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Fluctuations of the heat flux of a one-dimensional hard particle gas

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Abstract – Momentum-conserving one-dimensional models are known to exhibit anomalous Fourier's law, with a thermal conductivity varying as a power law of the system size. Here we measure, by numerical simulations, several cumulants of the heat flux of a one-dimensional hard particle gas. We find that the cumulants, like the conductivity, vary as power laws of the system size. Our results also indicate that cumulants higher than the second follow different power laws when one compares the ring geometry at equilibrium and the linear case in contact with two heat baths (at equal or unequal temperatures).

Understanding the fluctuations of the flux of heat or of the current of particles through systems in their steady state is a central question in non-equilibrium statistical mechanics. Since the discovery of the fluctuation theorem [1–6], one knows that the probability distribution of these fluctuations has some symmetry properties related to time-reversal symmetry. In most cases, the calculation of this distribution for a given microscopic model remains, however, a challenging issue.

Over the last few years, several exact expressions for the distribution of these fluctuations have nevertheless been obtained for diffusive systems, such as lattice gases [7–14] (for instance the one-dimensional symmetric simple exclusion process). For diffusive systems in their steady state, in the two geometries of fig. 1 (the ring geometry in equilibrium at temperature T and the open system, *i.e.* a finite system in contact with two heat baths at temperatures T_a and T_b), the cumulants $\langle Q_t^n\rangle_c$ of the flux of energy Q_t during a long time t take, for a large system size L, the following form:

$$\begin{cases} \lim_{t\to\infty} \frac{1}{t}\langle Q_t^2\rangle^{\text{ring}} & \simeq \frac{1}{L}A(T), \\ \lim_{t\to\infty} \frac{1}{t}\langle Q_t^{2n}\rangle_c^{\text{ring}} & \simeq \frac{1}{L^2}B_n(T), \\ \lim_{t\to\infty} \frac{1}{t}\langle Q_t^{n}\rangle_c^{\text{open}} & \simeq \frac{1}{L}C_n(T_a,T_b). \end{cases} \tag{1}$$

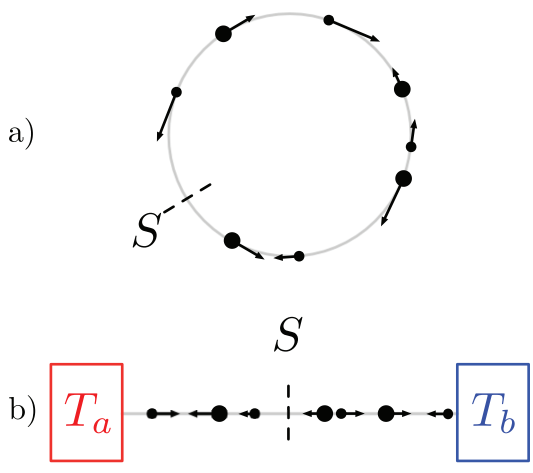

Fig. 1: (Colour on-line) We measure the cumulants of the integrated current Q_t of a one-dimensional hard particle gas with alternating masses 1 and $m_2>1$: a) for an even number of particles on a ring; b) for an odd number of particles in contact with two heat baths (open system). In our simulation, we measure the flux Q_t through a section S, located anywhere on the ring in a) and half-way between the two heat baths in b); we also measure the flux $\overline{Q}_t$ averaged over the whole system.

For the ring geometry (fig. 1a)), explicit expressions of the prefactors $A(T)$ and $B_n(T)$ have been obtained for the symmetric simple exclusion process, as well as for

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generic diffusive systems with one conserved quantity [10]. For the open case (fig. 1b)), the amplitudes $C_n(T_a, T_b)$ are also known for the one-dimensional symmetric exclusion process [7–9] (with expressions identical to those which had been previously determined for disordered one-dimensional conductors [15,16]); they are also known for generic diffusive systems with one conserved quantity [11–14,17–19].

The $1/L$-dependence of $\langle Q_t\rangle^{\text{open}}/t$ for the open case means that diffusive systems satisfy Fourier's law [20]. Together with the fluctuation-dissipation theorem, Fourier's law also implies the $1/L$ decay of $\langle Q_t^2\rangle^{\text{ring}}/t$ (or of $\langle Q_t^2\rangle^{\text{open}}/t$ for $T_a = T_b$).

It is remarkable that the L-dependence (1) of *all* the cumulants is generic for diffusive systems, with a few exceptions where some prefactors may vanish and the decay with L is faster [10]. All these L dependencies follow from the fact that, for large diffusive systems, local equilibrium holds and can be treated within the *macrosopic fluctuation theory* (MFT), a theory of diffusive systems which allows one to calculate explicitly a number of properties of non-equilibrium steady states [21–25]. For systems with more than one conserved quantity, much less has been done so far concerning the cumulants of the current but, as long as the system is diffusive, one expects, from the MFT, the same L dependencies of the cumulants as in (1).

Momentum-conserving systems in one dimension are known to exhibit anomalous Fourier's law [26–32], with an average current varying as a non-trivial power law of the system size L:

$$\lim_{t\to\infty} \frac{1}{t}\langle Q_t\rangle^{\text{open}} \sim L^{\alpha-1} C_1(T_a, T_b). \tag{2}$$

The exponent α is not easy to determine [33–37]. It seems to vary with the systems studied; even for a given system, numerical simulations or theoretical approaches do not always agree. The current consensus is that several universality classes exist depending on the nature of the non-linearity of the forces between the atoms [38,39].

As major numerical efforts have been already done to determine the exponent α, our goal here is to present numerical simulations, not to determine α more accurately, but rather to look at the L-dependence of higher cumulants of Q_t.

The numerical determination of the higher cumulants of Q_t requires much better statistics than the lower ones. This is why the system sizes for which we could obtain reliable data are significantly smaller than those which have been studied previously for the thermal conductivity, despite the fact that we used the same efficient algorithm as in [35].

Measurement of the cumulants for the hard particle gas. – The system we have decided to simulate is a one-dimensional gas [33,35,40,41] of point particles with hard-core interactions. It was mainly chosen for its simple dynamics: masses follow ballistic motions between successive collisions, which are elastic. If the particles were all of equal masses, the velocities of colliding particles would simply be exchanged, and the transport of energy would be the same as for an ideal gas; this is why, as in previous studies of hard particle gases, we chose here a two-mass system, with alternating particles of masses 1 and m_2.

For the ring geometry, we consider an even number N of masses on a circle of length $L = N$, initially in microcanonical equilibrium at fixed energy $E = N$ and zero total momentum: the total energy and the momentum remain of course conserved by the dynamics.

For the open case in contact with two heat baths at unequal (or equal) temperatures, we take an odd number N of particles in a one-dimensional box of size $L = N$, and we choose the particles closest to the boundaries to be of mass 1. The heat baths at these boundaries are implemented in the following way: whenever a particle hits a boundary, it is reflected as if a thermalized particle was entering the system from the bath, so that the total number of particles in the system remains N.

As the steady state is in general not known in the open case, we started our first sample with an initial condition chosen at random; then, the initial configuration of each new sample was taken to be the final configuration of the previous sample. Therefore, apart from transient effects affecting the first samples (which represent a very small fraction of the total), the initial configurations of our samples are typical of steady-state configurations.

Through any section of our system, the flux of energy Q_t is the algebraic sum of the kinetic energies of the particles crossing the section S during a time interval t. In the steady state, the statistical properties of Q_t depend on where the section is located (at least in the open geometry). On the other hand, one expects (under the assumption that the internal energy cannot grow indefinitely) that the long-time limit of the ratios $\langle Q_t^n\rangle_c/t$ are independent of where Q_t is measured. In our simulations, we measure for the same samples the flux of energy Q_t through a fixed section S located at position $L/2$ in the open geometry (and anywhere on the ring geometry) and its integrated value $\overline{Q}_t$ averaged over the whole system.

As shown in fig. 2a), the cumulants obtained from these two measurements behave differently at finite time, but both exhibit a linear growth for large t. Figure 2b) shows that, when the ratios $\langle Q_t^2\rangle_c/t$ are plotted *vs.* $1/t$, the two sets of data converge to a common value in the long-time limit. This was the case for all the cumulants we were able to measure: for all the results shown below, the procedure of fig. 2b) was used to estimate the asymptotic values of the cumulants $\langle Q_t^n\rangle_c/t$.

The $1/t$ convergence of fig. 2b) can easily be understood. For a finite system of size L, the correlation function $\langle J(t_1)J(t_2)\rangle_c = f(t_2 - t_1)$ of the energy current $J(t) = \partial_t Q_t$, decays like a power law until a cut-off time τ_L

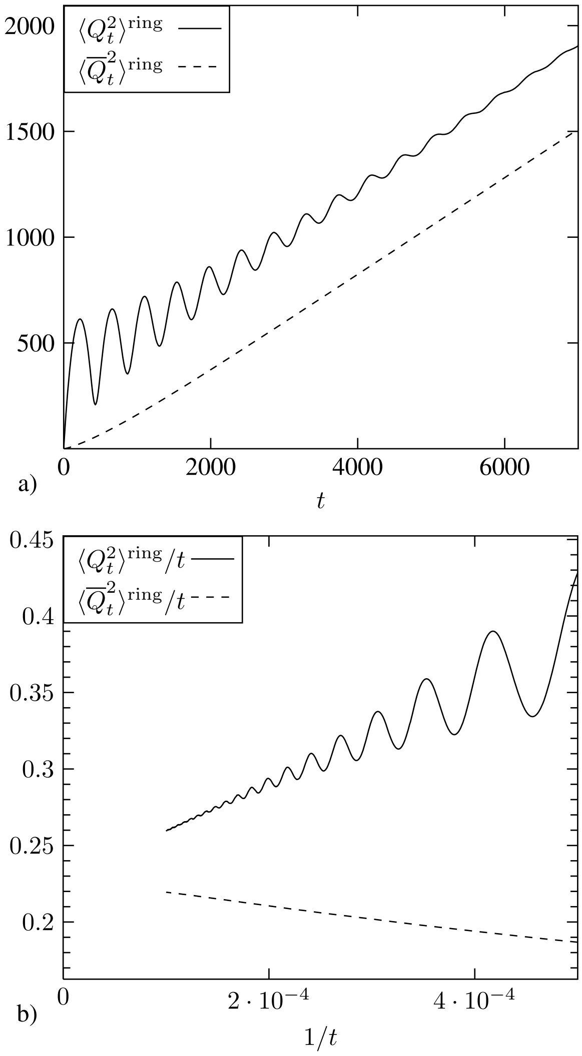

Fig. 2: Second cumulant of the energy flux through a section, Q_t, and of its space average, $\overline{Q}_t$, on a ring of $N = 800$ particles (a). When plotted as functions of $1/t$ (b), the two ratios $\langle Q_t^2 \rangle / t$ converge, when $t \to \infty$, to a common value $\simeq 0.23$. We took advantage of this expected $1/t$ convergence (see text) to obtain the limits $\lim\limits_{t\to\infty} \langle Q_t^n \rangle_c / t = \lim\limits_{t\to\infty} \langle \overline{Q}_t^n \rangle_c / t$.

which increases with L: for $t_2 - t_1 > \tau_L$, the decay is much faster (see, for instance, [35], fig. 4), so that $\int_0^\infty f(\tau)\,\mathrm{d}\tau$ and $\int_0^\infty \tau f(\tau)\,\mathrm{d}\tau$ are finite. Therefore, when $t \gg \tau_L$, $\langle Q_t^2 \rangle_c = \int\int_0^t \mathrm{d}t_1\,\mathrm{d}t_2 \langle J(t_1) J(t_2) \rangle_c = 2t \int_0^t f(\tau)\,\mathrm{d}\tau - 2\int_0^t \tau f(\tau)\,\mathrm{d}\tau$ becomes of the form $At + B$ so that $\langle Q_t^2 \rangle_c / t \sim A + B/t$. In the case of fig. 2, we estimated $\tau_L \sim 10^3$ and measured Q_t up to $t = 10^4$: the $1/t$ behavior can be observed well for $t \geqslant 5 \cdot 10^3$ or so.

Remark: all the cumulants we could measure grow linearly with time for large t. On the ring geometry, this growth was only observed when performing microcanonical sampling at fixed total energy E and momentum P (we chose $E = N$ and $P = 0$ for all our initial conditions). When E is allowed to fluctuate (canonical ensemble) while keeping $P = 0$, the cumulants exhibit a faster growth ($\langle Q_t^{2n} \rangle_c^{\text{can.}} \sim t^n$).

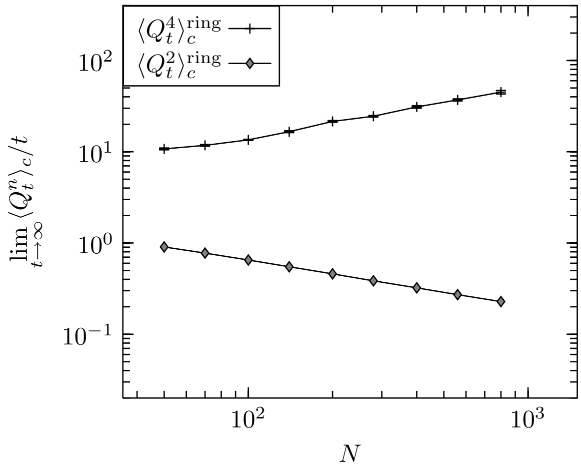

Fig. 3: Asymptotic values of $\langle Q_t^n \rangle_c / t$ on a ring of $50 \leqslant N \leqslant 800$ particles of alternating masses 1 and 2.62, with total energy N and total momentum 0. While the second cumulant decreases as $N^{\alpha - 1}$, with $\alpha \simeq 0.5$, the fourth cumulant increases with N.

This can be understood as follows. In the microcanonical case, because all of the system's energy is in kinetic form, multiplying the initial energy E by a factor λ is equivalent to speeding up time by a factor $\sqrt{\lambda}$: hence, one can write in the long-time limit

$$\begin{cases} \langle Q_t^2 \rangle^{\text{micro.}} \sim A\sqrt{E}t, \\ \langle Q_t^4 \rangle_c^{\text{micro.}} = \langle Q_t^4 \rangle^{\text{micro.}} - 3(\langle Q_t^2 \rangle^{\text{micro.}})^2 \sim B\sqrt{E}t, \end{cases}$$

with A and B independent of E. When performing a canonical average, the fourth cumulant grows like t^2:

$$\langle Q_t^4 \rangle_c^{\text{can.}} = \langle Q_t^4 \rangle^{\text{can.}} - 3(\langle Q_t^2 \rangle^{\text{can.}})^2 \sim 3A^2(\langle E \rangle - \langle \sqrt{E} \rangle^2)t^2.$$

For similar reasons, one expects $\langle Q_t^{2n} \rangle_c^{\text{can.}} \sim t^n$.

Size dependence of the cumulants. – Figures 3 and 4 show the asymptotic values of $\langle Q_t^n \rangle_c / t$ we obtained for $1 \leqslant n \leqslant 4$. The cumulants were calculated by averaging over a number of samples varying from $2 \cdot 10^8$ for $N = 50$ to $2 \cdot 10^6$ for $N = 800$, for the following systems:

- a ring of $50 \leqslant N \leqslant 800$ particles with total kinetic energy N and total momentum 0;
- an open system of $51 \leqslant N \leqslant 801$ particles between two heat baths at temperatures $T_a = 2$ and $T_b = 1$;
- the same open system between two heat baths at the same temperature $T_a = T_b = 1$.

In all cases, the particle density N/L was exactly 1. The mass of the heavier particles, m_2 was taken to be 2.62 (as in [33]); when we repeated some of our simulations with a different mass ratio, $m_2 = (1 + \sqrt{5})/2$ as in [35], we obtained qualitatively similar results (not shown here). In order to increase the efficiency of our simulations at large system sizes, we used a heap algorithm similar to the one in [35] to store the collision times.

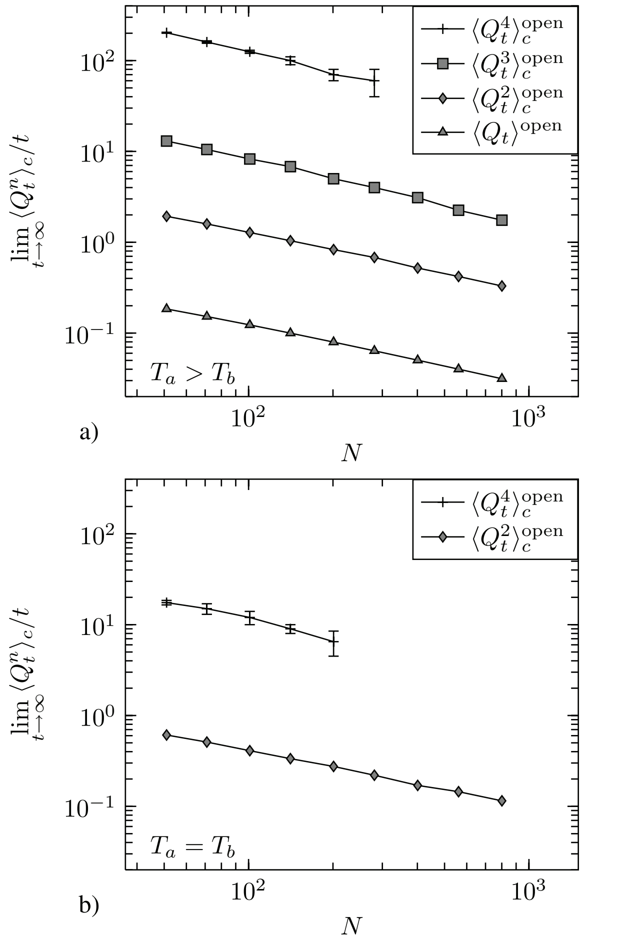

Fig. 4: Asymptotic values of $\langle Q_t^n\rangle_c/t$ on an open system with $51 \leqslant N \leqslant 801$ particles, with alternating masses 1 and 2.62, between heat baths at temperatures $T_a = 2$ and $T_b = 1$ (a) and $T_a = T_b = 1$ (b). All cumulants seem to decrease as $N^{\alpha-1}$, with $0.25 \leqslant \alpha \leqslant 0.4$.

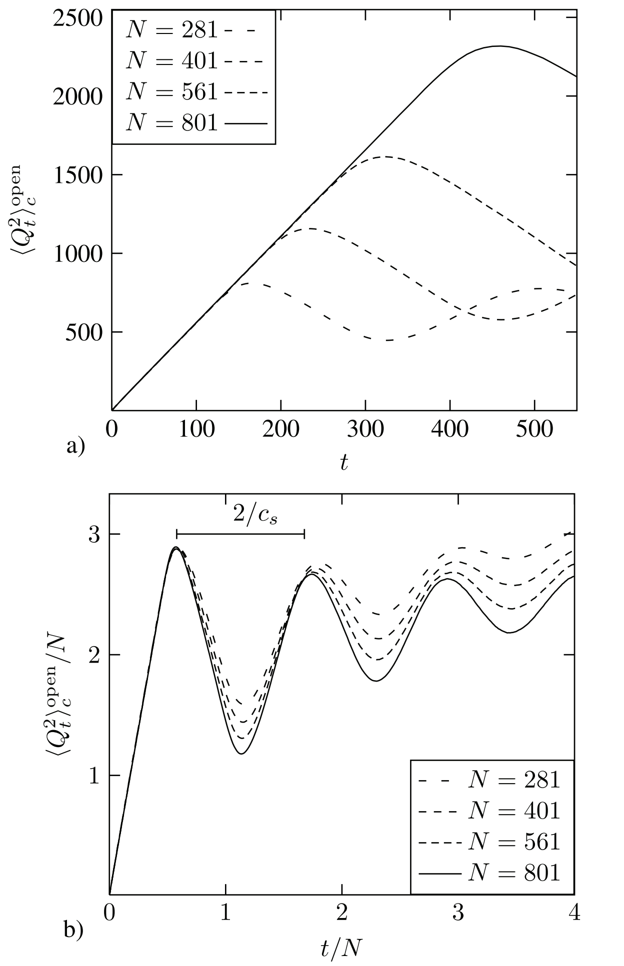

Fig. 5: Short-time behavior of $\langle Q_t^2\rangle_c$ on an open system of $281 \leqslant N \leqslant 801$ particles between heat baths at the same temperature $T_a = T_b = 1$. In a time range increasing with system size, the second cumulant behaves as on an infinite system at equilibrium (a); it then exhibits damped oscilllations on time scales of order N (b).

The fourth cumulant of Q_t is of course the hardest to obtain: we were only able to measure the asymptotic value of $\langle Q_t^4\rangle_c/t$ accurately for $N \leqslant 201$ in the open case.

For the ring geometry, while the second cumulant decays like a power law, the fourth cumulant increases with the system size. Hence the picture is very different from the diffusive case (1): in addition to the anomalous Fourier's law, we observe an increase of the fourth cumulant instead of a decay.

For the open case, the situation looks more similar to the diffusive case : all the cumulants seem to decrease with comparable power laws of the system size, albeit with a different exponent than in the diffusive case (1).

At the moment, we do not have any theroretical explanation for the different behaviors exhibited by the fourth cumulant on the ring and in the open case. We can only notice that the ring geometry, for which the fourth cumulant increases with system size (fig. 3), is reminiscent of the totally asymmetric exclusion process (TASEP) [42], where $\langle Q_t^2\rangle_c/t \sim L^{-1/2}$ and $\langle Q_t^4\rangle_c/t \sim L^{1/2}$.

Short-time behavior. – In our simulations (fig. 2a)), we measure the whole time dependence of the cumulants $\langle Q_t^n\rangle_c$. As fig. 5 shows, the short-time behavior of $\langle Q_t^n\rangle_c$ is independent of the system size N over a time range which increases with N. This can be interpreted as the fact that, over this time range, the system behaves as if it was infinite: in turn, this allows us to study the behavior of the cumulants on an infinite system. Figure 5a) shows that, for an infinite system at equilibrium, $\langle Q_t^2\rangle_c$ grows linearly with time; other results (not shown here) indicate that $\langle Q_t^4\rangle_c$ is also linear in time for the same system. This is another major difference with infinite diffusive systems [43], for which all the cumulants of Q_t grow asymptotically as $\sqrt{t}$.

At intermediate times, all the $\langle Q_t^n\rangle_c$ exhibit periodic oscillations for $n \geqslant 2$, with a period proportional to system size (as can be seen for the second cumulant in fig. 5b)): for the second cumulant, they can be fitted by an exponentially damped sine function [44]. The periods can be understood from the adiabatic sound velocity c_s in the hard particle gas, given by

$$c_s = \sqrt{\frac{\gamma P}{\rho}};$$

here, $\gamma = 3$ (for an one-dimensional monoatomic gas), $P = NkT/L = 2$ (since the average energy, $E/N = kT/2$, is taken to be 1), and $\rho = (1 + m_2)/2$, so that $c_s = 1.82$ for $m_2 = 2.62$. For the open system, the period is close to $2N/c_s$ (shown in fig. 5b)), which is the time for a sound wave originating in S to come back to S in the same direction, having been reflected once on each boundary; for the ring, our data (not shown here) exhibits a period close to N/c_s, the time for a sound wave starting from S to go around the ring.

Conclusion. – In this letter, we have shown that, for a hard particle gas at equilibrium and out of equilibrium, the cumulants of the flux of energy scale as power laws of the system size. These power laws differ from the ones expected for diffusive systems. Hence, our data shows that the anomalous Fourier's law of momentum-conserving systems is also characteristic of higher cumulants of the current.

The difference between the momentum-conserving system studied here and diffusive systems can also be seen (fig. 5) for an infinite system at equilibrium, in which $\langle Q_t^2 \rangle$ grows as t (instead of $\sqrt{t}$ in diffusive systems). An elementary calculation shows that, for an infinite ideal gas at equilibrium, all the cumulants of Q_t also increase linearly with t: it remains to be seen whether this linear growth is generic of momentum-conserving systems.

More numerical work is certainly needed to accurately determine the exponents characteristic of the cumulants of the energy flux, in particular to check whether, in the open case, all the cumulants decay with the same power law; one could try to compare the exponents seen for the ring and for the open geometry.

We have focused here on the fluctuations of the flux of energy, which is one of the conserved quantities of this hard particle gas. As momentum is also conserved, it would be interesting to study the size dependence of the fluctuations of the momentum flux in a similar way [45].

It would also be interesting to investigate whether similar power laws of the cumulants can be observed in other momentum-conserving systems, such as anharmonic chains like the Fermi-Pasta-Ulam models (which are known to exhibit anomalous Fourier's law). The study of the cumulants could be a good test for existing theoretical approaches [46,47], such as the mode-coupling theory [48–51] or the Boltzmann-Langevin equation [52,53]. In particular, one may wonder whether, for momentum-conserving systems, there exists an analog of the universal ratios of the cumulants which are expected for diffusive systems on a ring [10].

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