

Anomalous Fourier’s Law and Long Range Correlations in a 1D Non-momentum Conserving Mechanical Model

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Received: 22 July 2010 / Accepted: 11 October 2010 / Published online: 2 November 2010
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Abstract We study by means of numerical simulations the velocity reversal model, a one-dimensional mechanical model of heat transport introduced in 1985 by Ianiro and Lebowitz. Our numerical results indicate that this model, which does not conserve momentum, exhibits nevertheless an anomalous Fourier’s law similar to the ones previously observed in momentum-conserving models. This disagrees with what can be expected by solving the Boltzmann equation (BE) for this system. The pair correlation velocity field also looks very different from the correlations usually seen in diffusive systems, and shares some similarity with those of momentum-conserving heat transport models.

Keywords Current · Anomalous Fourier law · Hard particle gas

Introduction

Understanding the steady state of a system in contact with two heat baths at unequal temperatures is a central question in the theory of non-equilibrium systems [1]. With very few exceptions (such as zero range processes [2, 3]), non-equilibrium systems exhibit long range correlations in their steady state. These correlations have been studied theoretically by various approaches and measured experimentally [4–8].

For a one dimensional diffusive system of size L , for instance a stochastic lattice gas, these long range correlations take the following scaling form [4, 9–11]:

$$\langle A(r_1)A(r_2) \dots A(r_n) \rangle_c = \frac{1}{L^{n-1}} F_n \left(\frac{r_1}{L}, \dots, \frac{r_n}{L} \right), \quad (1)$$

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(where $A(r)$ is an observable at position r such as the density or the energy) when the distances between the positions r_i are macroscopic (i.e. $L \sim |r_i - r_j| \gg 1$).

The macroscopic fluctuation theory developed by Bertini et al. [12, 13] allows one to write down the general equations satisfied by the scaling functions F_n [9]. These partial differential equations are usually difficult to solve. The expressions of the F_n are however known in a number of examples [4, 14, 15], where they have been obtained either from exact solutions of microscopic models or by integrating the partial differential equations derived from the macroscopic fluctuation theory. Diffusive systems are also known to satisfy Fourier's law, meaning that, for large system sizes, the steady state flux $\langle J \rangle$ of energy through a system of size L scales like L^{-1} :

$$\langle J_L \rangle = \frac{1}{L} G(T_a, T_b), \quad (2)$$

where $G(T_a, T_b)$ is a function of the temperatures T_a and T_b of the heat baths at the two extremities of the system, which maintain it out of equilibrium; the function $G(T_a, T_b)$ vanishes linearly with the difference $T_a - T_b$ so that the flux becomes proportional to the temperature gradient.

Over the last 15 years [16–24] it has been realized on the basis of numerical simulations that one-dimensional mechanical systems which conserve momentum do not satisfy Fourier's law. Instead, they exhibit a power law decay, called anomalous Fourier's law, of the average flux J with system size:

$$\langle J_L \rangle = L^{\alpha-1} G(T_a, T_b). \quad (3)$$

So far, the exponent α has not been determined analytically for any microscopic model with non-quadratic interactions; however, numerical [25, 26] and analytic [19, 27–29] calculations, based on mode coupling theory or on other approaches [30, 31], indicate that, depending on the type of the non-linearities and on the accuracy of the simulations, α can take values ranging between 0.2 and 0.5. The main two systems for which this anomalous heat conduction has been observed are:

- the Fermi-Pasta-Ulam model, a chain of N harmonic oscillators with an additional cubic (FPU- α) or quartic (FPU- β) interaction potential [16, 31, 32]. For the latter case, most estimates indicate that $\alpha \sim 0.4$;
- a one-dimensional gas of N hard point particles with elastic collisions [26] (when the particles are identical, the collisions simply exchange the velocities of the incoming particles: hence the system has the same transport properties as an ideal gas, i.e. a ballistic transport with $\alpha = 1$). For the collisions to be non-trivial, one choice is to consider particles of alternating masses 1 and $m_2 \neq 1$ (2-mass model). In this case, it is commonly found that $\alpha \sim 0.33$ [25].

In comparison with diffusive systems, for which (2) holds, the main feature of these models is that their dynamics conserve momentum, and it is believed that this property plays a key role in the divergence of the heat conductivity. Note, however, that there is no proof for this behavior.

In this article, we consider a simpler model originally introduced in [33], the velocity reversal model, in order to better understand which features could be at the origin of the anomaly. This model consists of N particles (labelled by $i = 1, \dots, N$ from left to right) which, as in a 1D hard-particle gas, move freely between collisions. The collisions are, however, not elastic, but instead are given by the following simple rule:

- when two particles collide with velocities of opposite signs, $v_{i+1} < 0 < v_i$, their two velocities get reversed ($v_i \rightarrow -v_i, v_{i+1} \rightarrow -v_{i+1}$ at the collision);
- when they collide with velocities of the same sign, the particles simply pass each other, exchanging their velocities ($v_i \rightarrow v_{i+1}$ and $v_{i+1} \rightarrow v_i$).

In contrast with the Fermi-Pasta-Ulam chain and the hard-particle gas, these dynamics do not conserve momentum. It should be noted, however, that the absolute values of the velocities themselves are conserved, leading in general to more conserved quantities than in standard momentum-conserving models. One should also note that, when the velocities are reversed at independent exponential times instead of at collisions, the system becomes diffusive [33].

Here, the N particles of the velocity reversal model are in a one-dimensional box of length $L = N$ between two boundaries which play the role of heat baths. Whenever a particle hits a boundary, its velocity is changed as if the particle was reinjected instantaneously, with its velocity thermalized by the reservoir. The reservoirs are thus described by the velocity p.d.f. of these “reinjected particles”, $\rho_a(v)$ and $\rho_b(v)$. An obvious choice is to consider Maxwellian reservoirs at temperatures T_a and T_b , with velocity densities

$$\rho_a(v) = \theta(v) \frac{v}{T_a} e^{-\frac{v^2}{2T_a}} \quad \text{and} \quad \rho_b(v) = \theta(-v) \frac{|v|}{T_b} e^{-\frac{v^2}{2T_b}}, \quad \text{with } \theta(v) = \begin{cases} 1 & \text{for } v > 0 \\ 0 & \text{for } v \leq 0 \end{cases}. \tag{4}$$

We will study below this “Maxwellian case” for $T_a = 4$ and $T_b = 1$. For a system which thermalizes well, one would expect other choices of these reservoir velocity densities to only affect small regions near the boundaries, but not to influence the macroscopic behavior of the system. For the velocity reversal model, however, the conservation of the absolute values of the particle velocities prevents thermalization from taking place: for instance, one can easily see that, for another choice of reservoirs, where particles are always reinjected with velocities v_a from the left reservoir and v_b for the right reservoir,

$$\rho_a(v) = \delta(v - v_a) \quad \text{and} \quad \rho_b(v) = \delta(v + v_b), \tag{5}$$

the only possible velocities inside the system are $\pm v_a$ and $\pm v_b$. We will study this “two-speed case” with $v_a = 2$ and $v_b = 1$.

In a first part, we show, by studying the steady-state current of systems with $125 \leq N \leq 8000$ particles, that, both in the Maxwellian and the two-speed case, the velocity-reversal model exhibits anomalous Fourier’s law, in contrast to the prediction of the associated Boltzmann equation [33].

We then present, in a second part, measurements of the steady-state correlation functions of the momentum density for Maxwellian and two-speed systems of $100 \leq N \leq 400$ particles, as well as for a 2-mass hard-particle gas with $m_1 = 1$ and $m_2 = 1.6$ for comparison: they indicate a size dependence very different from (1), with an anomalous decay of the long-range correlations in a mesoscopic region.

1 Anomalous Fourier’s Law for the Velocity Reversal Model

The main advantage of the velocity reversal model described above, compared to the hard-particle gas for instance, is that its associated Boltzmann equation can be solved analytically, thanks to the simpler form of its collision term. By solving this Boltzmann equation in the steady state with the appropriate boundary conditions, the average current between the

reservoirs can be predicted, as done in [33]. The simplest case is the two-speed system (5) with velocities v_a and v_b , for which the Boltzmann equation relates the four densities $f_{\pm a}(x, t)$ and $f_{\pm b}(x, t)$ of the particles with respective velocities $\pm v_a$ and $\pm v_b$, with $0 \leq x \leq L = N$ the space coordinate:

$$\begin{cases} (\partial_t + v_a \partial_x) f_{+a} = (v_a + v_b)(f_{+b} f_{-a} - f_{-b} f_{+a}) \equiv A(x, t), \\ (\partial_t - v_a \partial_x) f_{-a} = -A(x, t), \\ (\partial_t + v_b \partial_x) f_{+b} = -A(x, t), \\ (\partial_t - v_b \partial_x) f_{-b} = A(x, t). \end{cases}$$

Setting the time derivatives to 0, these equations can be solved [33] to determine the steady state of the two-speed system:

$$\begin{cases} f_{+a}(x) = \frac{v_b}{v_a + v_b} \left(1 - x + \frac{x}{N+1}\right), \\ f_{-a}(x) = \frac{v_b}{v_a + v_b} \frac{N}{N+1} (1 - x), \\ f_{+b}(x) = \frac{v_a}{v_a + v_b} \frac{N}{N+1} x, \\ f_{-b}(x) = \frac{v_a}{v_a + v_b} \left(x + \frac{1-x}{N+1}\right), \end{cases}$$

yielding linear profiles for the four densities as well as a steady-state current $J = \frac{v_a v_b (v_a - v_b)}{2(N+1)}$ satisfying Fourier’s law (2). By a similar calculation, the Boltzmann equation predicts that the energy current will satisfy Fourier’s law in the Maxwellian case.

We studied numerically the Maxwellian (4) and the two-speed (5) velocity reversal models for $125 \leq N \leq 8000$ particles, with $T_a = 4, T_b = 1$ in the first case and $v_a = 2, v_b = 1$ in the second. Because the true steady state is unknown, our measurements were performed by starting the system in an equilibrium configuration at $T = 2$ in the Maxwellian case, and by choosing the velocity of each particle to be $\pm v_a$ or $\pm v_b$ with equal probabilities in the two-speed case.

We then let the system evolve from that initial state, and sampled the time evolution of $J_N, \rho_N(x)$ and $E_N(x)$: J_N was measured by a time average of the instantaneous energy flux, $J_N = \frac{1}{2N} \sum_{i=1}^N v_i^3$, while $\rho_N(x)$ and $E_N(x)$ were measured by counting the particles and energy within the boxes $k \leq x < k + 1$ for $k = 0, \dots, N - 1$. We considered our measurements to have reached their steady state values when they remained stable for the last 80% of the total simulation time t : this was reached for t varying between $2 \cdot 10^6$ (for $N = 125$) and $4 \cdot 10^7$ (for $N = 8 \cdot 10^3$).

As shown in Fig. 1, our data indicate that J_N decreases like a power law of N for both choices of reservoirs for the system sizes we considered. They are consistent with (3), with $\alpha \sim 0.3$ for the Maxwellian reservoirs and $\alpha \sim 0.4$ for the two-speed reservoirs. In the latter case, the density and energy profiles $\rho_N(x)$ and $E_N(x)$ shown in Fig. 2 also differ noticeably from the linear profiles predicted by the Boltzmann approach, at least for the sizes we were able to study.

2 Long-Range Correlations in Anomalous Systems

The main assumption in the derivation of the Boltzmann equation is that there are no correlations between the velocities of particles entering a collision in which their velocities are reversed. As it fails to predict the anomalous Fourier’s law observed in Fig. 1, it is interesting to investigate the form of the steady-state correlations for the velocity reversal model.

Fig. 1 Steady-state energy current J_N for the velocity-reversal model with $125 \leq N \leq 8000$ particles, in the Maxwellian case with $T_a = 4$ and $T_b = 1$ (left) and in the two-speed case with $v_a = 2$ and $v_b = 1$ (right). In both cases, the current decreases as a non-integer power of the system size: over the range of sizes we considered, our data are well-fitted by $J_N \propto N^{-0.69}$ in the Maxwellian case and $J_N \propto N^{-0.60}$ in the two-speed case

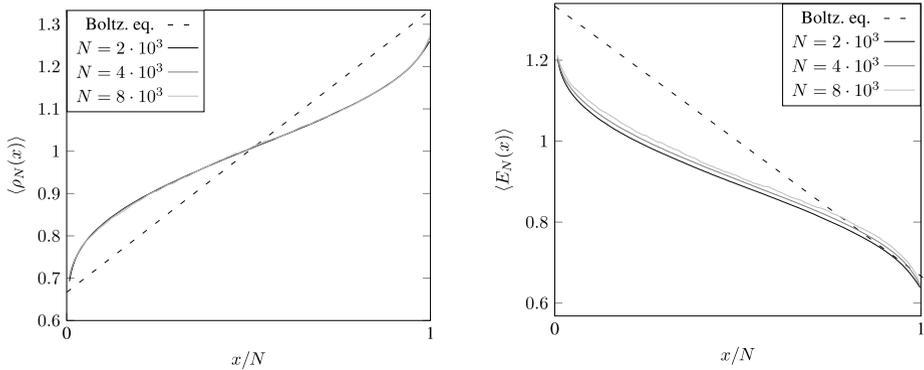
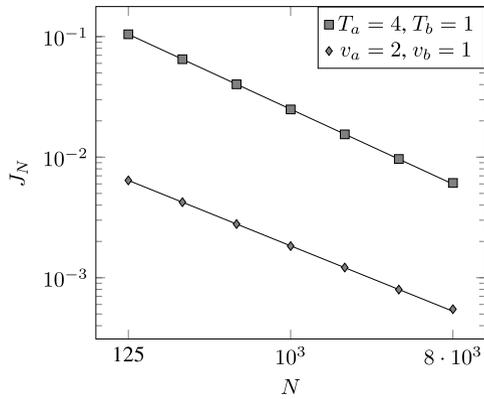


Fig. 2 Average density (left) and energy (right) profiles for the two-speed velocity reversal model between reservoirs for $v_a = 2$ and $v_b = 1$ and for system sizes $N = 2 \cdot 10^3, 4 \cdot 10^3$ and $8 \cdot 10^3$ (continuous lines). According to the Boltzmann equation, these profiles (given by $f_{+a} + f_{-a} + f_{+b} + f_{-b}$ and $\frac{v_a^2}{2}(f_{+a} + f_{-a}) + \frac{v_b^2}{2}(f_{+b} + f_{-b})$ respectively) should be linear in x (dashed lines)

We measured numerically the steady-state two-point correlation functions of the momentum field, $\langle p(x)p(y) \rangle_c$, for the velocity reversal model in the Maxwellian (Fig. 3) and in the two-speed (Fig. 4) cases, for systems of 100, 200 and 400 particles.

As in the previous section, we approximated the momentum density function $p_N(x)$ by its discretization over the boxes $k \leq x < k + 1$ for $0 \leq k < N$. We took the stationary-state correlations $\langle p(x)p(y) \rangle_c$, which we measured for $y = \frac{N}{4}$ and $y = \frac{3N}{4}$, to be the long-time limits of their time evolutions for a system started in the arbitrary initial state described in the previous section. In the following figures, the variances $\langle p(y)^2 \rangle_c$ were omitted, as they would be much larger than the off-diagonal correlations shown here.

For diffusive systems, one would expect $\langle p(x)p(y) \rangle_c$ to follow a scaling of the form (1): $\langle p(x)p(y) \rangle_c = \frac{1}{N} F_2(\frac{x}{N}, \frac{y}{N})$, except for $x = y$ with a variance $\langle p(x)^2 \rangle_c$ of order 1. For the velocity reversal models of Figs. 3 and 4, we observed $\langle p(x)^2 \rangle_c$ to be of order 1: however, when measuring $\langle p(x)p(y) \rangle_c$ for $y = N/4$ and $y = 3N/4$, as in Figs. 3 and 4, we observed an additional anomalous growth in $\langle p(x)p(y) \rangle_c$ for x close to y in a region growing with system size, but becoming narrower on a macroscopic scale.

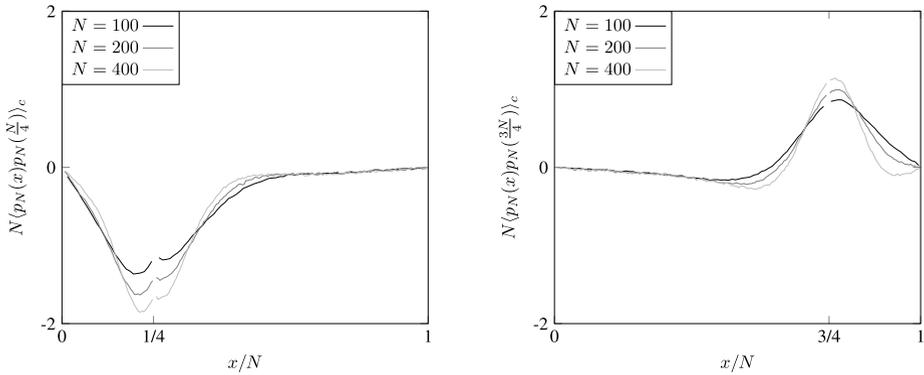


Fig. 3 Two-point correlation function $\langle p(x)p(y) \rangle_c$ of the momentum field $p_N(x)$ for the velocity reversal model in the Maxwellian case (4) with $T_a = 4$ and $T_b = 1$, for $y = \frac{N}{4}$ (left) and $y = \frac{3N}{4}$ (right)

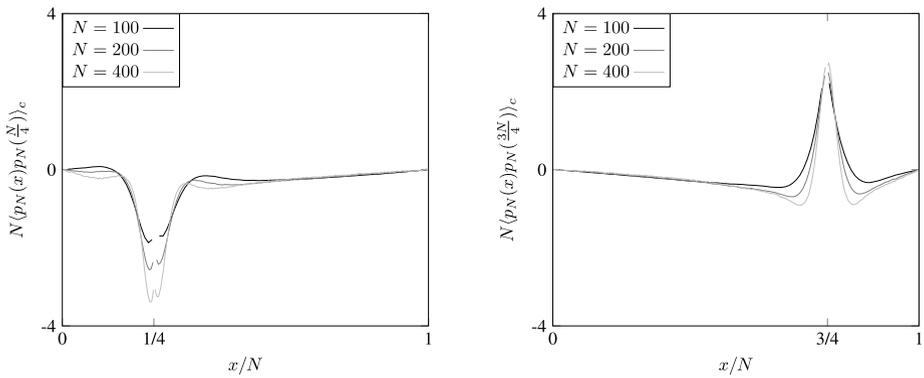


Fig. 4 Two-point correlation function $\langle p(x)p(y) \rangle_c$ of the momentum field $p_N(x)$ for the velocity reversal model in the two-speed case (5) with $v_a = 2$ and $v_b = 1$, for $y = \frac{N}{4}$ (left) and $y = \frac{3N}{4}$ (right)

The sign of $\langle p(x)p(y) \rangle_c$ seems to be always negative for y closer to the left (warmer) reservoir and positive for y closer to the right, colder reservoir. As shown in Figs. 3 and 4, where our data are multiplied by the system size N , the correlations seem to decay slower than $1/N$ as N grows, over a region which seems to grow slower than the system size.

In order to compare the behavior of these models with those of usual momentum-conserving models, we also measured the two-point correlation function of the momentum for a hard-particle gas of particles of alternating masses 1 and $m_2 = 1.6$ between Maxwellian reservoirs at $T_a = 4$ and $T_b = 1$: we observed a similar growth of the correlation functions at intermediate scales (Fig. 5).

For this hard-particle gas (Fig. 5), due to a faster relaxation to the steady state, we were able to simulate much larger system sizes than for the velocity reversal model: at these sizes, $10^3 \leq N \leq 4 \cdot 10^3$, the anomalous growth of $\langle p_N(x)p_N(y) \rangle_c$ of Fig. 4 is compatible with a scaling of the form

$$\langle p_N(x)p_N(y) \rangle_c \propto \frac{1}{N^\beta} F_2 \left(\frac{x-y}{N^\beta} \right), \tag{6}$$

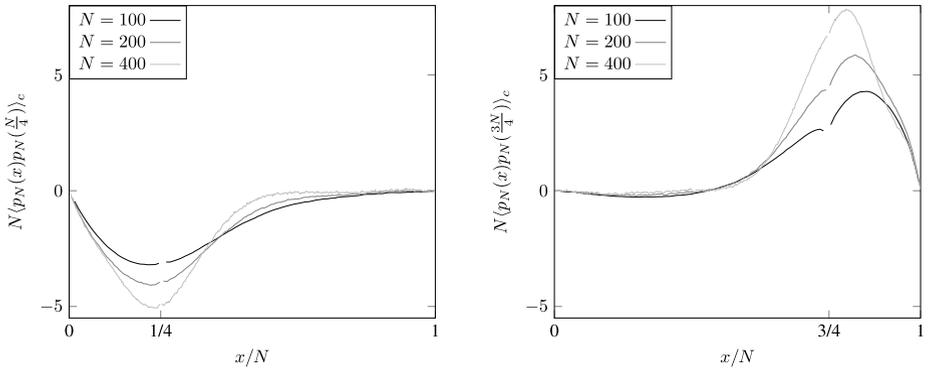


Fig. 5 Two-point function $\langle p(x)p(y) \rangle_c$ of the momentum field $p_N(x)$ for the 2-mass hard-particle gas with $m_2 = 1.6$ between reservoirs at $T_a = 4$ and $T_b = 1$, for $y = \frac{N}{4}$ (left) and $y = \frac{3N}{4}$ (right)

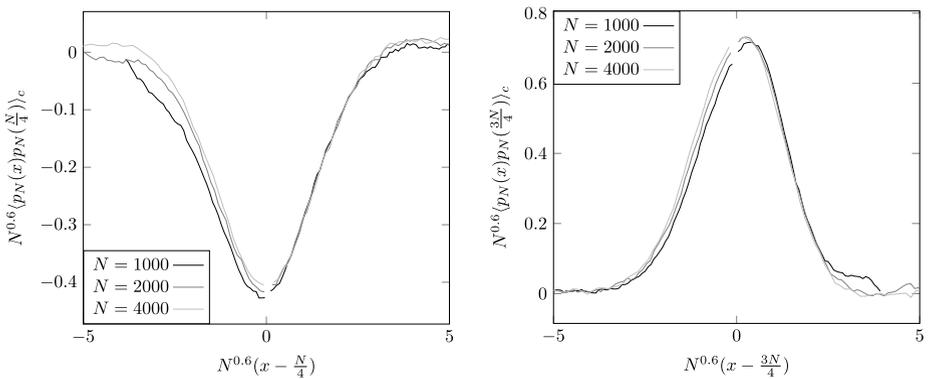


Fig. 6 Rescaling of the two-point function of the momentum field $\langle p_N(x)p_N(y) \rangle_c$, for $y = \frac{N}{4}$ (left) and $y = \frac{3N}{4}$ (right), for the 2-mass hard particle gas with $m_2 = 1.6$ between reservoirs at temperatures $T_a = 4$ and $T_b = 1$

with $\beta = 0.6$, as shown in Fig. 6. At the sizes we could reach for the velocity reversal models, the Maxwellian case of Fig. 3 seems to satisfy a similar scaling form with $\beta = 0.8$. Our data for the two-speed case, however, does not exhibit such a clear scaling.

For the velocity-reversal model as well as for the 2-mass hard particle gas, we also measured the correlations of the energy field $E_N(x)$, which exhibited a behavior very similar to the one shown above for the momentum field.

Conclusion

The numerical simulations presented in this work show that the velocity-reversal model exhibits an anomalous Fourier’s law, although it does not conserve momentum. Its density and energy profiles (Fig. 2) differ noticeably from those predicted by the Boltzmann equations. For the sizes we could achieve, however, they have not yet converged: this might question whether our data showing the anomalous Fourier’s law (Fig. 1) correspond to the asymptotic regime.

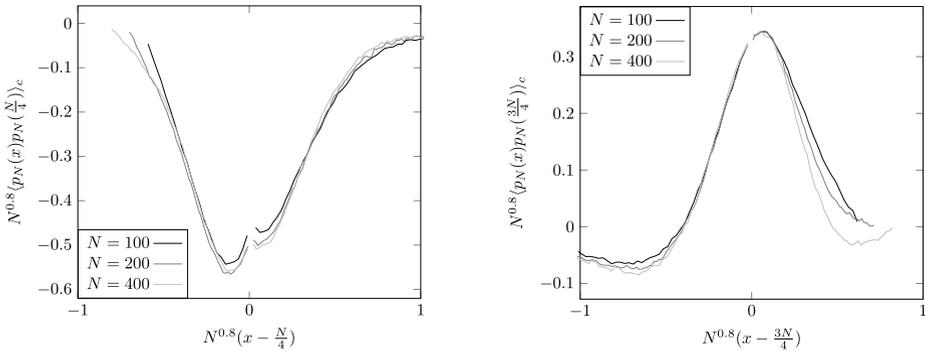


Fig. 7 Rescaling of the two-point correlation function $\langle p(x)p(y) \rangle_c$ of the momentum field $p_N(x)$ for the velocity reversal model in the Maxwellian case (4) with $T_a = 4$ and $T_b = 1$, for $y = \frac{N}{4}$ (left) and $y = \frac{3N}{4}$ (right)

Within the system sizes we could reach, the two-point function of the momentum also looks very different from those of diffusive systems: they seem to be concentrated on a mesoscopic scale, much larger than the microscopic scale, but smaller than the system size. Within this mesoscopic region, the decay of the correlations seems to be anomalous as well, i.e. it seems to be a non-integer power of the system size.

We have checked that the pair correlations seem to have a rather similar behavior for the 2-mass hard particle gas; they are also similar to those derived for an exactly solvable case [34, 35], a chain of harmonic oscillators with random exchange of momentum between nearest neighbors.

This leads us to believe that the shape of the correlation functions we have observed is probably another signature of the anomalous Fourier's law: it would therefore be interesting to see whether these anomalous correlations are also present for all other models known to exhibit an anomalous heat conductivity, such as the Fermi-Pasta-Ulam chain.

Looking at higher-order correlations would require major numerical efforts. They would however be very interesting to measure in order to guess what would replace (1) for systems exhibiting anomalous Fourier's law.

The present work is purely numerical in nature. It would of course be very interesting to see what the existing theories explaining the anomalous Fourier's law would predict for the pair correlation functions we have measured. For diffusive systems, the scaling (1) of the correlations with system size is closely linked to the scaling form of the large deviation function of the system's density profile [9, 11]: what such a large deviation function would look like for systems exhibiting anomalous Fourier's law is also an interesting open issue.

Acknowledgements We would like to thank J. Lukkarinen, H. Spohn, and H. van Beijeren for useful discussions. J.L. thanks the IHES and the IHP for their hospitality during this work. The work of J.L. was supported by NSF grant DMR-044-2066 and by AFOSR grant AF-FA9550-10.

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