Thermodynamic entropy production fluctuation in a two-dimensional shear flow model

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We investigate fluctuations in the momentum flux across a surface perpendicular to the velocity gradient in a stationary shear flow maintained by either thermostated deterministic or by stochastic boundary conditions. In the deterministic system the fluctuation relation for the probability of large deviations, which holds for the phase space volume contraction giving the Gibbs ensemble entropy production, never seems to hold for the flux which gives the hydrodynamic entropy production. In the stochastic case the fluctuation relation is found to hold for the total flux, as predicted by various exact results, but not for the flux across part of the surface. The latter appear to satisfy a modified fluctuation relation. Similar results are obtained for the heat flux in a steady state produced by stochastic boundaries at different temperatures.

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I. INTRODUCTION

There has been much effort during the past decade to connect the statistical mechanics of stationary nonequilibrium states (SNS's) with the theory of dissipative dynamical systems [1]. While most results obtained so far via this approach are more of mathematical than physical interest, there is one potential exception: the fluctuation theorem [2] and its generalizations [3–6]. The original fluctuation theorem was stated and numerically checked for a particular ''thermostated'' dynamical system in Ref. [7]. An heuristic connection with the relevant properties of reversibility and chaoticity of the system was also given in that paper. A rigorous proof of the fluctuation theorem together with a clarification of its connection with the theory of the invariant (SRB) measure for a chaotic dynamical system was given in Ref. [2].

The phase-space time evolution of such a system is given by an equation of the form

$$\dot{X}=\mathcal{F}(X), \tag{1.1}$$

with $\mathcal{F}$ chosen to keep $X(t)$ confined to a compact surface Σ in the phase space while forcing the system into a nonequilibrium state. The latter requires that $\mathcal{F}$ be non-Hamiltonian, with $\operatorname{div}\mathcal{F}(X)=\sigma(X)\neq 0$.

Using some very strong assumptions on dynamical system (1.1), Gallarotti and Cohen (GC) proved that in the SRB measure [8] describing the SNS of this system the probability distribution $P_\tau(p)=\langle\delta(p-\pi_\tau(X))\rangle$, of

$$\sigma_\tau(X)=\frac{1}{\tau\langle\sigma\rangle}\int_{-\tau/2}^{\tau/2}\sigma(X(t))dt, \tag{1.2}$$

satisfies the equality

$$\lim_{\tau\to\infty}\frac{1}{\tau\langle\sigma\rangle}\ln\frac{P_\tau(p)}{P_\tau(-p)}=p. \tag{1.3}$$

Here $\langle\cdot\rangle$ represents the average in the SNS.

The quantity $\langle\sigma\rangle$ is formally equal to the ''rate of change'' of the Gibbs entropy in the SNS. More precisely, if we start the system with a measure $\mu_0(dX)=\rho_0(X)dX$, where dX is the Liouville measure restricted to the surface Σ then, using evolution (1.1),

$$\dot{S}_G(t)=-\frac{d}{dt}\int\rho_t\log\rho_t dX=\mu_t(\sigma)\xrightarrow[t\to\infty]{}\langle\sigma\rangle, \tag{1.4}$$

where the existence of the limit will hold under the assumptions of the GC theorem. Furthermore we will have $\langle\sigma\rangle<0$ implying that $S_G(t)\to-\infty$ whenever the limiting state is not an equilibrium one with zero currents [9,10].

Based on relation (1.4), $\sigma_\tau(X)$ is often called the (normalized) ''average entropy production during a time interval τ'' in the SNS. The identification of σ_∞, the object of the GC theorem, with entropy production was further strengthened by the form of $\sigma(X)$ in many examples of bulk thermostated systems, e.g., those considered by Moran and Hoover [11] for electrical conduction, and in Ref. [12] for shear flow. In those systems $\sigma(X)$ is given by an expression related to the hydrodynamic entropy production and the validity of the fluctuation relation, Eq. (1.3), was confirmed by numerical simulations, despite the fact that the conditions of the GC theorem are not satisfied there.

However, such bulk thermostatted systems are very different from realistic systems which are typically driven to SNS by inputs at their boundaries: the motion in their interiors is governed by Hamiltonian dynamics which do not produce any phase-space volume contraction. It is therefore important, for a comparison with real systems, to consider models of dynamical systems in which the thermostats forcing the system into SNS operate only near boundaries. Such

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deterministic models were introduced by Chernov and Lebowitz [13] for shear flow and by Gallavotti [1] and van Beijeren [14] for heat flux.

We note that the GC theorem has been extended to open systems in contact with infinite thermal reservoirs which act on the system but are not changed by it. The simplest modeling of such a situation is via stochastic transitions, induced by the reservoirs, between different microstates of the system induced by the reservoirs [4,6]. Thus, to model a system carrying a heat current and/or a momentum flux, one may use Maxwellian boundary conditions. This means that a particle hitting the left (right) wall will be reflected with a Maxwellian distribution of velocities corresponding to temperatures $T_L(T_R)$ and mean velocities $u_L(u_R)$ parallel to these walls. For $T_L \neq T_R$ this will induce a SNS with a heat flux, while $u_L \neq u_R$ will (using periodic boundary conditions in the flow directions) induce a SNS with a shear flow; see Refs. [15,16]. It is expected (hoped) that deterministic (thermostatted) and stochastic kinds of boundary modeling will yield similar SNS's of a macroscopic system away from the boundaries. This is what happens in equilibrium systems at least when not in a phase transition region.

Such an ''equivalence of ensembles'' is far from established for SNS's. In fact there is, at some level, a profound difference between thermostatted and stochastically modeled SNS's as far as S_G is concerned. As already noted, the former have $S_G(t) \to -\infty$, and $\dot{S}_G(t) \to \langle \sigma \rangle < 0$, while the latter have $S_G(t) \to \overline{S}_G$, $\dot{S}_G(t) \to 0$. The origin of the difference lies in the differences in the measures describing these SNS's. Thermostatted SNS's are described by a SRB measure which is singular with respect to the induced Lebesgue measure dX, while the SNS's of stochastically driven systems are (this can be proven in some case and expected in general) described by measures that are absolutely continuous with respect to dX [17,18]. However, this difference need not mean much for a macroscopic system, since quantities of physical interest are sums of functions which depend only on a few variables. Their properties are therefore determined by the reduced distribution functions which can be expected to be absolutely continuous with respect to the local Lebesgue measure, i.e., expressible as densities, even when the full measure is singular and fractal [19].

Interestingly enough, it is possible for the boundary driven pure heat flow case to model the thermostat in such a way that the expression for $\sigma(X)$ appearing in the fluctuation relation is the same, up to terms whose average vanishes, for both the deterministic and stochastic case; see Ref. [1]. It can be written as

$$\sigma = \left(\frac{1}{T_L} - \frac{1}{T_R} \right) J_Q + \frac{dF(X)}{dt}, \tag{1.5}$$

so that

$$\langle \sigma \rangle = \left(\frac{1}{T_L} - \frac{1}{T_R} \right) \langle J_Q \rangle, \tag{1.6}$$

where $J_Q(X)$ is the heat flux through some surface in the middle of the system and the average of the time derivative dF/dt vanishes in the SNS. $\langle \sigma \rangle$ has a form of entropy production in the left and right heat ''reservoirs'' which is also equal to the hydrodynamic entropy production in the SNS [16].

The situation is different for the thermostatted boundary driven shear flow case considered in Ref. [13]. $\sigma(X)$ in Eq. (1.2), entering the GC theorem for that model, is not clearly related to the hydrodynamic entropy production. The latter now corresponds to a momentum flux through the system, $J_M(X)$, for which a fluctuation relation holds for the stochastically driven system. The question is then whether there is still enough equivalence between systems driven deterministically and stochastically so that the fluctuation relation for $J_M(X)$, derived for the latter, also holds in the former.

Another question which concerns both heat conduction and the shear case is whether the fluctuation relation can be observed in real macroscopic physical systems. More precisely, we know that in the linear regime the fluctuation relations imply an Onsager type reciprocity relations for the transport coefficients [20,4] which hold not only globally but also locally. Our question is therefore the following: assuming that the fluctuation relation holds for some flux crossing a surface S does it also hold (in some form) for the flux through part of S. The reason this is important for the applicability of the fluctuation relation to a real system is that for values of p for which $P_\tau(p)$ is of order unity, $P_\tau(-p)$ in Eq. (1.3), which corresponds to the flux J going in the opposite direction from its usual one, e.g., the heat flowing from the cold to the hot reservoir, is so small in a macroscopic system that the possibility of observing it is effectively zero. A local flux reversal, on the other hand, may be quite observable: an attempt in this direction was indeed made by Ciliberto and Laroche [21]. Here we describe numerical investigations of these questions for a deterministic and stochastically driven shear flow SNS's and for a stochastic heat flow model.

II. DESCRIPTION OF THE SHEAR FLOW MODEL

A. Deterministic

The system consists of N unit mass particles contained in an $L \times M$ box with periodic boundary conditions in the x direction, and reflecting boundaries on the walls perpendicular to the y direction. The dynamics in the bulk of the system is Hamiltonian, with hard core interactions (the particles have a radius r). When a particle collides with the reflecting walls its outgoing speed is the same as the incoming one, while the direction of the velocity is chosen in a way which simulates a moving boundary and creates a shear flow. The boundary transformation we consider is the same as in Refs. [13,22]. Let φ and ψ be the angle that the incoming (outgoing) velocity forms with the positive x direction if the particle collides with the upper wall or with the negative x direction if the particle collides with the lower wall. In the thermostatted system the outgoing angle ψ is given by a function of the incoming angle φ: $\psi = f(\varphi)$. The function f we choose is $f(\varphi) = (\pi + b) - \sqrt{(\pi + b)^2 - \varphi(\varphi - 2b)}$. This is time reversible, i.e., $\pi - f(\pi - f(\varphi)) = \varphi$; see Fig. 1.

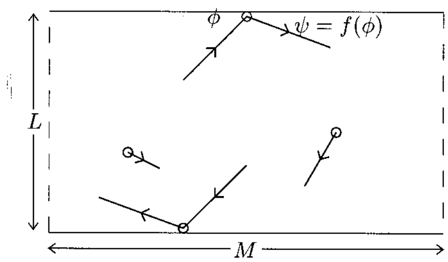

FIG. 1. Schematic representation of the dynamics of the system.

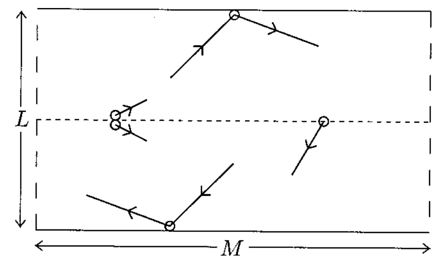

FIG. 2. Events producing momentum flux.

B. Stochastic

The dynamics in the interior of the system is the same as before, while the outgoing velocity at the upper (lower) wall is now chosen as if the particle was coming from a Maxwellian bath at temperature β^{-1} moving at velocity v_0 $(-v_0)$. More precisely we assume that after a collision with the boundary the particle emerges with a velocity that is randomly chosen from a distribution:

$$\mathcal{P}(v) = \frac{1}{Z} v_y \exp\left(\frac{\beta}{2}((v_x - \epsilon_y v_0)^2 + v_y^2)\right), \tag{2.1}$$

where Z is a normalization constant, v_0 is the mean x momentum of the particle after a collision, and ϵ_y is 1 if the collision is with the upper wall and -1 if it is with lower wall.

In Ref. [22] we checked the validity of the fluctuation relation for the phase-space contraction generated during the collisions of particles with the deterministic thermostatted boundary. We divided the phase-space contraction into a contribution due to the lower boundary and one due to the upper one. We found that the fluctuation relation was well verified for the total phase-space contraction $\sigma(X)$ but not for the partial ones.[1]

As already noted, there is no apparent connection between the phase-space contraction and the hydrodynamic entropy production which is proportional to the flux of the x component of the momentum across the system. In Ref. [13] an equality between the average phase space contraction rate and the average hydrodynamical entropy production rate was shown to hold to first order in the shear in the limit in which the system becomes large (at constant density), i.e., macroscopic, but the shear rate goes to zero in such a way as to maintain a constant total momentum transfer. This was done under the assumption that before a collision with either wall the particle velocities are distributed according to a Maxwellian. The equality between these averages was supported by numerical evidence.

In the present paper we further investigate the possible equivalence between phase-space contraction and entropy production. The momentum flux is equal to the momenta carried by particles crossing a line through the middle of the system plus the exchange of momentum between two colliding particles when their center are on opposite side of the line; see Fig. 2.

To be more precise we first introduce a discrete time for the system (in a slightly different way from what we did in Ref. [22]). Let $X = (q_i, v_i)$ be a phase space point, $\Phi_t(X)$ be the time evolution induced by the dynamics, and $\tau(X)$ be the first time at which a particle crosses the middle line or two particles on different sides of this line collide starting from the phase point X (we call such a situation a *timing event*) and let $S(X) = \Phi_{\tau(X)}(X)$. Finally, let $\pi(X)$ be the exchange of x momentum at the phase point X.

We now specify the quantity whose fluctuations we will check. Given an integer τ, let

$$\pi_\tau(X) = \sum_{i=-\tau/2}^{\tau/2} \pi(S^i(X)) \tag{2.2}$$

and

$$p_\tau(X) = \frac{\pi_\tau(X)}{\langle \pi_\tau(X) \rangle}, \tag{2.3}$$

where the mean $\langle \cdot \rangle$ is taken with respect to the stationary measure of the system. Now let $\Pi_\tau(p)$ be the distribution function of $p_\tau(X)$ and

$$\xi_\tau(p) = \frac{1}{\langle \pi_\tau(X) \rangle} \ln\left(\frac{\Pi_\tau(p)}{\Pi_\tau(-p)}\right).$$

We can formulate our ''fluctuation relation for the entropy production'' as follows:

$$\lim_{\tau \to \infty} \xi_\tau(p) = Cp. \tag{2.4}$$

Here C is the conversion constant between momentum flow and entropy production that, from hydrodynamics [22], is $C = 2u_b/T_b$ where u_b is the velocity of the particle near the upper boundary and T_b is the temperature near the boundary. Observe that this, as well as the following definitions, also make sense in the stochastic case when the phase-space contraction rate is not defined.

[1]We observe that based on the proof of GC we have no reason to expect that such a relation should hold for the partial phase-space contraction. We tested it anyway, since, as already noted, the fluctuation relation appears to hold in more general situations than those covered by the GC theorem, e.g., for the total σ here.

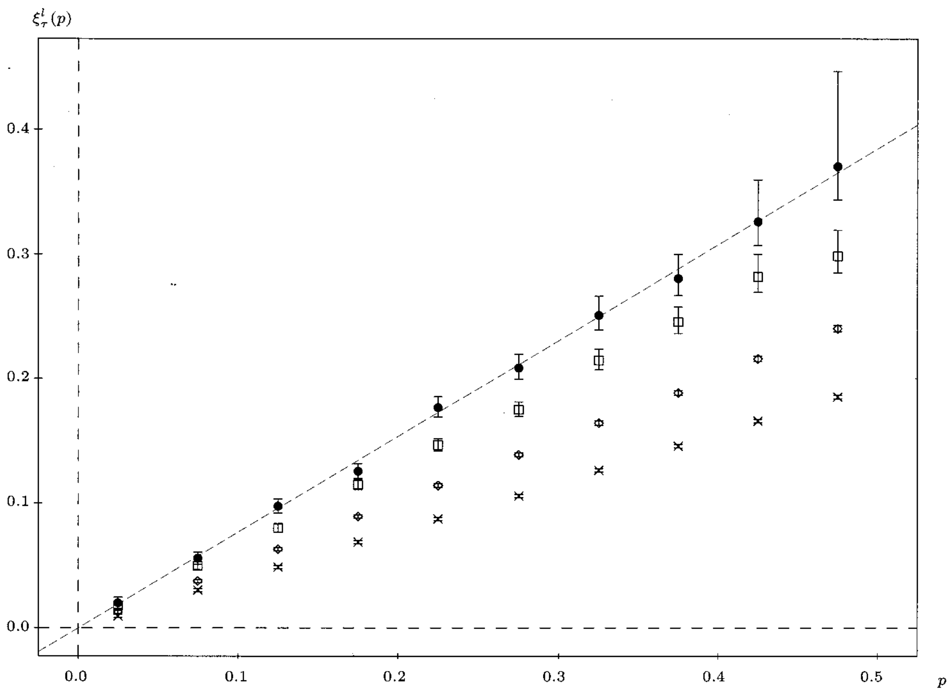

FIG. 3. Fluctuation relation for the momentum flux in the stocastic shear flow with a rectangular geometry. The filled circles (●) represent the experimental value for the total momentum flux, with error bars, for $\tau=400$ and $N=60$, while the dashed line is the theoretical prediction. The other data represent the partial fluctuation relation for $l=0.9$ (□), $l=0.6$ (◇), and $l=0.3$ (×). In all three cases, $\tau=400$.

In this setting we define a local entropy production by looking at all events like the ones described in Fig. 2, that occur in a specified part of the middle line of size lL. More precisely, let

$$\pi^l(X)=\pi(X)\chi_{[0,lL]}(X), \tag{2.5}$$

where $\chi_A(X)=1$ if the location of the momentum transfer event is at a point in A and 0 otherwise. We now define, in a way analogous to Eqs. (2.2) and (2.3), the quantities $\pi^l_\tau(X)$, $p^l_\tau(X)$, $\Pi^l_\tau(p)$, and $\xi^l_\tau(p)$, and state our ''local fluctuation relation'' for the entropy production as

$$\lim_{\tau\to\infty}\xi^l_\tau(p)=Cp. \tag{2.6}$$

More generally, we check if a relation of the form

$$\lim_{\tau\to\infty}\xi^l_\tau(p)=C_l p \tag{2.7}$$

holds.

The stochastic model also permits us to discuss different kind of transport phenomena. In fact we can set the reciprocal temperature β of the upper and lower walls to different values: β^+ and β^-. In this case we will also have a transport of heat through the middle of the system. We also ran a simulation for this case, setting $v_0=0$ for simplicity; we report the results in Sec. IV. Clearly the correct quantity to compute is the energy transfered across the middle line when a particle crosses or a collision happens.

III. NUMERICAL EXPERIMENTS FOR THE SHEAR FLOW

We simulated systems with $N=20$, 40, and 60 particles, and L and M such that the number density $\delta=N/LM=0.034$ was fixed. We chose two different ways to set L and M. In one case we fix $L=M$, i.e., a square domain. In the second case we keep M fixed at the value it had for $N=20$, and increase L proportionally as N is increased. In the deterministic case we fixed the energy per particle $(1/2N)\Sigma_i v_i^2=1$, while in the stochastic case we fixed the values of v_0 and β to reproduce the mean velocity u_b and temperature $T_b=\langle(v-u)^2\rangle$ observed in the $N=60$ simulation for the deterministic system. More precisely, we fixed $v_0=0.2$ and $\beta^{-1}=0.48$. Finally the radius r was fixed to 1. For each value of N and L we followed a single trajectory of the system for 5×10^8 timing events, and used it to compute the distributions $\Pi^l_\tau(p)$. As in Ref. [22] (differently than in Ref. [23]) we did not discard any events between two consecutive segments of length τ.

A. Stochastic case

As discussed in Sec. I (also see Sec. V A for further discussion) we expect the fluctuation relation to hold for the total momentum flux corresponding to the hydrodynamic entropy production. This can indeed be seen in Fig. 3, in which $\xi_\tau(p)$ is plotted for $\tau=300$ and $N=60$ for the rectangular geometry. The dashed line represent the theoretical prediction $\xi_\infty(p)=0.769p$. Similar results hold for $N=20$ and 40.

The relation in the strong form given by Eq. (2.6) appears not to hold for $l<1$, but Eq. (2.7) seems to hold as one always observes a linear behavior of $\xi^l_\tau(p)$ in Fig. 3.

The results for ξ^l_τ can be used to obtain the behavior of the slope C_l as a function of l. We report the result in Fig. 4

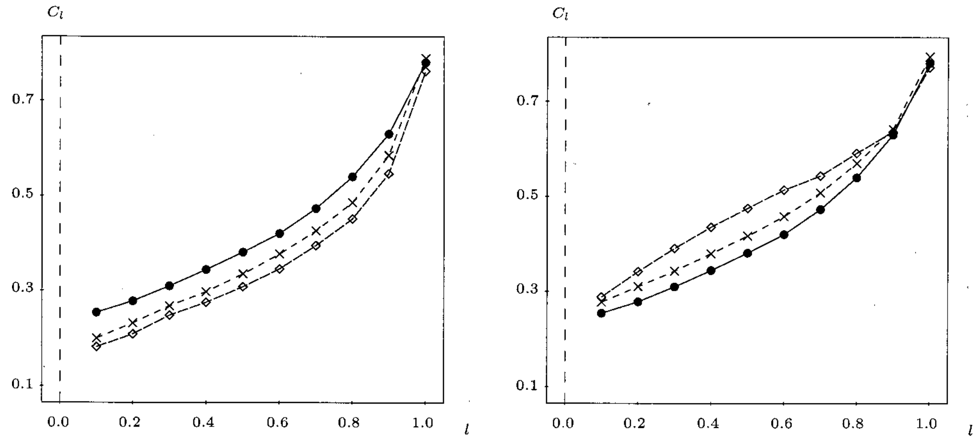

FIG. 4. Slope C_l as a function of l in the stochastic shear flow for $N=20$ (●), $N=40$ (×), and $N=60$ (◇). The left figure is for the square geometry, while the right one is for the rectangular geometry.

for the three value of N and the two different geometries we have used. We observe that in the square box case C_l decreases with N, and seems to reach a limit different from 1, when N grows. If we just increase the horizontal side of the box, keeping its height constant, C_l increases with N; it is not clear from the data what, if any, limit is reached when $N \to \infty$. Instead of fixing l we also tried fixing the length $l \times L$ but found nothing interesting.

B. Deterministic case

The situation looks very different in the deterministic case. No fluctuation relation seems to hold even when we consider the full momentum transfer. The result are shown in Fig. 5, where $\xi_\tau(p)$ is plotted for $\tau=100$, 200, and 300. The dashed line represents the value predicted by Eq. (2.4). Although we still observe a linear behavior, the slope appears to be increasing with τ so that no limit seems to be reached. We will attempt an explanation of this phenomenon in Sec. V.

We observe that a relation like Eq. (2.7) seems to hold if we look at the partial momentum flux. This is clearly shown in Fig. 6, where the behavior of $\xi_\tau^l(p)$ for $l=0.6$ and several values of τ is plotted for $N=60$ in the rectangular geometry. As in the stochastic case we can look at the behavior of C_l as a function of l for both geometries. The results are plotted in Fig. 7. As can be seen, the slope depends only very weakly

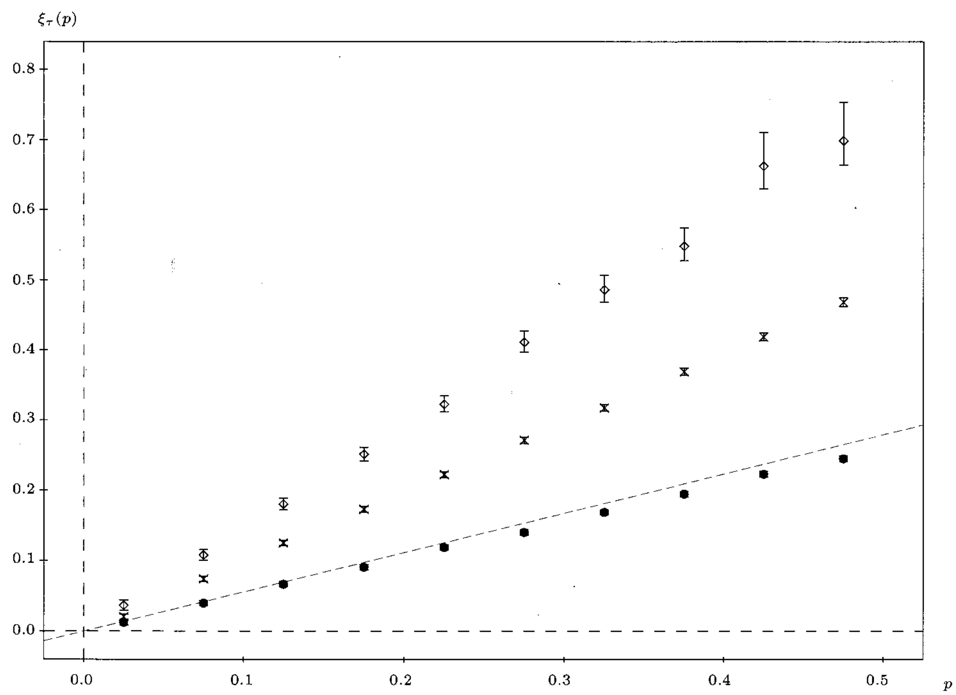

FIG. 5. Fluctuation relation in the deterministic shear flow in the rectangular geometry for the total momentum flux with $\tau=100$ (●), $\tau=200$ (×), and $\tau=300$ (◇).

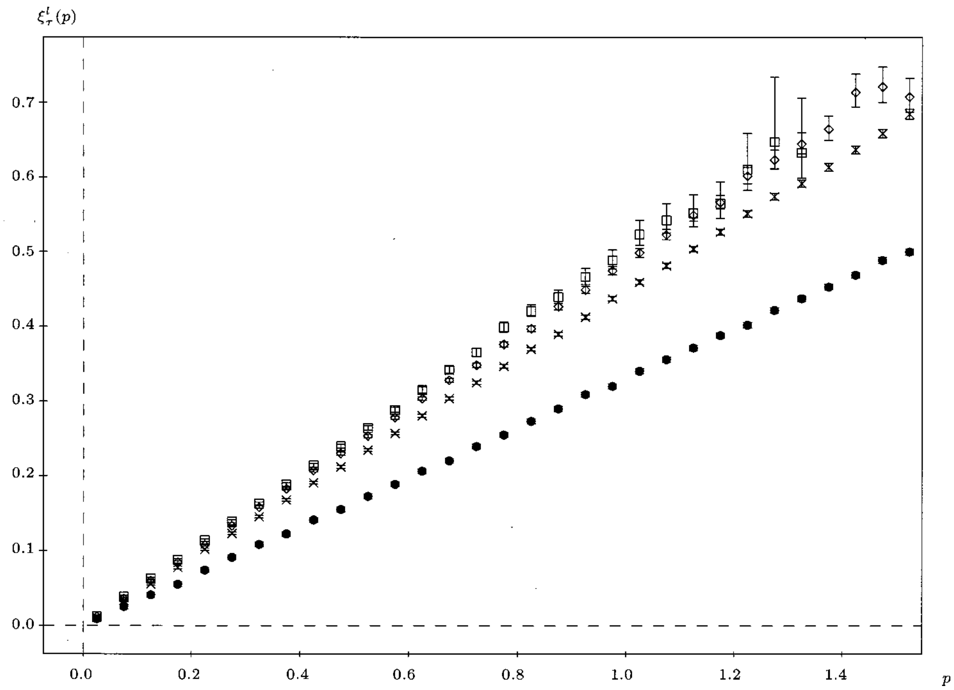

FIG. 6. Approach to a limit of the right hand side of Eq. (2.7) for the deterministic case. In this case $l=0.6$, while $\tau=100$ (●), 300 (×), 500 (◇), and 700 (□).

on the size of the system, at least for the square geometry. The only value for which C_l seems to depend on the size is $l=0.9$.

It is interesting to observe that if the fluctuation relation is true we would expect to observe a slope $C_l=2u_b/T_b$, as discussed for the stochastic system. In this situation, and mainly for the square geometry, the value of u_b varies significantly from $N=20$ to 60, while C_l remain almost constant. This and the result for the total momentum transfer suggest that the fluctuation of the phase-space contraction rate and those of the momentum flux behave differently.

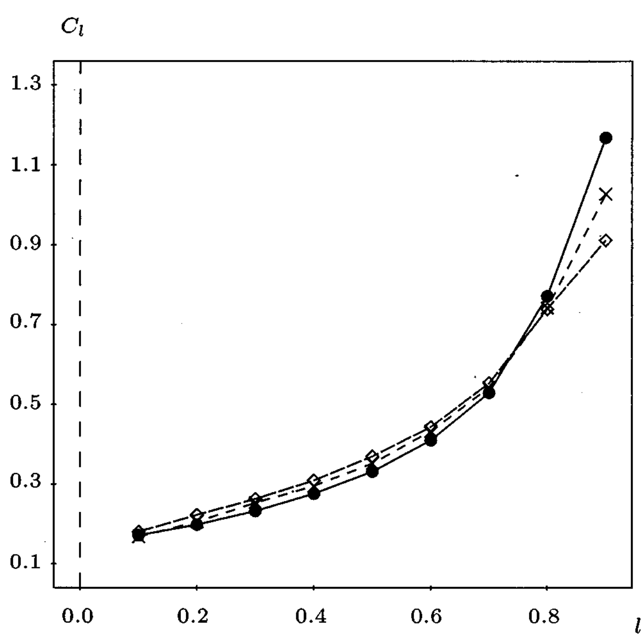

FIG. 7. Slope C_l as a function of l in the deterministic shear flow for $N=20$ (●), $N=40$ (×), and $N=60$ (◇) in the rectangular geometry. The graph of the square geometry is analogous.

IV. HEAT FLOW

The stochastic boundary condition permits us to study the case in which the two walls are kept at different temperatures T_+ and T_-. In this case the hydrodynamics entropy production is proportional to the heat current or energy flux from the upper wall of the system to the lower one. The events contributing to an exchange of energy are the same as those considered in Fig. 2, but now we consider the kinetic energy of a particle passing through the middle line or the exchange of energy in a collision between two particles that are on different sides of the middle line.

Analogously to what we did in Sec. II we define $\varepsilon(X)$ as the energy exchange for a point X that is on the Poincaré section with

$$\varepsilon_\tau(X)=\sum_{i=-\tau/2}^{\tau/2}\varepsilon(S^i(X)) \tag{4.1}$$

and

$$e_\tau(X)=\frac{\varepsilon_\tau(X)}{\langle\varepsilon_\tau(X)\rangle}. \tag{4.2}$$

Now let $E_\tau(e)$ be the distribution function of $e_\tau(X)$, and

$$\xi_\tau(e)=\frac{1}{\langle\varepsilon_\tau(X)\rangle}\ln\left(\frac{E_\tau(e)}{E_\tau(-e)}\right).$$

As before, we expect that

$$\lim_{\tau\to\infty}\xi_\tau(e)=Ce, \tag{4.3}$$

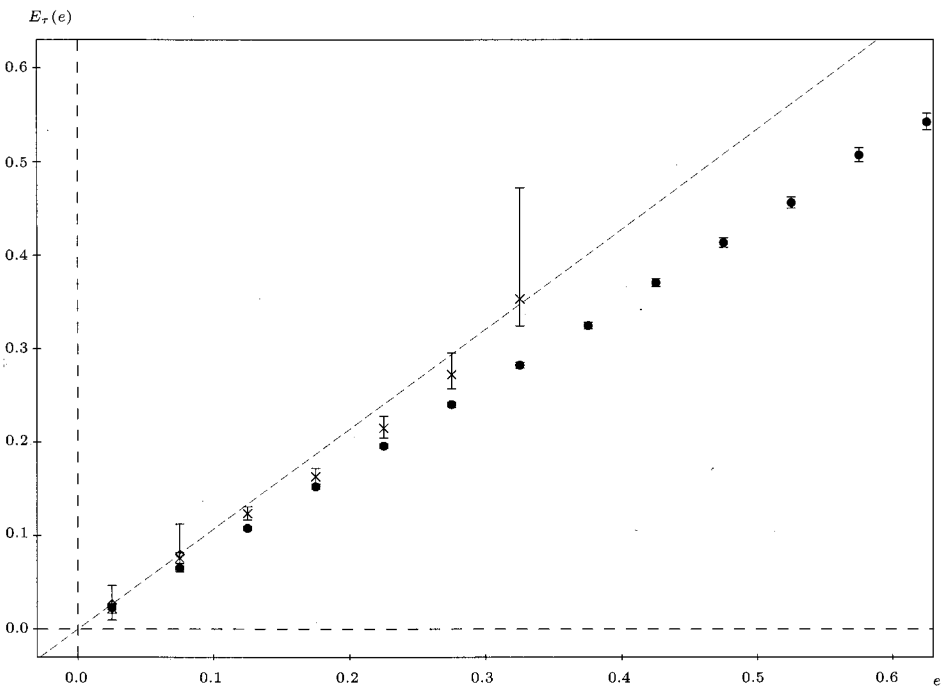

FIG. 8. Fluctuation relation for the total energy flux in the heat flow model. The experimental values are plotted with an error bar for $\tau=100$ (●), $\tau=200$ (×), and $\tau=300$ (◇) and $N=20$. The dashed line is the theoretical prediction.

where C is the proper conversion constant between heat flow and entropy production:

$$C=\frac{1}{T_+}-\frac{1}{T_-}.$$

Similarly we define $\varepsilon_l(X)$, $e_l(X)$, $E^l_\tau(e)$, and $\xi^l_\tau(e)$, and check whether

$$\lim_{\tau\to\infty}\xi^l_\tau(e)=C_l e. \tag{4.4}$$

The numerical experiments are very similar to the ones described in Sec. III, but we considered only stochastic boundary conditions with a rectangular geometry. Finally, we fixed $T_+=0.7$, $T_-=0.4$, and all the other parameters as in the shear flow case. The global fluctuation relation is shown in Fig. 8. There it can be observed that the fluctuations are smaller than the shear flow case. In fact, for $\tau=300$, when in the shear flow case the limiting behavior was reached, we have just two points for the fluctuation. We interpret the results as showing an approach to the expected limit. Similar result are obtained for $N=40$ and 60. The plots for $\xi^l_\tau(e)$, again, appear very linear, and their slopes C_l are shown in Fig. 9. Comments similar to those for the rectangular geometry shear flow hold here.

V. CONCLUSIONS

We now try to summarize the results of our numerical experiments.

A. Global fluctuation

In the case of the stochastic boundary conditions the fluctuation relation appears to be satisfied for both shear flow and heat conduction. This is not surprising. As in Refs. [4,5,16], we consider the stationary probability $P_\tau(X(t))$ on the space of the trajectories of the system from time $-\tau$ to time τ. (This can be assumed to be unique; see for example, Refs. [17,24]). Then define the time reversal operation $I((q_i,v_i))=(q_i,v_i)$; then, if $X(t)$ is a possible trajectory so is $I(X(t))$, and we can consider the measure $\overline{P}=IP$. Then as in Refs. [4,5] one finds

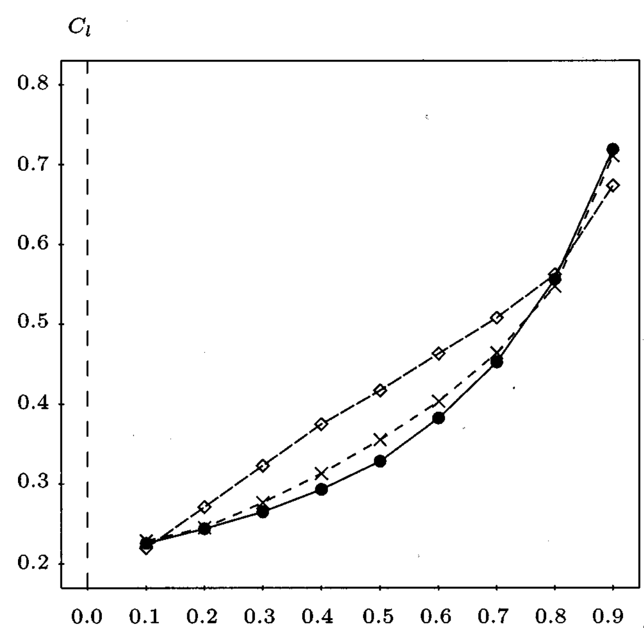

FIG. 9. Slope C_l as a function of l in the heat flow model for $N=20$ (●), $N=40$ (×), and $N=60$ (◇).

$$\frac{dP}{d\bar{P}}(X)=\exp\left\{R(X(\tau))-R(X(-\tau))+\int_{-\tau}^{\tau}\sigma(X(t))dt\right\} \tag{5.1}$$

for some appropriate function $\sigma(X)$. Here the left-hand side represents a Radon-Nykodyn derivative and $R(X)$ is a boundary term. The relation of Ref. [2] then follows.

It is easy to see that in the shear flow model $\sigma_\tau = \int_{-\tau}^{\tau}\sigma(X)$ is proportional to the momentum entering the system from the lower wall, minus the momentum leaving the system from the upper wall. Due to the conservation of momentum in the bulk of the system the total momentum flux π_τ through the middle of the system is proportional to σ_τ plus corrections due to the variation of momentum in the upper and lower halves of the system. We expect these two quantities to fluctuate much less than the momentum flux, at least if the system is large enough so that we can expect to have a fluctuation relation for π_τ.[2] Similar considerations hold for the heat conduction model.

The deterministic case is far less clear. We know that the average phase-space volume contraction rate is equal to the hydrodynamic entropy production rate only in some limiting situation; see Ref. [13]. Our numerical results, together with those of Ref. [22], show that this equality does not extend to their fluctuations. We observe, first of all, that although the GC fluctuation relation appears not to hold $\xi_\tau(p)$ is linear in p, so that we can rewrite Eq. (2.4) as

$$\xi_\tau(p)=C_\tau p. \tag{5.2}$$

The most striking effect appears to be the divergence of the slope C_τ. A possible explanation for this can be based on the assumption that the distribution $\Pi_\tau(p)$ is close to a Gaussian (see [22]), so that

$$C_\tau=\frac{2}{S(\tau)},$$

where

$$S(\tau)=\frac{2}{\tau}\sum_{t=-\tau}^{2}D(t)-\frac{2}{\tau^2}\sum_{t=-\tau}^{\tau}|t|D(t) \tag{5.3}$$

is the integral of the π-autocorrelation function $D(t) = \langle\pi(\Phi^t(\cdot))\pi(\cdot)\rangle-\langle\pi\rangle^2$.

Now, when $\Sigma_{t=-\tau}^{\tau}D(t)$ converges to a finite value, the fluctuation relation reduces to the usual Green-Kubo relation. On the other hand, if we assume that $\Sigma_{t=-\tau}^{\tau}D(t)$ approaches 0 when $\tau\to\infty$, then C_τ has to diverge as τ^{-1}, which is in good agreement with our numerical data. We were not able to check this relation more directly due to the lengthy simulations involved, but we hope to come back to this in future work.

We already noted that the quantity that enters the GC theorem for our deterministic shear flow model, i.e., the phase space contraction rate due to collisions, appears to have little in common with the hydrodynamic entropy production. This is different from models of deterministically boundary thermostatted heat conduction systems in which the phase space contraction rate assume the form of an entropy production [1,4,14]. We expect that it is possible to introduce a deterministic forcing term for the shear flow acting only at, or near, the boundary and producing a phase space contraction rate equal to the hydrodynamic entropy production; see Ref. [13]. This would make the fluctuation relation dependent on the form of the boundary forcing term.

B. Local fluctuation

As we already noted in Ref. [22] local fluctuations, in both the stochastic and deterministic case, do not satisfy a fluctuation law in the form of Eq. (2.6) but they appear to be in good agreement with the more general relation, Eq. (2.7). This seems to be contrary to the results obtained in Refs. [25] and [5].

To resolve this apparent contradiction we note that in Ref. [25] Gallavotti considered a chain of weakly interacting Anosov dynamical systems,[3] and took as a subsystem a finite piece of the chain. The phase-space contraction rate is an extensive quantity, as in the bulk thermostatted systems. Furthermore, correlations in the chain decay exponentially in both space and time. In a system with these characteristics one can prove that fluctuations of the phase space contraction rate due to the degree of freedom of the subsystem satisfy a fluctuation relation with corrections proportional to the boundary of the subsystem times the correlation length.

In our situation none of the above characteristics is present. First of all, we are not able to divide the degrees of freedom between the subsystem and the rest of the system. Moreover the phase-space volume contraction is present only at the boundary of the system, and the subsystem does not include any portion of the boundary. Finally, we expect the correlation length in our system to be very long (potentially infinite), i.e., larger that the size of the subsystem considered. For these reasons we do not expect the arguments in Refs. [25] and [5] to be applicable to our situation. However, we observe that our system is closer to the experimental situation described in Ref. [21], and to possible other experiments one can imagine doing.

As in Ref. [22] we do not have any real explanation for the apparent validity of Eq. (2.7). We think that the fluctuation relation can be extended to a partial relation of the form

[2]We observe, however, that differently from the analysis in Ref. [4] we do not have an *a priori* bound on the fluctuation of the total momentum of the system.

[3]The paper by Maes deals with a rather more general situation, but similar arguments also apply there.

of Eq. (2.7) in a wide range of situations. These include a system of particles under the influence of an electric field and a Gaussian thermostat; see Refs. [23] and [26] for more details. We think that for the asymmetric simple exclusion process, one should be able to find an analytical justification of this behavior.

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