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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).

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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 \( \langle Q^n \rangle_c \) of the flux of energy \( Q_t \) during a long time \( t \) take, for a large system size \( L \), the following form:

\[
\begin{align*}
\lim_{t \to \infty} \frac{1}{t} \langle Q^2 \rangle_{\text{ring}} & \simeq \frac{1}{2} A(T), \\
\lim_{t \to \infty} \frac{1}{t} \langle Q^{2n} \rangle_{\text{ring}} & \simeq \frac{1}{2^n} B_n(T), \\
\lim_{t \to \infty} \frac{1}{t} \langle Q^n \rangle_{\text{open}} & \simeq \frac{1}{2^n} C_n(T_a, T_b).
\end{align*}
\]

(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 \( \overline{Q}_t \) 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

\[(a)\text{E-mail: gerschen@lps.ens.fr}\]
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 \( \langle Q_2 \rangle^{\text{open}}/t \) 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 \( \langle Q_2^2 \rangle^{\text{ring}}/t \) (or
of \( \langle Q_2^2 \rangle^{\text{open}}/t \) 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
macropscopic 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 \( L \):

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

The exponent \( \alpha \) 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 \( \alpha \), our goal here is to present
numerical simulations, not to determine \( \alpha \) 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
\( \langle Q_t^2 \rangle_c/t \) 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 \( \langle Q_t^2 \rangle_c/t \).

The \( 1/t \) convergence of fig. 2b) can easily be under-
stood. 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 \( \tau_L \)
which increases with $L$; for $t_2 - t_1 > \tau_L$, the decay is much faster (see, for instance, [35], fig. 4), so that $\int_0^\infty f(\tau) \, d\tau$ and $\int_0^\infty \tau f(\tau) \, d\tau$ are finite. Therefore, when $t \gg \tau_L$, $(Q_\tau^2)c = \int_0^\infty dt_1 \int_0^\infty dt_2 \langle J(t_1)J(t_2) \rangle_c = 2t \int_0^\infty f(\tau) \, d\tau - 2 \int_0^\infty \tau f(\tau) \, d\tau$ becomes of the form $At + B$ so that $(Q_\tau^2)c/t \sim A + B/t$.

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 $t \geq 5 \cdot 10^3$ 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 ($\langle Q_\tau^n \rangle_c^{\text{can}} \sim t^\alpha$).

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 $\lambda$ is equivalent to speeding up time by a factor $\sqrt{\lambda}$: hence, one can write in the long-time limit

$$\left\{ \begin{array}{l} \langle Q_\tau^2 \rangle^{\text{micro}} \sim A\sqrt{Et}, \\ \langle Q_\tau^4 \rangle^{\text{micro}} = \langle Q_\tau^2 \rangle^{\text{micro}} - 3 \langle (Q_\tau^2)^{\text{micro}} \rangle^2 \sim B\sqrt{Et}, \end{array} \right.$$  

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

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

For similar reasons, one expects $(Q_\tau^n)^{\text{can}} \sim t^n$.

**Size dependence of the cumulants.**—Figures 3 and 4 show the asymptotic values of $\langle Q_\tau^n \rangle_c/t$ we obtained for $1 \leq n \leq 4$. The cumulants were calculated by averaging over a number of samples varying from $2 \cdot 10^8$ to $2 \cdot 10^9$ for $N = 50$ to $2 \cdot 10^6$ for $N = 800$, for the following systems:

- a ring of $50 \leq N \leq 800$ particles with total kinetic energy $N$ and total momentum 0;
- an open system of $51 \leq N \leq 801$ 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, $m_2 = (1 + \sqrt{3})/2$ 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.
The fourth cumulant of $Q_t$ is of course the hardest to obtain: we were only able to measure the asymptotic value of $\langle Q^4_t \rangle_c/t$ accurately for $N \leq 201$ 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 theoretical 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 $\langle Q^2_t \rangle_c \sim L^{-1/2}$ and $\langle Q^4_t \rangle_c \sim L^{1/2}$.

**Short-time behavior.** – In our simulations (fig. 2a)), we measure the whole time dependence of the cumulants $\langle Q^n_t \rangle_c$. As fig. 5 shows, the short-time behavior of $\langle Q^2_t \rangle_c$ 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, $\langle Q^2_t \rangle_c$ grows linearly with time; other results (not shown here) indicate that $\langle Q^4_t \rangle_c$ 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 $\langle Q^n_t \rangle_c$ exhibit periodic oscillations for $n \geq 2$, 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 heat flux of a one-dimensional hard partice gas at equilibrium and out of equilibrium, the cumulants of the heat flux of a one-dimensional hard partice gas (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.

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