim L^\alpha \), with \( \alpha \) close to 1/3. If the masses of all the particles are taken to be equal, the estimated value of \( \alpha \) is 0.29 ± 0.01, while when the particle masses alternate with a mass ratio of 2.62, one obtains \( \alpha \) 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.

We also show results for the autocorrelation function of the energy current, which is related to the conductivity through the Kubo formula [14]. The autocorrelation function has a zero frequency limit that scales close to \( L^{1/3} \), in accordance with previous predictions and our numerical results for the conductivity. However, the full correlation function \( C(\omega; L) \) shows quite complicated behavior, not easily described by any simple scaling form, possibly indicating the existence of multiple time scales.

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. Although this makes the hydrodynamic equations more complicated, and increases their number from three to four, 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 of 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 \( P(v_x, v_y) \propto v_x \exp[-m(v_x^2 + v_y^2)/(2kBT)] \), 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 1024. 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 Figure 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 \( \alpha \)) would be smaller than obtained from the curves. However, prior experience with the one dimensional system [8] 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 \( \alpha \) from the figure, and must conclude that the corrections to scaling are large for this model [15].

In order to randomize the dynamics further, enabling faster convergence to the asymptotic scaling form for large \( L \), we modify the model above. Firstly, 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. Secondly, the particles are no longer
In this RC model, each particle has both x and y components of momentum, becoming redundant, and they effectively move along the direction of impact. For any collision, we take the recoil angle in the center of mass frame to be a uniform random variable [10]. The result of both these modifications together is that the transverse coordinate becomes redundant, and they effectively move along the x-axis. However, the transverse velocities $v_y$ are retained. In this RC 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.

Figure 2 shows a log log plot of the conductivity as a function of $L$ for the RC model. The particles are now disk shaped, but highly 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 uniform random variable [10]. The result of both these modifications together is that the transverse coordinate $v_y$ of the particles becomes redundant, and they effectively move along the $x$ axis. However, the transverse velocities $v_y$ are retained. In this RC 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.

Figure 2: Log-log plot of the conductivity as a function of the number of particles for the RC 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.

Disk shaped, but highly 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 uniform random variable [10]. The result of both these modifications together is that the transverse coordinate $v_y$ of the particles becomes redundant, and they effectively move along the $x$ axis. However, the transverse velocities $v_y$ are retained. In this RC 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.

Figure 3 shows the log-log plot of the conductivity as a function of $L$ for the RC 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 $\alpha = 0.29 \pm 0.01$ and $\alpha = 0.335 \pm 0.01$ 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 $\alpha$ 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 $\alpha$ that differ from 1/3 by the desired amount. Thus the numerical results of Figure 2 are a strong indication of the validity of the prediction of $\alpha = 1/3$.

We have also measured the autocorrelation function for the energy current, $C(\omega)$, with periodic boundary conditions in the $x$ direction (without heat reservoirs), for the case when all the particles have identical mass. Based on the analytical prediction [10], we show $L^{-1/3}C(\omega L)$ for a range of system sizes. The $\omega \rightarrow 0$ limit of all the curves appears to be the same, in accordance with the numerical results we have obtained for the conductivity, although...
The existence of a well defined limit in the longitudinal direction. The straight lines correspond to a functional form of $C(\omega, L) \sim \omega^{-1/4}$, where $L$ is the system size. The upper curve corresponds to a system with 512 particles and the lower curve to a system of 1024 particles. The two curves have been shifted with respect to each other for clarity. All particles have equal mass, and periodic boundary conditions are imposed in the longitudinal direction. The straight lines correspond to a system of 1024 particles. The two curves have been curve corresponds to a system with 512 particles and the lower curve to a system with 256 particles. The collapse of the curves to a single plot appears (for $L > L_c$) to decrease slightly faster than $\omega^{-1/4}$, indicating that there are important dynamics on the $t \sim L$ timescale.

It is not clear whether the correlation function converges to the simple scaling form for much larger system sizes, or whether there are indeed multiple time scales in the dynamics: $t_1(L) \sim L$ and $t_2(L) \sim L^{3/2}$ with $\beta \approx 4/3$. However, earlier work on the one dimensional KPZ equation has found it difficult to obtain universal critical exponents from numerical simulations, even with large system sizes. The hydrodynamic description used to obtain $\alpha$ is similar to the KPZ equation, but with three equations instead of one. In fact, $\alpha$ was correctly estimated earlier from the KPZ equation. Thus the slow convergence that we see for $\alpha$ for the pencase model — and, to a lesser extent, for the RC model — may be a similar phenomenon to that seen for the KPZ equation. Of course, even the hydrodynamic description for one-dimensional conduction does involve two time scales: for propagation and decay of the sound modes.

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 $\kappa$ as a function of system size $L$. This has allowed us to probe the scaling regime better than has been possible with previous models that show a slower approach to the large $L$ limit and less robust behavior. Over a wide range of length scales, we find good agreement with the earlier analytical prediction of $\kappa \sim L^{1/3}$.

We thank Abhishek Dhar and M.A. Moore for very useful discussions.

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{figure4.png}
\caption{Unscaled plot of the autocorrelation function of the energy current, $C(\omega)$, as a function of frequency $\omega$. The upper curve corresponds to a system with 512 particles and the lower curve to a system of 1024 particles. The two curves have been shifted with respect to each other for clarity. All particles have equal mass, and periodic boundary conditions are imposed in the longitudinal direction. The straight lines correspond to a $\sim \omega^{-1/4}$ functional form.}
\end{figure}

\begin{thebibliography}{10}
\bibitem{1} Z. Rieder, J.L. Lebowitz and E. Lieb, J. Math. Phys. \textbf{8}, 1073 (1967).
\bibitem{2} A. Casher and J.L. Lebowitz, J. Math. Phys. \textbf{12}, 1701 (1971); R.J. Rubin and W.L. Greer, J. Math. Phys. \textbf{12}, 1686 (1971); A.J. O’Connor and J.L. Lebowitz, J. Math. Phys. \textbf{15}, 692 (1974); H. Spohn and J.L. Lebowitz, Commun. Math. Phys. \textbf{54}, 97 (1977); H. Matsuda and K. Ishii, Prog. Theor. Phys. Suppl. \textbf{45}, 56 (1970).
\bibitem{3} A. Dhar, Phys. Rev. Lett. \textbf{86}, 5882 (2001).
\bibitem{4} S. Lepri, R. Livi and A. Politi, Europhys. Lett. \textbf{43}, 271 (1998).
\bibitem{5} S. Lepri, R. Livi and A. Politi, Phys. Rev. Lett. \textbf{78}, 1896 (1997); A.V. Savin, G.P. Tsironis, A.V. Zolotaryuk, Phys. Rev. Lett. \textbf{88}, 154301 (2002); T. Hatano, Phys. Rev. E \textbf{59}, R1 (1999); A. Dhar Phys. Rev. Lett. \textbf{86}, 3554 (2001).
\bibitem{6} P. Grassberger, W. Nadler and L. Yang, Phys. Rev. Lett. \textbf{89}, 180601 (2002).
\bibitem{7} G. Casati and T. Prosen, cond-mat/0203331.
\bibitem{8} P. Grassberger and L. Yang, cond-mat/0204247.
\bibitem{9} T. Prosen and D.K. Campbell, Phys. Rev. Lett. \textbf{84}, 2857 (2000).
\bibitem{10} O. Narayan and S. Ramaswamy, Phys. Rev. Lett. \textbf{89}, 200601 (2002).
\bibitem{11} G. Casati, J. Ford, F. Vivaldi, and W.M. Visscher, Phys. Rev. Lett. \textbf{52}, 1861 (1984).
\bibitem{12} Ya. G. Sinai and N.I. Chernov, Russian Math. Surveys (3) \textbf{42}, 181 (1977).
\bibitem{13} N. Simányi and D. Szász, Math. Res. Lett. \textbf{2}, 751 (1995).
\bibitem{14} R. Kubo, J. Phys. Soc. Japan \textbf{12}, 570 (1957).
\bibitem{15} Although the possibility that $\alpha$ could be non-universal is also allowed by the data.
\bibitem{16} The range of recoil angles is of course taken to be $[0, \pi]$, i.e. the particle that is incident from the left in any collision also emerges on the left.
\bibitem{17} F. Bonetto J.L. Lebowitz and L. Rey-Bellet, cond-mat/0002052; see also J.A. McLennan, Non-equilibrium statistical mechanics, (Prentice Hall, Englewood Cliffs NJ 1989).
\bibitem{18} P. de los Rios, Phys. Rev. Lett. \textbf{82}, 4236 (1999).
\bibitem{19} M. Kardar, G. Parisi and Y.-C. Zhang, Phys. Rev. Lett. \textbf{56}, 889 (1986).
\bibitem{20} T. Halpin-Healy, R. Novoseller cond-mat/0004251.
\end{thebibliography}