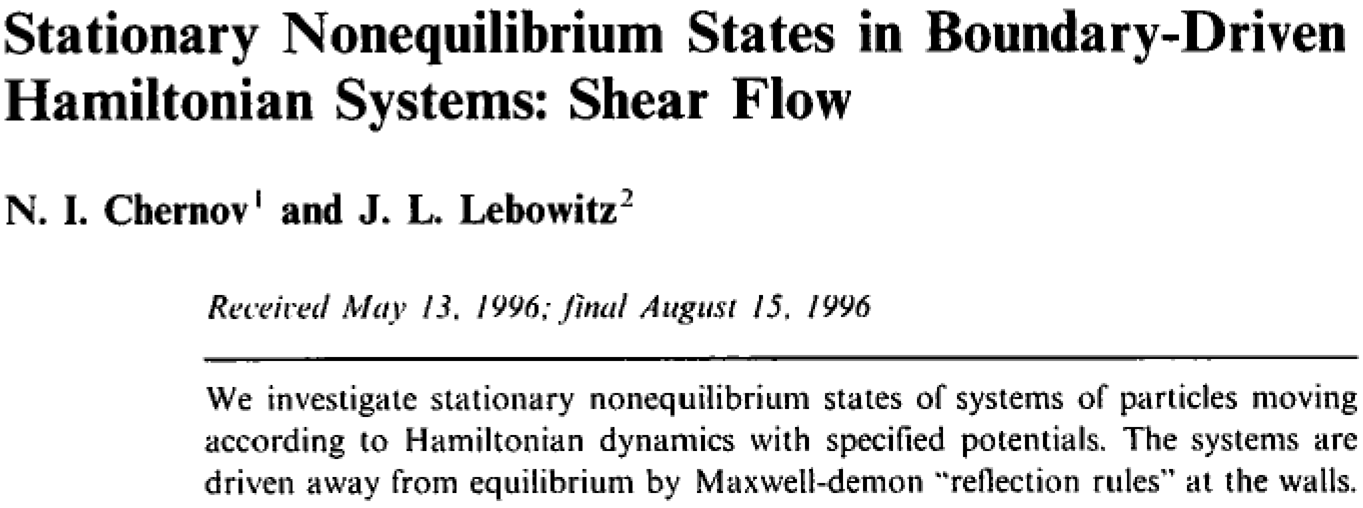
Part 2.



Stationary Nonequilibrium States in Boundary-Driven Hamiltonian Systems: Shear Flow

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We investigate stationary nonequilibrium states of systems of particles moving according to Hamiltonian dynamics with specified potentials. The systems are driven away from equilibrium by Maxwell-demon "reflection rules" at the walls.

Introduction

“ In the present paper we investigate a new class of models in which the microscopic dynamics in the bulk of the system are Hamiltonian and reflection at the boundaries are deterministic and energy conserving. This permits us to define a phase space flow $\dot{X} = \mathcal{F}(X)$, X a point in (a fixed energy surface of) the system’s phase space. In this respect our model is similar to the bulk thermostatting schemes mentioned earlier [6–8].

Unlike those schemes, however, which modify the equations of motion in the bulk of the fluid, something which is computationally useful but has no counterpart in real physical systems, our model is fully realistic away from the boundaries. In this respect it is similar to models in which the driving force is a “boundary layer” of reservoir particles or is given by stochastic thermal boundaries [4, 5, 19]. Our combination of realistic bulk dynamics and deterministic boundary drives offers a simple model of an mSNS [micro stationary nonequilibrium state] which can be investigated by means of classical dynamical systems theory. It will hopefully lead to a better understanding of SNS representing real systems.

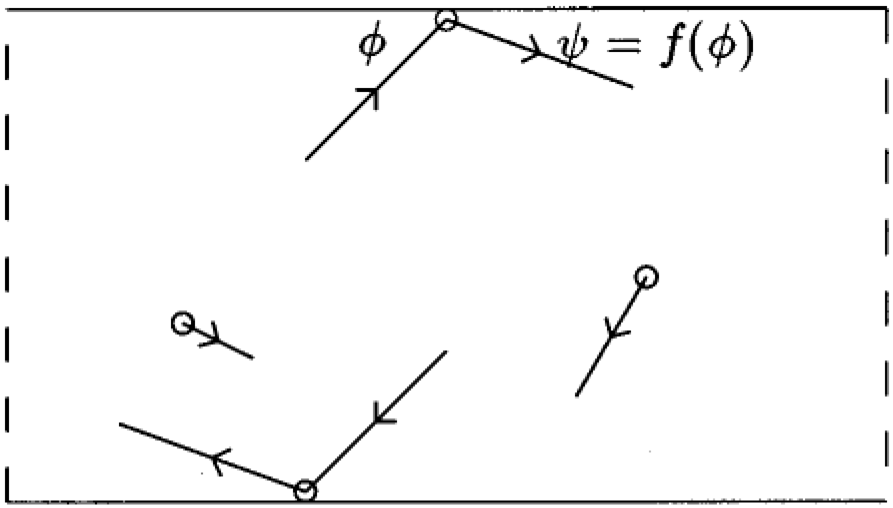

Figure 1: A schematic representation of the dynamics of the system.

Our main conclusion can be summarized as follows: Deterministic boundary driven models, reversible or not, accurately represent the bulk behavior of MSNS. There is an equality in these models between phase-space volume contraction, and hydrodynamic bulk entropy production for SNS of macroscopic systems in LTE. Plausible arguments of why this should be so and of how to connect entropy production in nonequilibrium states generated by different modelings of the inputs are given in section 8. ”

Lyapunov Instability of the Boundary-Driven Chernov–Lebowitz Model for Stationary Shear Flow

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We report on the computation of full Lyapunov spectra of the boundary-driven Chernov–Lebowitz model for stationary planar shear flow. The Lyapunov exponents are calculated with a recently developed formalism for systems with elastic hard collisions. Although the Chernov–Lebowitz model is strictly energy conserving, any phase-space volume is subjected to a contraction due to the reflection rules of the hard disks colliding with the walls. Consequently, the sum of Lyapunov exponents is negative. As expected for an inhomogeneously driven system, the Lyapunov spectra do not obey the conjugate pairing rule. The external driving makes the system less chaotic, which is reflected in a decrease of the Kolmogorov–Sinai entropy if the driving is increased.

KEY WORDS: Nonequilibrium steady states; Lyapunov instability; shear flow; computer simulations; many-body hard-disk systems.