Eur. Phys. J. B **25**, 135–138 (2002)
DOI: 10.1140/epjb/e20020015

THE EUROPEAN PHYSICAL JOURNAL B
EDP Sciences

Separation of dissipation from diffusion

Tong Zhou[a]

Department of Physics, University of California, Santa Barbara, CA 93106, USA

Received 30 August 2001

Abstract. We study velocity correlations induced by diffusion and dissipation in a simple dissipative dynamical system. We observe that diffusion, as a result of time reversible microscopic processes, leads to correlations with different spatial parity from those caused by dissipation, consisting of time irreversible microscopic processes. The velocity correlations observed conflict with the "molecular chaos" assumption of the Boltzmann equation. To account for the apparent correlation structures in our simple model system, we propose that they indicate geometric distortion of the phase space.

PACS. 05.70.Ln Nonequilibrium and irreversible thermodynamics – 05.60.Cd Classical transport – 02.40.-k Geometry, differential geometry, and topology

The second law of thermodynamics states that a system left to itself will evolve towards a state with maximum entropy, *i.e.* maximum randomness. We are familiar with order due to interaction where, for example for systems in equilibrium at certain temperature, different strength of interaction among microscopic constituents leads to states with different degrees of order – solid, liquid, or gas. In this paper we study a different type of order, order purely induced by diffusion and dissipation.

Nonequilibrium phenomena have long attracted much research interest. The Boltzmann equation is probably the most celebrated theory, yet its crucial assumption of "molecular chaos" needs scrutiny before it can be applied to specific systems, see for example [1]. Linear response theory [2] also has wide applications in condensed matter physics. Some of recent studies include derivation of Ohm's Law for the periodic Lorentz gas [3], the connection between the smoothness of distribution function and the number of degrees of freedom [4], finite and anomalous thermal conductivity in 1d lattices [5] and directed current in a 1d system [6], on nonequilibrium phase transition [7], and on violation of the fluctuation-dissipation equality [8], among others. However many theoretical works done on nonequilibrium phenomena, to different extent, assume certain mathematical forms as the starting point of their investigations, which, though making the problems at hand mathematically attackable, may miss generic properties of real physical systems because of the limitation of the forms being used. On the other hand, with the development of modern computer technology, numerical experiments have become a very powerful tool. Here we carry out our investigation by applying extensive numerical studies on a simple model system, and try to form an understanding based on these results, without introducing any *ad hoc* mathematical functional forms to characterize the system.

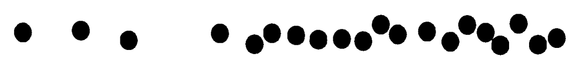

Fig. 1. A snapshot of the thin pipe system. The periodic side walls are indicated by dashed lines. The coordinate system is set up so that the x-axis is along the pipe.

We study a two-dimensional system of identical non-interacting hard disks confined in a thin pipe (Fig. 1). The width of the pipe is set so that two disks cannot pass each other. Thus the motion of the disks is two dimensional, while at the same time their sequence is preserved. The two side walls are periodic and the two end walls are energy sources kept at the same temperature. For more details, see [9,10]. We use the simplest collision model – after a collision between two disks, the normal relative velocity changes sign, and decreases by a factor of the restitution coefficient r, with $0 \leq r \leq 1$. In the collision, the other components of the velocities are unchanged. Thus the total momentum is conserved while a portion of kinetic energy is lost when $r < 1$. Simulations are for 80 disks and the average spacing between two neighboring disks are much larger than their radii. Statistical analysis is done for the steady state. Different versions of one-dimensional diffusion models are used in [5–7]. However, they rely on preset diffusion equations as their starting point, while we are attempting to find out the physical rules which will lead to those equations. For a review of the current status for such effort, see [11].

[a] e-mail: tong@physics.ucsb.edu

Even with this simple model, we nevertheless limit ourselves to situations close to equilibrium. Extensive works have been done on such systems where linear deviations from equilibrium are generally observed and studied [2–4,12]. In our system, the details of the setting are so clearly defined that we may attempt to obtain a thorough understanding of the linearity, which then may point to the direction for further study on situations farther away from equilibrium.

One of the cornerstones of classical kinetics theories, Liouville's theorem states that the phase space volume is a conserved quantity [12–14]. The importance of underlying geometry of the phase space is especially stressed in [15]. It is long recognized that energy dissipation makes phase space tend to shrink [9]. We would like to investigate the effects of this deviation from Liouville's theorem on the dynamics. The set up of the system is to create a very small, yet uniform dissipation and look for its first order effects. To stay away from disturbing the internal dynamics, we put energy sources only at the end walls. However, in this way we cannot have energy dissipation without energy diffusion. There are two processes going on in the system. First, energy dissipation due to inelastic collisions, which to the first order is uniform. Second, energy diffusion, meaning energy conduction from the end walls into the system, which at a certain location is proportional to its distance to the center – at the center there is no net diffusion in either direction due to symmetry. Energy conduction also exists in a similar system with elastic collisions between disks but two end walls at different temperature, which we will treat later. The coexistence of diffusion and dissipation is a general feature in dissipative systems. We will demonstrate that they can be separated due to different spatial parities they exhibit in our system.

We concentrate on correlations among x-components, *i.e.* along the pipe, of velocities as an indicator of internal orders. For a system at equilibrium, even when there are interactions among its constituents, their velocities obey Gaussian distribution and thus are uncorrelated. The influence of a particle's motion on other particles' velocities is an indicator of order, and we quantify this order with velocity correlations. Specifically, among other things, we look at $\langle u_i|v_j\rangle$, meaning the conditional time average of the x-component of velocity of the ith disk when v_j is given, where $v_j \equiv u_{j+1} - u_j$. Of course, $\langle u_i\rangle$ by itself vanishes because in the statistical steady state there is no average drift in disks' positions.

A somewhat more simplified quantity is the collision average [10], denoted by $\langle u_i\rangle_j$, which is the average of u_i when the jth disk is colliding with the $(j+1)$th disk. For a system in equilibrium, this quantity vanishes when i is neither j nor $j+1$. However, in our system, it does not vanish, but exhibits regular and interesting patterns. We can plot $\langle u_i\rangle_j$ as a function of i for several different j's – the resulting curves are confusing. But if we plot the odd and even parity components of these curves, they are easily identified as dissipation and diffusion, respectively.

The odd parity component, *i.e.* $\langle u_i - u_{2j+1-i}\rangle_j$ is for dissipation – they overlap for different value of j's (Fig. 2),

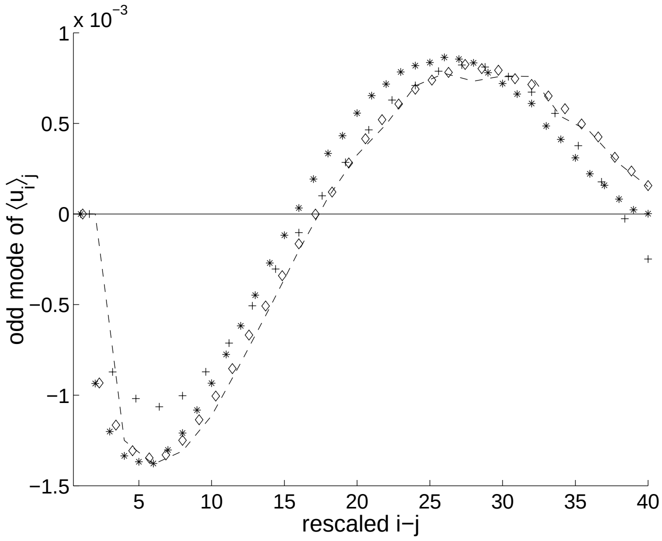

Fig. 2. The odd parity component of $\langle u_i\rangle_j$. $(*)$ is for $j=40$, $(\diamond)$ for $j=35$ and $+$ for $j=25$. The horizontal axis is for $i-j$ rescaled so that the closest boundary to j is shown at 40. Only the positive half of $i-j$ is shown. The system has 80 disks, $r=0.995$ and the two end walls are set to the same temperature. The vertical axis is without rescaling, demonstrating a uniform correlation structure from uniform dissipation. The dashed line is the corresponding rescaled curve for a system of 40 disks and $r=0.99$.

a clear signature for uniform dissipation. Apparently, dissipation due to collision between two neighboring disks has effects on the motions, not just of several disks close to them, but of all the disks in the system. The even parity component, *i.e.*, $\langle u_i + u_{2j+1-i}\rangle_j$ is for diffusion—they are proportional to the distance between j and the center $j=40$ (Fig. 3), a signature that they are caused by energy conduction which is also proportional to this distance.

For a further test, we run simulations for a system with similar set up, but with elastic collisions and the two end walls are kept at different temperatures so that no dissipation, only diffusion occurs. The odd parity component of the curves vanishes. And $\langle u_{i-j}\rangle_j$ is independent of j, corresponding to uniform diffusion. Also $\langle u_i\rangle_j$ can be rescaled to overlap with the even parity components from the dissipative system (Fig. 3).

Heuristically, we can explain the different spatial parities by pointing out that dissipation consists of time irreversible microscopic processes while diffusion consists of only time reversible microscopic processes. In the system with no dissipation but only constant diffusion, when the jth disk is colliding with the $(j+1)$th disk, let us consider the following two operations: time reverse and a spatial parity operation that reverses the direction of x-axis and interchanges ith disk with $(2j+1-i)$th disk. These two operations leave the energy flux unchanged and connect two equally probable microscopic states. Because u_i in one state is the same as u_{2j+1-i} in the other state, we see the correlation curve from diffusion has even spatial parity. The odd parity for the

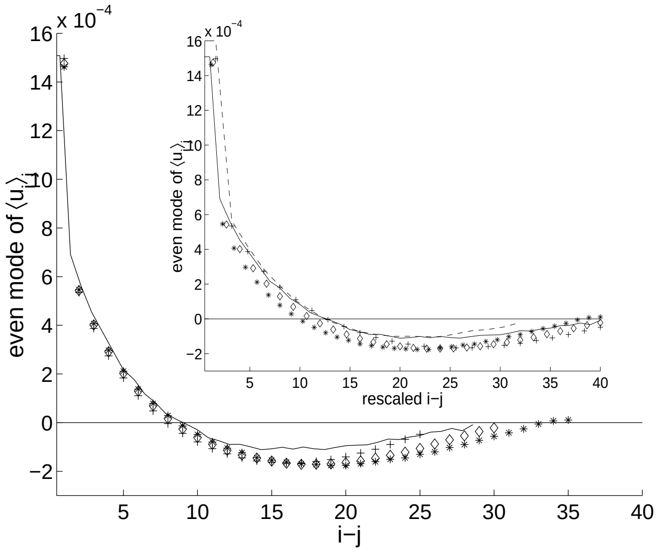

Fig. 3. The even parity component of $\langle u_i \rangle_j$. ($*$) is for $j = 35$, ($\diamond$) for $j = 30$ and $+$ for $j = 25$. The horizontal axis is for $i - j$ without rescaling. Only the positive half of $i - j$ is shown. For $j = 35$, the vertical coordination plotted is the real number divided by 5 for the energy flux at $j = 35$ supplies dissipation caused by 5 disks; for $j = 30$, it is the real number divided by 10; for $j = 25$, it is the real number divided by 15. These three curves overlap, showing that the even mode is proportional to the distance between j and the center. The solid line is the corresponding rescaled curve for an elastic system with only energy diffusion; its $i-j$ value is rescaled. The inset is a similar plot, with rescaled $i - j$ as the horizontal axis, also shown as the dashed line is a corresponding curve from a elastic system with 40 disks.

correlation curve from dissipation is intuitively reasonable, given dissipation causes the shrinkage of phase space volume.

The correlation curves from diffusion and dissipation have following properties. They are independent of the width of the pipe. The diffusion curves are not sensitive as to where the boundaries are – curves for different collision number j's can overlap though the distances from j's to the boundaries are different. However, they are not for local structures. The inset of Figure 3 shows the overlapping between diffusion curves for systems with 80 disks (solid line) and 40 disks (dashed line), only after suitable rescaling of $i - j$, which suggests they are roughly functions of $(i - j)/N$. This is true also for dissipative curves, which only overlap with one another after rescaling of $i-j$ (Fig. 2). These observations suggest that the structures from dissipation and diffusion are global.

In the rest part of this paper, we describe our detailed investigation of correlation curves for diffusion. For this purpose, the simulations are for systems with elastic collisions and different temperatures at two ends. We look at the conditional time average of u_i when v_j and x_j are given, where x_j is the spacing between jth and $(j + 1)$th disks, and find (Fig. 4),

$$\langle u_i | v_j, x_j \rangle = c_{i-j} \left[(v_j^2 - \langle v_j^2 \rangle) + f(x_j - \langle x_j \rangle) \right], \qquad (1)$$

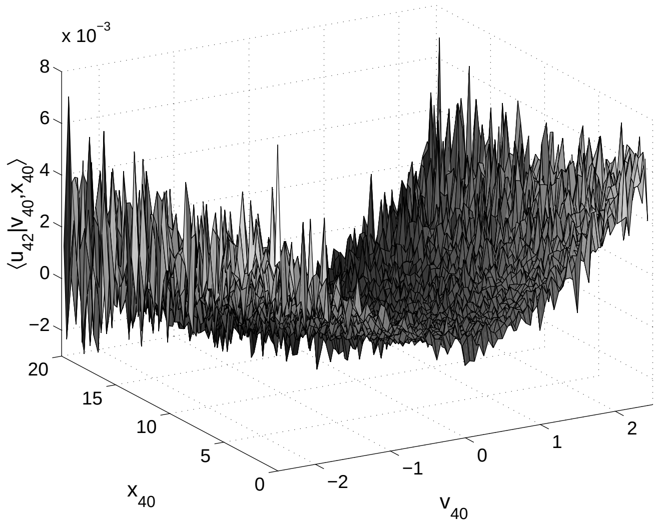

Fig. 4. $\langle u_{42} | v_{40}, x_{40} \rangle$. Though noisy, the surface plot shows a linear dependence on x_{40} and a quadratic dependence on v_{40}.

where f is a constant. This suggests that the effects of v_j on u_i are independent of those from x_j and we can concentrate on just the velocities:

$$\langle u_i | v_j \rangle = c_{i-j} (v_j^2 - \langle v_j^2 \rangle). \qquad (2)$$

It is not difficult to understand this relation for $i = j$. Let us consider $\langle u_j + u_{j+1} | v_j \rangle$ as a function of v_j. It cannot be a constant because $\langle (u_j + u_{j+1}) v_j \rangle = \langle u_{j+1}^2 - u_j^2 \rangle < 0$ while $\langle v_j \rangle = 0$. It cannot have a linear term proportional to v_j either because when jth disk collides with $(j+1)$st disk, v_j changes sign while $u_j + u_{j+1}$ is unchanged due to momentum conservation. Then the simplest form $\langle u_j + u_{j+1} | v_j \rangle$ can have is a constant times $v_j^2 - \langle v_j^2 \rangle$, as in (2). Though conforming to quite general arguments, the above observation is in contrast to the "molecular chaos" assumption of the Boltzmann equation, the assumption that makes the equation time irreversible.

It is counterintuitive that (2) does not vanish when i is neither j nor $j + 1$. The evidence shown in Figure 3 implies a global structure yet depending on local inhomogeneity. We propose an approach based on geometric distortion of the phase space. Let us think the phase space as a Riemannian manifold with a metric g for the usual (p, q) coordinate system [15]. The statistical probability density ρ is a scalar. But the probability of the system in the neighborhood of a point is proportional to $\rho\sqrt{g}$. One approach would be to view the phase space as a simple Euclidean manifold with a trivial g, then ρ has to account for the interesting but puzzling correlation structure. Another approach, which we prefer, is to set ρ to a constant, and view the correlation pattern as an indication of the distortion of the phase space and thus a non-constant g.

In this approach, because the distortion of the phase space, the variables u_i's are no longer statistical independent and the corresponding coordinate system no longer orthogonal. Let us assume a new set of independent variables u_i''s deviates from the original set to the first

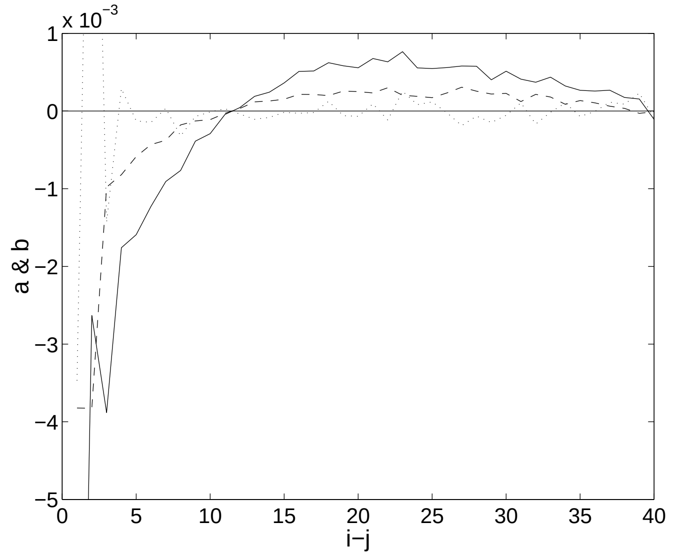

Fig. 5. Coefficients $a(i-j)$ and $b(i-j)$ in (4). Solid line is for a and dashed line for b. The first data point of a is not shown, which at about -0.01. The dotted line is $a-2.5b$ and is close to 0.

order:

$$u_i' = u_i + \epsilon F(\Gamma), \qquad (3)$$

where ϵ is proportional to the small inhomogeneity, and Γ denotes the set of u_i's. Because $\langle u_i'|v_j\rangle = 0$ by definition, we have $\langle u_i|v_j\rangle = -\epsilon\langle F(\Gamma)|v_j\rangle_0$. The subscript 0 in the last expression indicates that only the zeroth order is needed, which can be extracted from numerical data. From the somewhat noisy data, we find (3) takes the form,

$$u_i' = u_i + \sum_{j=1}^{N-1} a_{i,j} v_j^2 + \sum_{j=1}^{N-2} b_{i,j} v_{j-1} v_j + C, \qquad (4)$$

where C is a constant that keeps $\langle u_i'\rangle = 0$. Let us for the moment ignore boundaries and write the coefficients as $a(i-j)$ and $b(i-j)$ respectively. $b(i-j)$ can be obtained by noticing:

$$\langle u_i|v_{j-1}, v_j\rangle - \langle u_i|v_{j-1}, -v_j\rangle = -2b(i-j)v_{j-1}v_j. \qquad (5)$$

Then in turn $a(i-j)$ can be obtained by substituting $b(i-j)$ into

$$\langle u_i|v_j\rangle = \left[-a(i-j) - \frac{1}{4}a(i-(j-1)) - \frac{1}{4}a(i-(j+1)) + \frac{1}{2}b(i-j) + \frac{1}{2}b(i-(j+1))\right] v_j^2. \qquad (6)$$

We use numerical data from $\langle u_i|v_{40}, v_{41}\rangle$ to extract values of $a(i-j)$ and $b(i-j)$ and plot the result in Figure 5.

We can assume the metric under the coordinate system u_i' diagonal. Then by the relation between two coordinate systems (3), we can obtain the metric g under the original coordinate system of u_i's. Because the metric g is connected to the strain tensor [16], we see how the correlations indicate the distortion of the phase space.

Because we study the behavior of the system very close to equilibrium, we expect a smooth distribution function in the phase space, agreeing with the approach of Tuckerman *et al.* [15]. However, when the inhomogeneity is stronger [17], there is likely to be a transition in the dynamics and the distribution function becomes fractal as suggested by Hoover, *et al.*

In this paper, we present numerical results of velocity correlations in a simple model of nonequilibrium system and propose to interpret the observation as an indication of geometric distortion of the phase space. However, most theoretical reasonings in the paper are heuristic arguments. We did not attempt to formulate a fundamental theoretical framework because we feel further data collecting, and more importantly, different, more general setting of the system should be tested before a better understanding can be reached. A simple extension would be the testing of a similar system, but with two dimensional close-packed disks.

This work was supported by EPRI/DoD through the Program on Interactive Complex Networks, and NSF Grant No. DMR-9813752, and by a grant from the Keck Foundation.

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