Heat Conduction and Entropy Production in a One-Dimensional Hard-Particle Gas

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(Received 13 March 2002; published 11 October 2002)

We present large scale simulations for a one-dimensional chain of hard-point particles with alternating masses and correct several claims in recent literature based on much smaller simulations. We find heat conductivities κ to diverge with the number N of particles. These depended strongly on the mass ratio, and extrapolations to $N \to \infty$, and $t \to \infty$, are difficult due to very large finite-size and finite-time corrections. Nevertheless, our data seem compatible with a universal power law $\kappa \sim N^{\alpha}$ with $\alpha \approx 0.33$ suggesting a relation to the Kardar-Parisi-Zhang model. We finally discuss why the system leads nevertheless to energy dissipation and entropy production, in spite of not being chaotic in the usual sense.

DOI: 10.1103/PhysRevLett.89.180601 PACS numbers: 05.60.–k, 44.10.+i, 66.60.+a

Low-dimensional systems are special in many ways. Second order phase transitions have anomalous exponents, chemical reactions do not follow the mass action law [1], hydrodynamics breaks down due to divergent transport coefficients caused by long time tails [2], and electrons in disordered systems are localized [3]. A last item in this list is the divergence of heat conductivity [4] in ≤ 2 spatial dimensions.

For ordered (periodic) harmonic systems, it is well known that all transport coefficients are infinite due to the ballistic propagation of modes. Thus, one needs either disorder or nonlinear effects in order to have finite conductivity κ. For electric conductivity, disorder in 1D leads to zero conduction. The main difference between heat and (electronic) charge conduction is that there is no background lattice in the former; i.e., translation invariance is not broken even if the system is disordered. Of course, one can study the electronic contribution to heat conduction, but experimentally one never can neglect the ionic contribution [5]. Thus, one has always soft (Goldstone) modes in heat conduction. These soft modes are not localized by disorder [6], and they are not affected by nonlinearities. Thus, they propagate essentially freely. In high dimensions, this has no dramatic consequences. But in low dimensions they become important and lead to the above mentioned divergence. More precisely, one expects a power divergence $\kappa \sim N^{\alpha}$ in $d = 1$ and a logarithmic divergence in $d = 2$. Simulations and calculations using the Green-Kubo formula give $\alpha \approx 0.35$ to 0.45 [4]. It is not clear whether the slight discrepancies found between different models are true or artifacts. Theoretically, one would of course prefer a universal value.

There are some exceptions to this general scenario. Apart from models with external potentials and broken translation invariance, the best known 1D model with finite κ is the rotor model of [7,8]. Here very fast rotors effectively decouple from their less fast neighbors. Thus, very steep jumps of temperature are effectively stabilized and act as barriers to energy transport.

Another model which was recently claimed to have κ finite [9] is the 1D hard-point gas with alternating masses. The same gas with all particles having the same mass is trivial (a collision between particles is indistinguishable from the particles just passing through each other undisturbed), and perturbations just propagate ballistically, leading thus to infinite κ (i.e., no temperature gradients can build up inside the gas). To break this integrability, it is sufficient to use alternating masses: every even-numbered particle has mass m_1, and every odd has $m_2 = rm_1$ with $r > 1$ [9–15].

The arguments given above for a divergence of κ with N hold also for the hard-point gas. It is obviously nonlinear, sound waves dissipate, it is translation invariant, and there is no obvious special feature as in the rotor model. Indeed, prior to [9], heat conduction has been studied in this system by means of simulations in [13,14]. In these papers, it was claimed that κ diverges. But the simulations of [13] had presumably low statistics (very few details were given), while the simulations of [14] are obviously not yet in the scaling regime (N is too small) and are compatible with $\kappa \to$ const for $N \to \infty$. In any case, the exponent α suggested by the simulations of [14] is ≤ 0.22, much smaller than for all other models.

In view of this confusing situation, and suspecting that the simulations of [9,13,14] were not done most efficiently, we decided to make some longer simulations.

We followed [14] in setting $m_1 = 1$ and using Maxwellian heat baths at the ends with $T_1 = 2$, $T_2 = 8$ (i.e., after hitting the end, a particle is reflected with a random velocity distributed according to $P(v) = \Theta(\pm v) mv/T \exp(-mv^2/2T_{1,2})$. The heat baths sit at $x = 0$ and $x = N$; i.e., the density of the gas is 1. When an even particle with velocity v_1 collides with an odd one with velocity v_2, their velocities after the collision are

$$v_1' = \frac{(1-r)v_1 + 2rv_2}{(1+r)}, \qquad v_2' = \frac{2v_1 + (r-1)v_2}{(1+r)}. \tag{1}$$

Between two collisions, the particles propagate freely. Thus, a fast simulation algorithm is event driven: For each particle i, we remember its velocity, the time t_i of its last collision (initially, t_i is put to zero), and the position x_i it had at that time. In addition, we maintain a list of future collision times τ_i for each neighboring pair $(i, i+1)$ (here the walls are treated formally as particles with $v_0 = v_{N+1} = 0$, $x_0 = 0$, $x_{N+1} = N$). The system is evolved by searching the smallest τ_i, updating the triples (t_i, x_i, v_i) and $(t_{i+1}, x_{i+1}, v_{i+1})$, and calculating the new future collision times τ_{i-1} and τ_{i+1} (the new τ_i is infinite). Since the list $\{\tau_i\}$ is essentially a priority queue [16], we use for it the appropriate data structure of a *heap* [16]. Using heaps, searching for the next collision takes a CPU time $O(\ln N)$. In comparison, a naive search would take $O(N)$. This allowed us to make much larger simulations than in previous works. Our largest systems contained 16 383 particles and were followed for $> 10^{12}$ collisions. In spite of this, we had to start with carefully tailored initial configurations to keep transients short. When obtaining statistics, one should not forget that measurements should *not* be made after a fixed number of collisions, but at fixed intervals in real time. The correctness of the results and the absence of transients were checked by verifying that the energy density is constant, as proven in [14].

Before presenting results, let us discuss the expected dependence on the mass ratio r. For $r \to 1$, equilibration becomes slow (it takes a long time until a fast particle is slowed down to average speed), but perturbations propagate ballistically. Thus, a perturbation will be damped out slowly at first, but it will have no long time tails and is damped exponentially. In the other extreme, for $r \to \infty$ the light particles bounce between pairs of heavy ones which are hardly perturbed. Thus, if a heavy particle is perturbed, we have a situation very similar to the one for $r \to 1$. If a light particle is perturbed, its energy is soon given to its two nearest heavy neighbors, which then behave again as for $r \approx 1$. In contrast, in the intermediate region $1 \ll r \ll \infty$, we expect the perturbation to spread nonballistically for all times. It is in this regime that we expect the fastest convergence to asymptotic behavior, both with respect to time and to N.

In Fig. 1(a), we show κ, defined as total energy flux $J = \sum_i m_i v_i^3/2$ divided by ΔT, versus N, for four values of r. The value $r = 1.22$ is in the small-r region and was studied most intensively in [14]. The value $r = 2.62$ is near the center of the intermediate regime, while $r = 5$ is clearly above it. Finally, $r = 1.618 = (1+\sqrt{5})/2$ was chosen because it was used in [9], not because of its irrationality (problems with ergodicity related to rational values of r exist only for very small N [11,12]).

A power law would give a straight line with slope α in Fig. 1(a). None of the four curves is really straight. For small N the curve for $r = 1.22$ agrees perfectly with Fig. 3 of [14] (which extends only to $N = 1281$). It shows the strongest curvature (in agreement with the above discussion), and the small-N data alone would suggest a crossover to $\kappa = \text{const}$. But this curvature stops for large N and a closer look shows that the slope *increases* for $N > 8000$. The same is true also for the other curves: They all bend down for small N but veer up for larger systems [Fig. 1(b)]. This is most clearly seen for $r = 1.618$ and 2.62. It is less clear for $r = 5$, but the most rational expectation is that also this curve will have the same slope for $N \to \infty$. Our best estimate $\alpha = 0.32^{+0.03}_{-0.01}$ has asymmetric errors because we do not know how much more the curves will bend upwards for very large N.

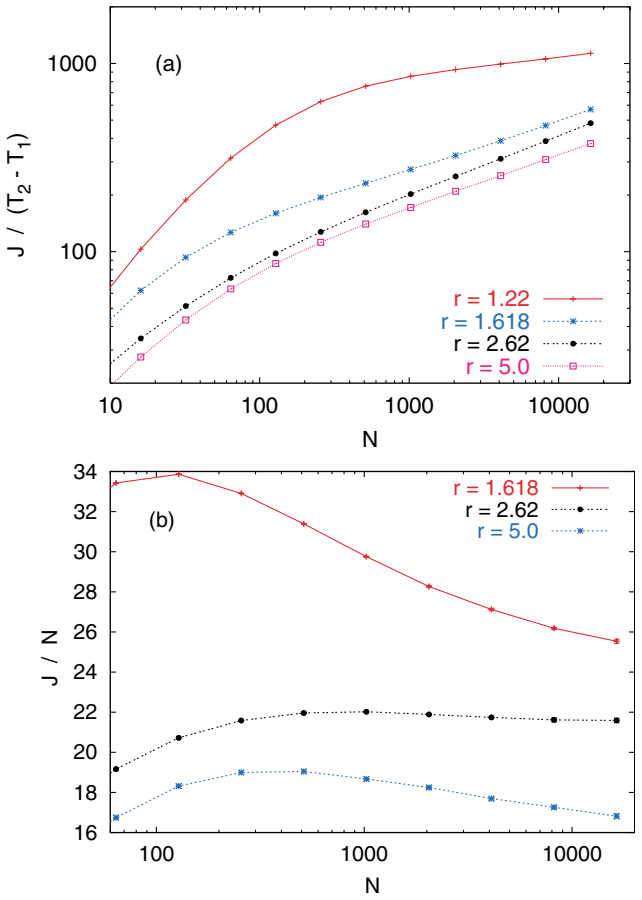

FIG. 1 (color). (a) Log-log plot of $J/(T_2 - T_1)$ versus N for four values of r. Statistical errors are always smaller than the data symbols. (b) Part of the same data divided by N^α with $\alpha = 0.32$, so the y axis is much expanded.

The rescaled temperature profiles for $r = 1.22$ are shown in Fig. 2. To verify the claim of [14] that $T(x)$ approaches the profile $T_k(x)$ predicted by kinetic theory with an inverse power of N, i.e., $T(x) - T_k(x) \sim N^{-0.67}$, we plot $T(x) - T_k(x)$ against x/N. For $N < 2000$, we see indeed this convergence in perfect agreement with [14], but not for $N > 2000$. Instead, it seems that $T(x) - T_k(x)$ remains different from zero for $N \to \infty$. The analogous results for $r = 1.618$ are shown in Fig. 3. In that case, the scaling observed in [14] is confined to very small N, not

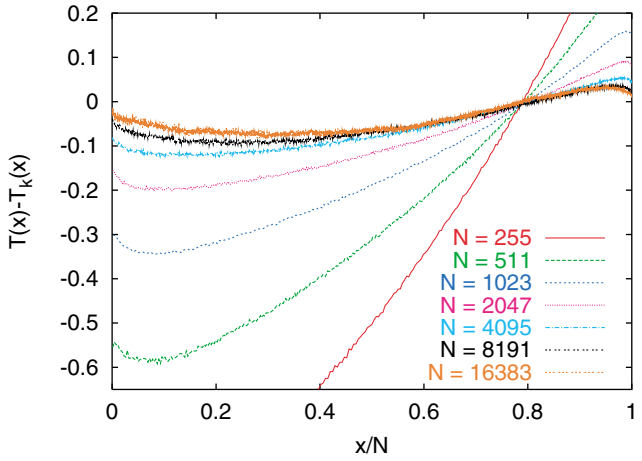

FIG. 2 (color). $T(x) - T_k(x)$ against x/N for $r = 1.22$, where $T_k(x) = [T_1^{2/3} - (T_1^{2/3} - T_2^{2/3})x/N]^{2/3}$ is the temperature profile according to kinetic theory. In order to reduce statistical fluctuations, we averaged in the curves for $N \geq 1023$ over three successive values of x.

shown in the figure. The fact that $T(x) - T_k(x)$ remains finite for $N \to \infty$ is now obvious. In contrast to a conjecture in [9], the temperature profile also does not become linear for large N. All results for $r = 1.618$ are qualitatively also true for $r = 2.62$ (not shown).

These results are easily understood. For $r = 1.22$, we are in the small-r regime. This explains the slow convergence of α with N and the weakness of long time tails, manifested in the agreement with kinetic theory. Only at very large N, we do see the correct asymptotics. For $r = 1.618$ and 2.62, we are no longer in this regime, the long time tails are stronger, and the disagreement with kinetic theory is more obvious.

In addition to systems driven by thermostats at different temperatures, we also studied systems in equilibrium with periodic boundary conditions. Here the Green-Kubo formula allows κ to be calculated from an integral over the heat current autocorrelation $\langle J(t)J(0)\rangle$ [4]. In Fig. 4 we show this, after suitable normalization and after multiplication by a power of t which makes it constant for large N and t. We see strong oscillations with periods $\propto N$ which reflect the dominance of (damped) sound waves with a fixed velocity of sound (see also [15]). They were mistaken for statistical fluctuations in [9], showing clearly that the simulations of [9] have not reached the asymptotic regime in contrast to what the authors assumed. Our data suggest that $\langle J(t)J(0)\rangle \sim t^{-0.66}$ for large N with a cutoff at $t \propto N$, giving $\alpha = 0.34$ in perfect agreement with our previous estimate.

A 1D hard-particle gas should be described macroscopically by hydrodynamics, i.e., by the Burgers, respectively, Kardar-Parisi-Zhang (KPZ), equation [17]. If we assume that heat diffusion scales similar to diffusion in KPZ, we might expect $\alpha = 1/3$ in agreement with our numerics. But we should warn that *particle* spreading in the 1D hard-particle gas is *not* superdiffusive (unpublished data; for $r = 1$ see [18]), so the relation with KPZ is not trivial.

It is easy to prove that the 1D hard-point gas is not chaotic in the usual sense. Consider an infinitesimal perturbation $v_i(t) \to v_i(t) + \delta v_i(t)$ and its weighted L_2 norm, $||\delta v(t)||_2 = \{\sum_{i=1}^N m_i(\delta v_i(t)]^2\}^{1/2}$. Since the $\delta v_i(t)$ change during a scattering according to the same Eq. (1) as the velocities $v_i(t)$ themselves, energy conservation leads to $||\delta v(t)||_2 \equiv 1$. Indeed the absence of chaos is quite obvious since there is no local instability. It seems to contradict a widespread folklore that dissipation and entropy production are tightly related to chaos (which sometimes is true; e.g., [19], page 231)—although it is also appreciated that this might not be always the case [20].

One solution to this puzzle is the observation [21], going back to work by Wolfram on cellular automata [22], that the notion of chaos in systems with infinitely many degrees of freedom is ambiguous and is not necessarily related to any *local* instability. In a spatially extended system, it makes perfect sense to use a norm

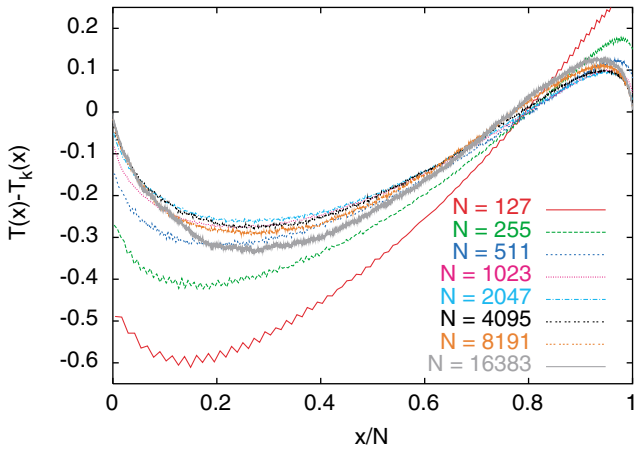

FIG. 3 (color). $T(x) - T_k(x)$ against x/N for $r = 1.618$.

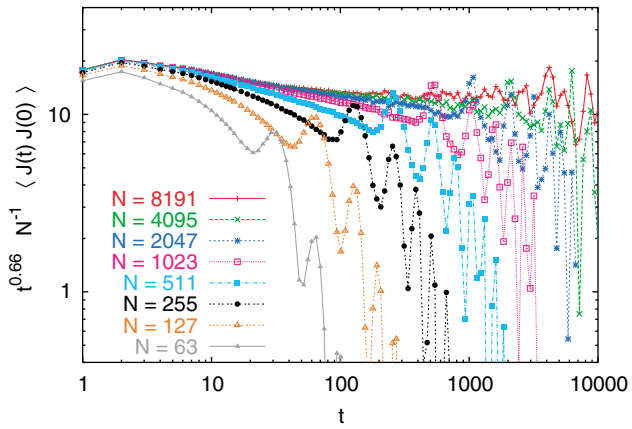

FIG. 4 (color). Total heat current autocorrelation, $t^{0.66}N^{-1}\langle J(t)J(0)\rangle$ for $r = 2.2$ and $T = 2$. Total momentum is $P = 0$.

which, in contrast to the L_2 norm used above, puts most weight on nearby regions and exponentially little weight on far-away regions. With such a definition, the norm of a perturbation moving towards (away from) the observer with constant velocity will increase (decrease) exponentially. More generally, also perturbations spreading diffusively will lead to an increase of the uncertainty about the local state for a short-sighted observer. For the 1D hard-point gas, this means that there is no need for any local instability to generate dissipation, local thermal equilibrium, and mixing. In a nonequilibrium case, entropy *flow* is provided by the stochastic thermostats at the ends, while (coarse-grained) entropy is *produced* by the diffusive propagation of perturbations.

In summary, we have given compelling evidence that heat conduction in the 1D hard-point gas shows the anomalous divergence with system size expected for any generic 1D system, in spite of strong finite-size and finite-time effects. This "normal" anomalous behavior holds in spite of the fact that the system is not chaotic in the usual sense, proving again that chaos in the form of local instabilities is not needed for mixing behavior and dissipation. Finally, we have discussed a possible connection to KPZ scaling.

We are indebted to Roberto Livi and Antonio Politi for very helpful correspondence. W. N. is supported by the DFG, Sonderforschungsbereich 237. P. G. thanks Henk van Beijeren and Tomaz Prosen for discussions.

Note added.—A careful study of 1D hydrodynamics [23] shows indeed that $\alpha = 1/3$ as conjectured in the present paper.

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