Boundary Dissipation in a Driven Hard Disk System

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Abstract

A simulation is performed aiming at checking the existence of a well defined stationary state for a two dimensional system of driven hard disks when energy dissipation takes place at the system boundaries and no bulk impurities are present.
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Bulk dissipation is often assumed to explain stationary states in driven systems as in the well known example of Drude's theory of electrical conduction where three mechanisms act over a given interacting particle system:
(1) a constant force that accelerates the particles in a given direction,
(2) a thermal bath that should drive the system to an equilibrium state absorbing energy excess due to the action of the driving and
(3) an array of bulk impurities that introduce a strong chaotic behavior on the particle dynamics.

The stationary state is characterized by a net current of particles in the field direction generated by the external work per unit time done by the field over the particles equals the heat flux absorbed by the thermal bath. The existence of such stationary state is physically intuitive: bulk forcing is compensated by bulk dissipation and it can be seen in several computer simulations (see for instance [1]). Moreover, it is expected that the thermostat model used does not influence the system statistical properties [2, 5], but some other dynamical properties may depend on the particular dissipation scheme used [7].

Existence of a stationary state is, however, not so clear if the action of the thermostat is at the system boundaries and no impurities are present: the field tends to align the particles trajectories and the boundaries introduce a disorder "transversal" to the field and this is a bulk versus a surface effect.

In this case, a similar system studied in hydrodynamics seems to lead to a well defined stationary state: a model for the Poiseuille flow in the weak-flow regime. There, a group of interacting particles are subject to a small external gravitational field that drives the particle flow between two parallel plates that are kept at constant temperature while strongly interacting via long range forces. Several computer simulations of these system confirm that the heat generated by a bulk force is efficiently removed by the thermostats even though the dynamics in the bulk of the system is conservative: and the system evolves tending to a stationary state [3, 2]. This is different from other studies showing thermostats efficiency in cases in which thermostats act on the system through its boundaries but the driving force also acts on the boundary only, [4].

It appears uncertain, more generally, whether the boundaries and the likely intrinsic chaotic behavior of the system would compensate the action of a strong external field leading to establish a stationary state (the question has been recently again

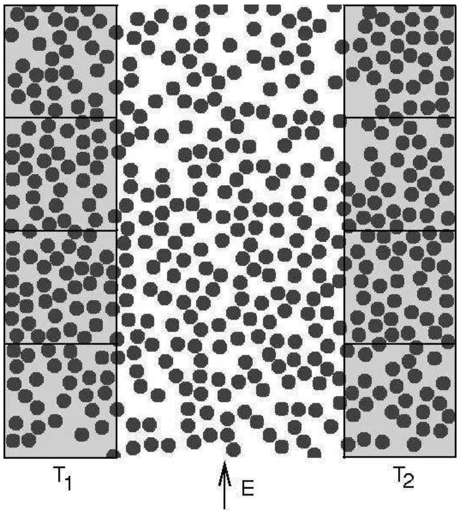

Figure 1: *Typical configuration of the model simulated. The disks in the white part (bulk particles) are accelerated in the y direction by a driving field E. The disks at the grey boxes act as thermal baths, keep constant their overall respective kinetic energies (temperatures T_1 and T_2) for all times. The disks interact each other with normal elastic collisions. The center of the disks may also elastically collide with the walls (black lines).*

raised in the literature, [5, 6, 8], and called the problem of *efficiency* of a thermostat mechanism) we consider worth studying in other cases the problem of whether a thermostat acting only on the boundary of the system is efficient enough to thermalize a system subject to *bulk* driving forces looking for other similar instances to add to the basic result in [3, 2]. The latter has been, to our knowledge, the first to show that such thermostats can actually be efficient to remove the heat generated by a bulk force even though the dynamics in the bulk of the system is conservative: and the system evolves tending to a stationary state.

A thermostat is "efficient" if it absorbs enough energy ("thermalizes") to forbid indefinite energy growth of a forced system.

In this note therefore we consider a system of hard disks under the action of a driving field and check that, within the range of external force strength that we are able to simulate, it appears to reach a well defined stationary state. Even for "strong" driving fields, although the thermostat acts only near the system boundaries, *i.e.* through very short range forces (in fact we consider hard core forces) between pairs of particles of the system and of the thermostats and between "mixed pairs" of system and thermostats particles.

The model consists of hard disks confined to a *unit box* and initially placed on a triangular lattice structure. The disks radius, r, is fixed so that the maximum number N_{max}, of particles in close-packing for a unit surface have a preassigned value. That is, $r = (\rho_{cp}/N_{max}\pi)^{1/2}$ where $\rho_{cp} = \pi/2\sqrt{3} \sim .9069$ is the close-packing mass density for hard disks: we take here $N_{max} = 10^4$ and hence $r = 5.3710^{-3}$.

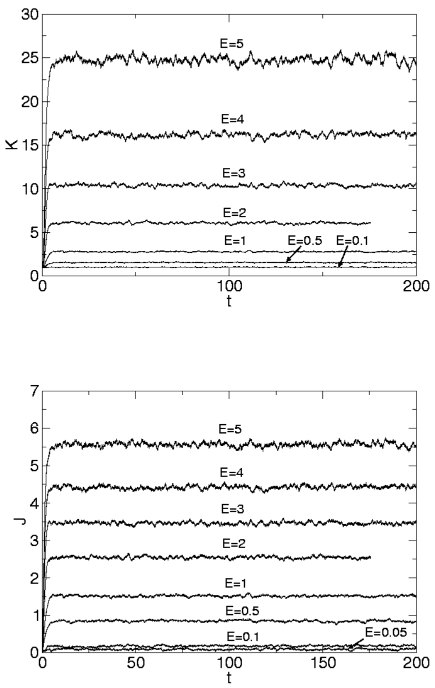

Figure 2: *Evolution of* $K = \frac{1}{2N}\sum_{i=1}^{N_{bulk}}(v_{xi}^2 + v_{yi}^2)$, *kinetic energy per particle (top) and particle current* $J = \frac{1}{N}\sum_{i=1}^{N_{bulk}} v_{yi}$ *on the y direction (bottom) for the bulk disks and for different values of the driving field.*

The box will be divided in three parts (see figure 1): a central part of width $1-2\alpha$ ("bulk") with top and bottom identifies ("vertical periodic boundary conditions") and two equal lateral parts of width α ("baths").

The actual number of disks placed in the bulk and in the bath parts are controlled by the corresponding densities of disks: ρ_{bulk} and ρ_{bath}. In our simulations we have chosen $\rho_{bulk} = 0.4$ and $\rho_{bath} = 0.5$. This implies that in our simulations the number of disks present in the bulk part is $N_{bulk} = 2301$, at each bath $N_{bath} = 1318$ and the total number is then $N = 4937$.

Disks dynamics depends on the sector they are. If a disk is in the bulk part it is subject *between collisions* to a uniform acceleration of magnitude E in the y direction while in the x direction its velocity keeps constant. The disks pertaining to the baths move at constant speed along its velocity vector.

In all cases, when the boundaries of two disks meet ("collision") they undergo an elastic collision. When the *center* of a disk hits any of the walls that define the region in which it is contained, it is elastically reflected. In this way we manage to keep disks confined at their respective regions and particles from the bulk may interact with particles in the thermal baths only across the walls.

Four equidistant walls along the x direction, see figure (1), in each bath prevent the disks of the bath having a net movement along the y direction induced by the interaction with the disks on the bulk.

The disks in each bath keep their total kinetic energy constant: $K_{1,2} = N_{bath} T_{1,2}$. This is achieved by the following prescription: when a disk from the bath collides with another of the bulk, the increment, Δ, of kinetic energy (positive or negative) that the bath particle suffers is immediately shared with the other particles of the bath by rescaling their speeds by the factor $(1 + \Delta/K_{1,2})^{-1/2}$ respectively.

Initially we let the system evolve during $100\,N$ collisions with $E = 0$: this is empirically sufficient to homogenize it spatially; next we turn on the driving field. Then, we take measures at intervals of N collisions during $10^5\,N$ collisions. We have simulated the cases with driving fields $E = 0.0001$, 0.0005, 0.001, 0.005, 0.01, 0.05, 0.1, 0.5, 1, 2, 3, 4 and 5 with $T_1 = T_2 = 1$.

Figure 2 shows typical evolutions of the kinetic energy per particle and the average current

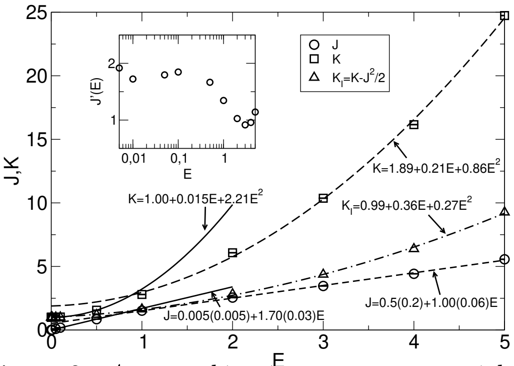

Figure 3: *Average kinetic energy per particle (K) and averaged particle current (J) at the system stationary state for the bulk disks. Lines are linear or square regression fits of the data. K_I is the internal kinetic energy per particle. Inset shows the forward discrete derivative of $J(E)$. Error bars are present.*

along the field direction of the bulk disks. After some short initial transient, apparently the system reaches a stationary state with a well defined current and kinetic energy.

Figure 3 shows the measured stationary values of the kinetic energy per particle and the particle current. We see that the hard disk system follow a nonlinear current-field response with: $J \simeq E$ and $K \propto E^2$ for large E while for small fields ($E < 1$) we see Ohm's law with a *larger* conductivity: $J \simeq 1.7E$ (see inset in Figure 3).

This behavior is consistent with the picture that the driving (that tends to align particles) seems to generate an intense enough interaction with the boundaries that disorders efficiently the bulk particles. If we consider the internal kinetic energy, $K_I = K - J^2/2$, (total kinetic energy minus the kinetic energy of the center of mass in the vertical direction) then we find that K_I increases quadratically with E exhibiting such disordering effect of the boundary interactions which has the effect of lowering the conductivity.

We have also studied the fluctuations distribution of $J(t)$ and $K(t)$ around its stationary average value. In particular the top of figure 4 shows the distribution of the observed values of $p(t) = J(t)/J$, $\Pi(p)$. We see that for $E \leq 1$ the measured distribution is compatible with a gaussian distribution

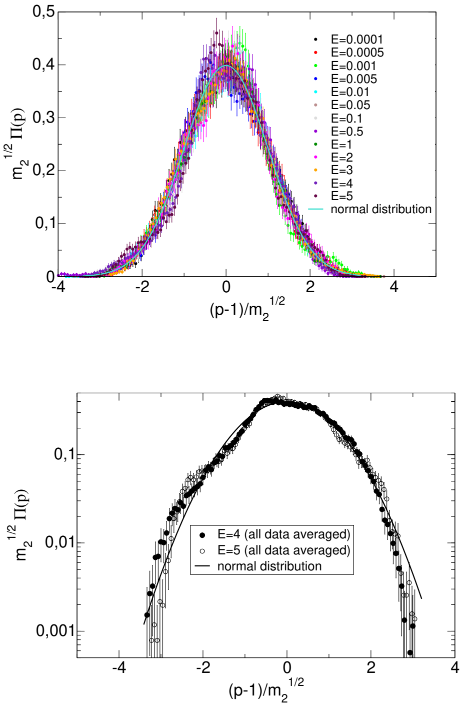

Figure 4: *Top: The measured probability distribution of $p(t) = J(t)/J$, $\Pi(p)$, at the stationary state for different electric fields. $m_2(E)$ is the observed variance of the $p(t)$ variable. Solid line is the normal distribution with zero average and variance one. Bottom: $\ln \Pi(p)$ vs. $(p-1)/m_2(E)$ plot for $E = 4$, $E = 5$.*

with an average value 1 and a variance $m_2(E)$ that depends on the electric field. However, systematic deviations from gaussianity is observed for large electric field (see bottom of figure 4). Moreover, in figure 5 we show the variance, $m_2(E)$, of $J(t)/J$ and $K(t)/K$ for different values of E. We see while $m_2(E)$ for the kinetic energy depends weakly on the electric field, the variance for the current decays with E as a power: $m_2(E) \simeq E^{-1.7}$ from $E = 0.001$ to $E = 1$. That is, for $E << 1$ a large set of particles are able to move in the $-E$ direction. This behavior is strongly suppressed as the field increases and, for $E > 1$ most of the particles move along the field. Note that the large error bars due to the limited amount of data obtained in this simulation obscures the analysis of the large deviations properties of $p(t)$ and so we are not able to check the fluctuation theorem as proposed in [6].

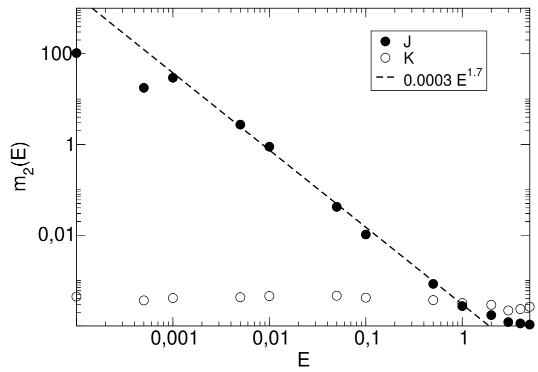

Figure 5: *The observed variance $m_2(E)$ of $J(t)/J$ and $K(t)/K$ versus the electric field. Dashed line is guide to the eye showing the power law behavior $E^{-1.7}$.*

Finally we have computed the correlation between the current and the energy at the stationary state: $C_{J-K} = \langle J(t)K(t)\rangle/JK - 1$. For all cases C_{J-K} is compatible with zero within error bars. That is, on the stationary state both magnitudes are uncorrelated and, for instance, the value of the system kinetic energy is independent on the sign of the current for a given configuration.

Further investigations could be done by changing the temperatures of the thermostats to two different values.

References

[1] T. Yuge, N. Ito and A. Shimizu, *Nonequilibrium molecular dynamics simulation of electric conduction*, Journal of the Physical Society of Japan, Vol. 74, 1895-1898 (2005).

[2] G. Ayton, E. Evans and D. Searles, *A local fluctuation theorem*, Journal of Chemical Physics, Vol. 115, 2033–2037, 2001.

[3] B.D. Todd, D.J. Evans and P. Daivis, *Pressure Tensor for inhomogeneous fluids*, Physical Review E, Vol. 52, 1627-1638, 1995; B.D. Todd and D.J. Evans, *Temperature profile for Pouiseuille flow*, Vol. 55, 2800-2807, 1997.

[4] F. Bonetto, N. Chernov and J. L. Lebowitz, *(Global and Local) Fluctuations in Phase-space Contraction in Deteministic Stationary Nonequilibrium*, Chaos, Vol. 8, 823–833, 1998.

[5] G. Gallavotti, *Nonequilibrium Thermodynamics?*, in Meteorological and geophysical fluid dynamics: ed. Wilfried Schroeder, Science, Bremen 2004 (and cond-mat/0301172) and in G.Gallavotti, F.Bonetto, G.Gentile, *Aspects of the ergodic, qualitative and statistical properties of motion*, Springer–Verlag, Berlin, 2005, p. 397–409.

[6] G.Gallavotti, *Stationary nonequilibrium statistical mechanics*, in Encyclopedia of Mathematical Physics, ed. J.P. Francoise, G.L. Naber, T.S. Tsun, Vol. 3, 530–539, 2006, Elsevier, (cond-mat/0510027) and *Irreversibility time scale*, Chaos, Vol. 16, 023130 (+7), 2006 (and cond-mat/0601049).

[7] R. Klages, *Microscopic chaos and transport in thermostated dynamical systems*, nlin/0309069.

[8] D. Ruelle. *Nonequilibrium statistical mechanics and entropy production in a classical infinite system of rotators*, cond-mat/0603760.