Stationary Shear Flow in Boundary Driven Hamiltonian Systems

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We investigate stationary nonequilibrium states of particles moving according to Hamiltonian dynamics with Maxwell demon "reflection rules" at the walls. These rules simulate, in an energy but not phase space volume conserving way, moving boundaries. The resulting dynamics may or may not be time reversible. In either case the average rates of phase space volume contraction and macroscopic entropy production are shown to be equal for stationary hydrodynamic shear flows, i.e., when the velocity distribution of particles incident on the walls is a local Maxwellian. Molecular dynamic simulations of hard disks in a channel produce a steady shear flow with the predicted behavior.

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Stationary nonequilibrium states (SNS) of macroscopic systems are usually maintained by external inputs at their boundaries. Since a full microscopic description of such inputs is not feasible, it is necessary to represent them by some type of modeling. An important open problem is how much of the universality, or insensitivity to boundary conditions, exhibited by equilibrium systems (not inside a coexistence region of the phase diagram) remains true for SNS of macroscopically stable nonequilibrium systems, e.g., fluids in regimes of laminar flow. While there is ample experimental evidence that the gross macroscopic behavior of such systems is determined by the unique solution of the compressible Navier-Stokes equations, with specified boundary conditions on the hydrodynamic velocity and temperature [1], different modelings of the external drives [2,3] produce very different types of microscopic states [4–7]. Thus stochastic thermal boundaries generally lead to statistical ensembles absolutely continuous with respect to Liouville measure, while deterministic themostatting schemes yield singular measures [3–7].

While it is reasonable to expect that these differences do not have any consequences for the bulk properties of such systems, i.e., an equivalence of ensembles such as can be proven for systems in equilibrium, it is far from clear how to characterize the essential features of nonequilibrium stationary measures and just how far the universality of SNS goes [5,7]. This question and a desire to have a physically reasonable microscopic dynamical model of SNS motivates the present work in which we investigate various models which produce shear flow in a channel with walls perpendicular to the y axis and periodic in the x direction. Our models, which are deterministic, differ from bulk thermostatting schemes involving specification of local macroscopic functions, in that the microscopic dynamics in the bulk of the system are Hamiltonian. To induce shear flow the reflections at the walls are specified by a function $\psi = f(\phi)$ where ϕ and $-\psi$, $0 \le \phi, \psi \le \pi$, are the angles which the incoming and outgoing velocities at the top (bottom) wall make with the positive (negative) x axis, the direction of the "wall velocity" induced by these rules, for $\psi \le \phi$. (The use of a two-dimensional system and of identical rules for top and bottom is for simplicity only.)

Two particularly simple reflection rules used in our molecular dynamics simulations to produce an approximately linear shear flow in the x direction are

$$\psi = c\phi\,, \tag{1}$$

$$\psi = f(\phi) = (\pi + b) - [(\pi + b)^2 - \phi(\phi + 2b)]^{1/2}, \tag{2}$$

with $c, b \ge 0$ and $c \le 1$: $c = 1$ and $b^{-1} = 0$ representing stationary walls with normal reflection. Rule (2) has the symmetry $\phi = f^{-1}(\psi) = \pi - f(\pi - \psi)$, which makes the system retrace its trajectory backwards in time following a velocity reversal of all the particles. This time reversal symmetry, which is automatically satisfied by Hamiltonian dynamics, is also present in bulk thermostatted dynamics [3–6]. It was beautifully exploited in [7] to deduce, under suitable additional assumptions, certain large deviation properties of such SNS. Somewhat surprisingly, time reversal symmetry turns out not to be necessary for hydrodynamical behavior or for obtaining equality between phase space volume contraction and macroscopic entropy production—at least for systems in local equilibrium (which can still be far from global equilibrium). This suggests a "robustness" of the connection between macroscopic and microscopic "dissipation" in hydrodynamic regimes which goes beyond that considered previously.

To understand the nature of the SNS that can be expected to result from our microscopic dynamics, we begin with the hydrodynamical or compressible Navier-Stokes description of a macroscopic shear flow in a uniform channel of width L in which top and bottom walls move with velocities $\pm u_b$ in the x direction and have the same temperature T_b [1,4,8]. The laminar stationary fluid velocity in the x direction $u(y)$ is maintained by a constant x-momentum flux Π in the y direction. In addition to $u(y)$, the system is characterized by a temperature $T(y)$ and density $n(y)$. Calling $J(y)$ the

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heat flux in the y direction, the hydrodynamic entropy production σ per unit volume is

$$\sigma = \left[-\Pi \frac{du}{dy} - J(y) \frac{d\ln T}{dy} \right] \Big/ T(y) = -\Pi \frac{d}{dy}(u/T). \tag{3}$$

The second equality uses the fact that in the stationary state $\Pi u + J$ (whose divergence is the rate of change of the local energy density) is zero by symmetry so $J(y) = -\Pi u(y)$. The total hydrodynamic entropy produced in the steady state is then

$$\begin{aligned} R &= \int_{\text{volume}} \sigma \, dr = -\int_{\text{surface}} [\Pi u/T] \, ds = \int_{\text{surface}} J/T \, ds \\ &= -2L\Pi u_b/T_b = -2(L^2)\Pi(u_b/L)/T_b \\ &= (\text{volume}) \, |\Pi\gamma|/T_b \, , \end{aligned} \tag{4}$$

where $\gamma = 2u_b/L$ is the average shear rate; we have taken the channel to be of length L in the x direction and unit height in the z direction, with periodic boundary conditions in those directions.

Equation (4) is interpreted in the macroscopic formulation of irreversible thermodynamics [4,9] as an equality, in the stationary state, between the hydrodynamic entropy produced in the interior and the entropy carried by the heat flux to the walls of the container. To maintain such a steady state in an experimental situation requires external forces acting on the walls to make them move with velocities $\pm u_b$. The work done by these forces, $|\Pi u_b|$ per unit wall area, is converted to heat by the viscosity and absorbed by the walls acting as thermal reservoirs at temperature T_b.

The existence of such macroscopic steady states, satisfying the compressible Navier-Stokes equations from which (3) and (4) follow, can be proven starting from the Bolzmann equation, when the walls are modeled by thermal boundaries, i.e., following collisions with the walls, particles have a Maxwellian velocity distribution with mean $\pm u_b$ and temperature T_b [8]. It is expected (but very far from proven) that such thermal boundaries would produce similar SNS for general fluid systems. We would then have on the microscopic level a steady state described by an ensemble or phase space measure with a density $\tilde{\mu}$ absolutely continuous with respect to Liouville measure [5]. The hydrodynamic quantities would be given by ensemble averages, and R would equal the corresponding average heat flux to the thermal walls [8,9]. In general, it is possible to show [9] that the total ensemble entropy production $dS_G(t)/dt + \sum_b J_b/T_b \geq 0$. Here $S_G(t) = -\int \mu(X,t) \ln \mu(X,t) \, dX$ is the Gibbs ensemble entropy, X being a point in the phase space, and J_b is the ensemble average heat flux to the top or bottom wall. In the stationary state $\tilde{\mu}$ we would have S_G constant (proportional to the number of particles in the system), so S_G would be zero and $J_b = -\Pi u_b$.

Let us turn now to our models where the flow is deterministic and collisions with the boundaries conserve energy. It is not clear at all *a priori* what should now correspond at the microscopic level to entropy production in our system. Following the work in Refs. [3,4], we note that since our dynamics does not conserve Liouville volume on the energy surface the quantity $\dot{S}_G(t) = \int \mu(x,t)(\text{div}\dot{\mathbf{X}}) \, d\mathbf{X}$ will generally not vanish in the stationary state. In fact, we expect that any initial ensemble density $\mu_0(\mathbf{X})$ absolutely continuous with respect to the microcanonical ensemble will evolve, as $t \to \infty$, to a unique stationary measure $\overline{\mu}$ which is singular with respect to the Liouville measure on the energy surface [3–7]. We would then have that $S_G(t) \to -\infty$ with $\dot{S}_G(t) \to \int \overline{\mu}(\mathbf{X}) \, (\text{div}\mathbf{X}) \, d\mathbf{X} = -M$, $M \geq 0$, being the average compression of phase space volume per unit time in the stationary state. Such behavior is in fact proven in [6] for a related simpler model and is to be contrasted with the case of stochastic boundaries considered earlier when $\tilde{\mu}$ is smooth and $\dot{S}_G(t) \to 0$ as $t \to \infty$ [9].

In the models treated in [3,4,6] the equations of motion are such that M is automatically equal to the ensemble averages of microscopic quantities, which can be identified with thermodynamic forces and fluxes appearing in the macroscopic entropy production (3) and (4). This is not the case for the models considered here where there is no *a priori* prescription of u or T anywhere in the system and phase space volume gets compressed only at collisions of a particle with the wall: the bulk dynamics being Hamiltonian. The amount of compression there, computed from the reflection rules [10], is

$$m = \left| \frac{\sin\psi \, d\psi}{\sin\phi \, d\phi} \right| = \left| \frac{\sin f(\phi)}{\sin\phi} f'(\phi) \right| . \tag{5}$$

The time average of $\ln m$ along a trajectory in phase space then gives the mean exponential contraction rate M of the phase space volume per unit time. Since there are no thermodynamic parameters in (5), it is not at all clear *a priori* what relation, if any, between M and R will be in the SNS produced by our model. [This problem remains even when we consider time reversible models, such as (2), which are the limit of a continuous thermostatted model in which the thermostat acts only in the vicinity of the walls [10]].

Before answering that question we note that if only the top wall of the channel was moving in the x direction, i.e., if we put $f(\phi) = \phi$ in Eqs. (1) and (2) for the bottom wall, corresponding to specular reflection there, then no matter how close $f(\phi)$ is to ϕ for the top wall, a stationary state would be one in which all particle velocities are parallel to the x axis (pointing in the + direction). Hence the deviation from specular reflection required to produce a given, $\pm u_b$, gets smaller as the width of the channel, L, gets larger; keeping the density and kinetic energy per particle fixed. Since we are interested in macroscopic systems, $L \to \infty$, we should consider the case where $f(\phi)$ in Eqs. (1) and (2) is close to the identity. Formally we write

$$\psi = f(\phi) = \phi + \delta f_1(\phi) + O(\delta^2), \tag{6}$$

with $\delta = 1 - c, f_1 = -\phi$, for model (1) and $\delta = b^{-1}, f_1 = -\phi(\pi - \phi)$ for model (2). As we shall see later, fixing $\pm u_b$ requires that $\delta \sim L^{-1}$, for $L \to \infty$.

To compute R and M we call $v_1 = r\cos\phi$, $v_2 = r\sin\phi$, $0 \le \phi \le \pi$, the x and y components of the velocity of a particle entering a collision with the top wall, and let $v_2 g(v_1, v_2) dv_1\, dv_2 = r^2 \sin\phi\, g(r, \phi) dr\, d\phi, v_2 \ge 0$ the average number of particles in $dv_1\, dv_2$ incident on the top wall per unit length and unit time in the stationary state. We then have, for the x component of the momentum flux,

$$\Pi = -\int_0^\pi d\theta \int_0^\infty dr\, r[\cos f(\theta) - \cos\theta] r^2 \sin\theta\, g(r, \theta) = \delta \int_0^\pi d\theta \int_0^\infty dr\, f_1(\theta) r^3 \sin^2\theta\, g(r, \theta) + o(\delta), \tag{7}$$

where we have set the mass of each particle equal to unity. In a similar way

$$M = -2L \int_0^\pi d\theta \int_0^\infty dr \ln[f'(\theta) \sin f(\theta)/\sin\theta] r^2 \sin\theta\, g(r, \theta) = -2L\delta \int_0^\pi d\theta \int_0^\infty dr\, f_1(\theta) r^2 \sin\theta \frac{dg}{d\theta} + o(\delta), \tag{8}$$

where the factor 2 comes from combining the top and bottom contributions (equal by symmetry) and we have carried out an integration by parts. Recalling now from (4) that $R = -2L\Pi u_b / T_b$ we note that keeping δL fixed as $L \to \infty$ and $\delta \to 0$ we obtain

$$R = M[1 + o(\delta)]$$

whenever $g(r, \theta) = G(r) e^{u_b r \cos\theta / T_b}$, i.e., $g(\mathbf{v}) = A(v^2) \exp\{-\frac{1}{2}(\mathbf{v} - \mathbf{u}_b)^2 / T_b\}$.

Taking $A(v^2)$ to be a constant independent of v corresponds to the assumption that the distribution of particles entering a collision with the wall is a local Maxwellian. Calling n_c the number of collisions with the wall per unit time and unit length gives $A = n_c / \sqrt{2\pi}\, T_b^{3/2}$. This is just what would be expected from local equilibrium in the hydrodynamic limit [5,8,9]. We have thus obtained an equality between M and R for general collision rules $f(\theta)$ for macroscopic fluids in regimes of hydrodynamic behavior. This is consistent with the results of our simulations which we now describe.

In our computer simulation we used a system of N hard disks of unit diameter; this sets the length scale. The positions of the particle centers were chosen randomly (without overlap) in a domain $0 \le x \le L, |y| \le \frac{1}{2}(L - 1)$. The system evolved according to Hamiltonian dynamics with periodic boundary conditions in the x direction and reflection rules (1) and (2) whenever the particle reached the walls at $y = \pm\frac{1}{2} L$. The value of L was chosen so that the volume fraction occupied by the disks, $\rho = \frac{\pi}{4} N/L^2 = 0.1$. For $N = 200$ this corresponds to $L = 39.6$. The particles were all started with mean speed 1 (which sets the time scale) as we varied b and c, so we always had $\sum v_i^2 = N$. We believe that the results to be described are statistically reliable within a few percent. This is based on various checks comparing different N and runs: For each value of b and c we averaged over many thousand collisions per particle with other particles and many hundreds with the wall [10]. Higher accuracy can be obtained by additional simulations, which are planned. There is no reason to expect any change in our conclusions.

In each run the vertical height, occupied by the centers, $L - 1$, was divided into 20 equally spaced horizontal layers and time averages of the density $n(y)$, mean x velocity $u(y)$, variances $\langle (v_x - u)^2 \rangle$, $\langle v_y^2 \rangle$, and cross variance $\langle (v_x - u) v_y \rangle$ were taken. We also recorded time averages of x-momentum transfer from the walls, Π, and the contraction rate M.

We summarize our results by saying that they were consistent with the solution of the Navier-Stokes equation for stationary shear flow in a channel [4,8]. In particular, we observed an approximately linear profile $u(y) \simeq \gamma y$, with measured ratio of stress Π to strain γ within a few percent of the shear viscosity η_E computed by Gass [11] from Enskog theory for hard disks. The x and y "temperatures" $\langle (v_x - u)^2 \rangle$ and $\langle v_y^2 \rangle$ were approximately the same, with small variations of $T(y)$ consistent with hydrodynamical behavior. The velocity distribution was also consistent with a local Maxwellian with cross covariance $\langle (v_x - u) v_y \rangle \sim -3 \times 10^{-3}$. The density variations were small except near the walls where the density was higher as expected [2]. They became quite large when u_b exceeded one-half the mean thermal velocity and was the reason for not going to higher shear rates than 0.05 in units of thermal velocity per mean free path. To get higher rates we need to go to higher densities where the fluid is less compressible.

For the conditions used in the simulations we could, in fact, assume constant values of the density and transport coefficients and compute $u(y), T(y)$, and Π consistently from hydrodynamics using Enskog values for the viscosity and heat conductivity in Eq. (7) with $g(v_1, v_2)$ a Maxwellian with $u_b = \gamma L/2$. A comparison of these "theoretical" and "experimental" values for the mean velocity and temperature in the top layer is given in the first two columns in Table I. The agreement is not bad.

More important is the impressive agreement between theory and experiment for M and R given in columns 3 and 4. Here theory corresponds to the (numerical) evaluation of the integrals in Eqs. (7) and (8) using a Maxwellian g with $u_{ex}^{top}, T_{ex}^{top}$ and measured $n_c \simeq 0.046$.

TABLE I. Theoretical and experimental values of u_{top}, T_{top}, M, and R. The last column gives the leading term of both M and R expansion in δ. The first five rows represent the b model and the last five rows the c model, both with 200 particles and $L = 39.6$.

b/c	$u_{\text{th}}^{\text{top}}/u_{\text{exp}}^{\text{top}}$	$T_{\text{th}}/T_{\text{exp}}$	$M_{\text{th}}/M_{\text{exp}}$	$R_{\text{th}}/R_{\text{exp}}$	M_{lead}
200.0	0.038/0.041	0.500/0.499	0.00288/0.00275	0.00282/0.00282	0.00284
100.0	0.077/0.087	0.499/0.498	0.0121/0.0116	0.0118/0.0118	0.0120
70.0	0.108/0.118	0.497/0.494	0.0235/0.0228	0.0230/0.0231	0.0236
45.5	0.162/0.171	0.493/0.491	0.0515/0.0507	0.0501/0.0497	0.0521
26.7	0.263/0.268	0.483/0.480	0.134/0.132	0.130/0.131	0.139
12.5	0.478/0.518	0.443/0.427	0.532/0.518	0.493/0.513	0.584
0.99	0.055/0.068	0.499/0.498	0.0092/0.0089	0.0067/0.0067	0.0067
0.98	0.109/0.130	0.497/0.496	0.0321/0.0320	0.0249/0.0255	0.0247
0.97	0.160/0.175	0.494/0.489	0.063/0.061	0.050/0.051	0.049
0.95	0.252/0.280	0.484/0.479	0.150/0.148	0.126/0.132	0.125
0.93	0.335/0.370	0.472/0.464	0.260/0.256	0.226/0.238	0.223
0.90	0.441/0.491	0.451/0.437	0.454/0.446	0.404/0.438	0.402

The last column gives the leading term in δ, for which $M = R$, computed from the right sides of Eqs. (7) and (8).

We note that while the agreement in columns 4 and 5 is equally good for the b and c models, Eqs. (2) and (1), we are much closer to the hydrodynamic regime $L \to \infty$ for the b dynamics than for the c dynamics. The reason for the difference between the b and c dynamics appears to be due to the fact that there is a jump in $f(\phi)$ at $\phi = \pi$ for the c dynamics, because $f(\pi) = \pi$ for the b but not the c dynamics. As a consequence, the corrections to the linear term in δ are much larger for the latter—in fact, the second derivative of M with respect to δ diverges for the c dynamics at $\delta = 0$. A simple calculation shows that for the top velocities in the first two rows in Table I we would have to make $L \geq 980$ or 870 for the c dynamics and $L \geq 30$ or 28 for the b dynamics to have M and R agree within 3%. [The mean separation between particle centers is ~2.76, while the measured (and theoretical) mean free path is approximately 2.2 in our units, so the effective ratio of macrolength or microlength scale is about 20 [5,8,9].

We mention finally that we also carried out simulations with different reflection rules, different densities, and different shear rates. They all seemed to lead to hydrodynamic behavior. A complete description will be given in [10].

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