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IRREVERSIBILITY IN THE TWO-BODY HARD-DISK LORENTZ GAS

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Abstract—Time-reversible modifications of Newton's equations of motion have been used to simulate irreversible isothermal shear flows. The modified equations have stable solutions for periodic systems with as few as two or three particles. These small-system solutions exhibit thermodynamic irreversibility, entropy production and realistic nonlinear constitutive behavior.

1. INTRODUCTION

IT IS PARADOXICAL that the basis of macroscopic irreversibility lies in reversible microscopic equations of motion. The unidirectional dissipation described by the second law of thermodynamics is a subtle consequence of instabilities in the reversible equations of motion of Newton and Schroedinger. Boltzmann clarified the origin of thermodynamic irreversibility in isolated dilute-gas systems obeying reversible Newtonian dynamics [1]. He pointed out that a statistical distribution of dynamically reversible Newtonian collisions must result in macroscopic irreversibility. This surprising result was challenged by Poincare and Zermelo, who pointed out that an isolated system will eventually return arbitrarily closely to its initial coordinate-velocity state. Thus there could hardly be long-time net motion away from even an "unlikely" starting point. To this "recurrence" objection Loschmidt added a "reversal" objection. Suppose a Newtonian system did develop "irreversibly." Then, because Newton's equations of motion are reversible in the time, a reversed version of the irreversible trajectory would run back to the initial spatial configuration. The objections of Poincare, Zermelo and Loschmidt were damaging to kinetic theory, but not disabling. Boltzmann countered these objections with physical arguments. Both objections are unreasonable, but for slightly different reasons: recurrence typically requires a time of order $\exp(N)$ for N particles, greatly exceeding the age of the universe; reversibility over a time span of this length would require a knowledge of the trajectories to a precision of one part in $\exp(N)$. The information required to implement either recurrence or reversibility greatly exceeds the precision with which coordinates and velocities can be known or predicted. More recently, Prigogine has devoted a book [1] to the understanding of irreversibility's basis. He concludes that "Theoretical reversibility arises from the use of idealizations in classical or quantum mechanics that go beyond the possibilities of measurement performed with any finite precision."

Nevertheless, it is still difficult to "understand" irreversibility, due to the lack of systems which are not only simple to analyze but also thermodynamically irreversible. Fast computers have enhanced our understanding of the microscopic basis of irreversibility. Computer simulations of many-body systems have been carried out for about 40 years. The simulations have led to a fairly thorough understanding [2] of the equilibrium thermodynamic properties of simple systems. The transport properties for these same systems are now undergoing intensive investigation. This transport work has led to special equations of motion, designed to simulate shear flows and heat flows. The new transport methods have been applied to a variety of fluid [3] and solid [4] systems. Because these systems typically involve hundreds of degrees of freedom there is no prospect for understanding their behavior analytically. For this reason we have studied very small, two- and three-body, systems using the same many-body techniques. These small systems exhibit the same thermodynamic irreversibility as do the larger many-body systems [5]. Here we exploit this parallel to shed new light on the microscopic mechanism for macroscopic irreversibility.

In Section 2, we review the equations of motion describing steady isothermal shear. In Section 3, we discuss the numerical and statistical solutions of these equations, applied to the two-body problem. This two-body problem reduces to the study of a periodic "Lorentz gas," in which a light particle scatters from a shearing periodic lattice of massive scatterers. In Section 4 we consider, from a physical standpoint, the nature of irreversibility exhibited by these formally-reversible two-body systems.

2. EQUATIONS OF MOTION

Homogeneous periodic shear is the simplest hydrodynamic fluid flow exhibiting irreversibility. Here we consider the case in which the horizontal (x) velocity increases linearly with the vertical (y) coordinate:

$$\dot{x} = \dot{\epsilon} y. \tag{1}$$

For values of the strain rate $\dot{\epsilon}$ which are not too large, (1) describes a steady laminar flow. This macroscopic description is still incomplete because the source of the work driving the flow and the sink for the heat produced have not yet been specified.

Now consider a microscopic description of the same flow (1). In a microscopic many-body system, made up of particles obeying atomistic equations of motion, individual particles have velocities distributed about the mean hydrodynamic value, $\dot{\epsilon} y$. From the microscopic point of view the temperature of such a system is described by the fluctuations of the atomistic velocities about this mean value. By considering these fluctuations explicitly, we can base a treatment of hydrodynamic shear on a modification of microscopic Hamiltonian mechanics. Let the momentum $p = (p_x, p_y)$ describe the thermal velocity fluctuations around the mean value, so that the velocity of a particle at $q = (x, y)$ has x and y components $(p_x/m) + \dot{\epsilon} y$ and (p_y/m), respectively, where m is the

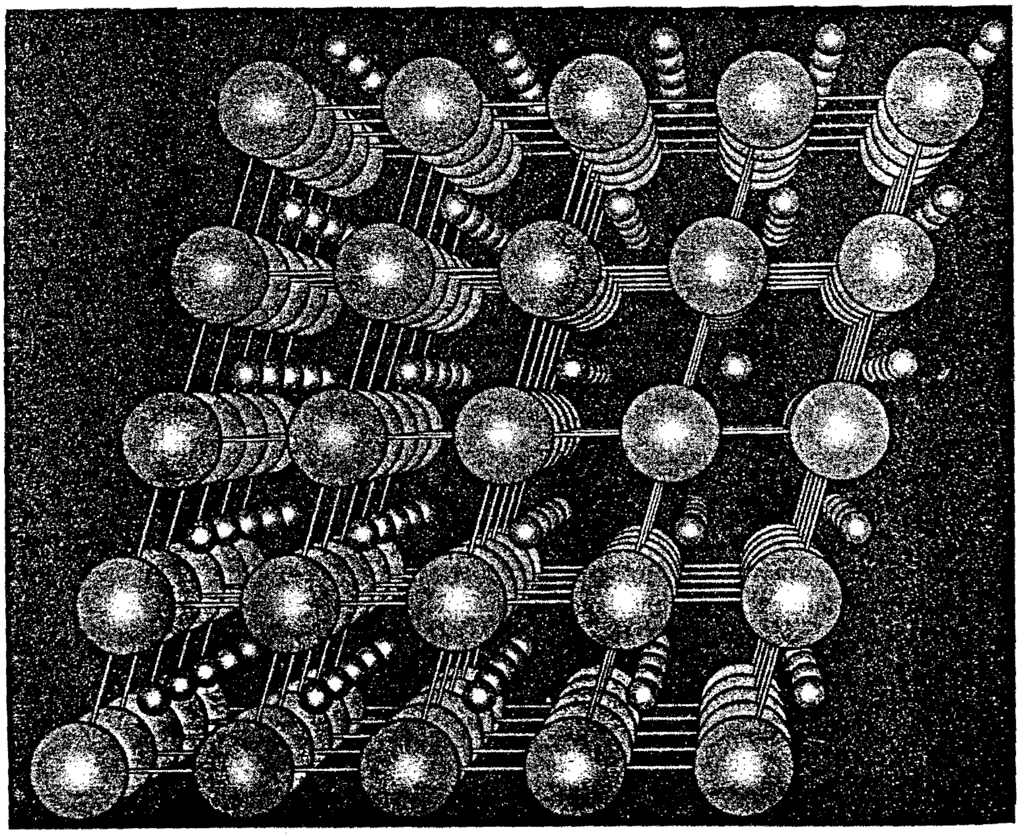

Fig. 1. A two-particle hard-sphere system undergoing periodic homogeneous shear. Figure generated using the Nelson Max "ATOMLLL" computer program.

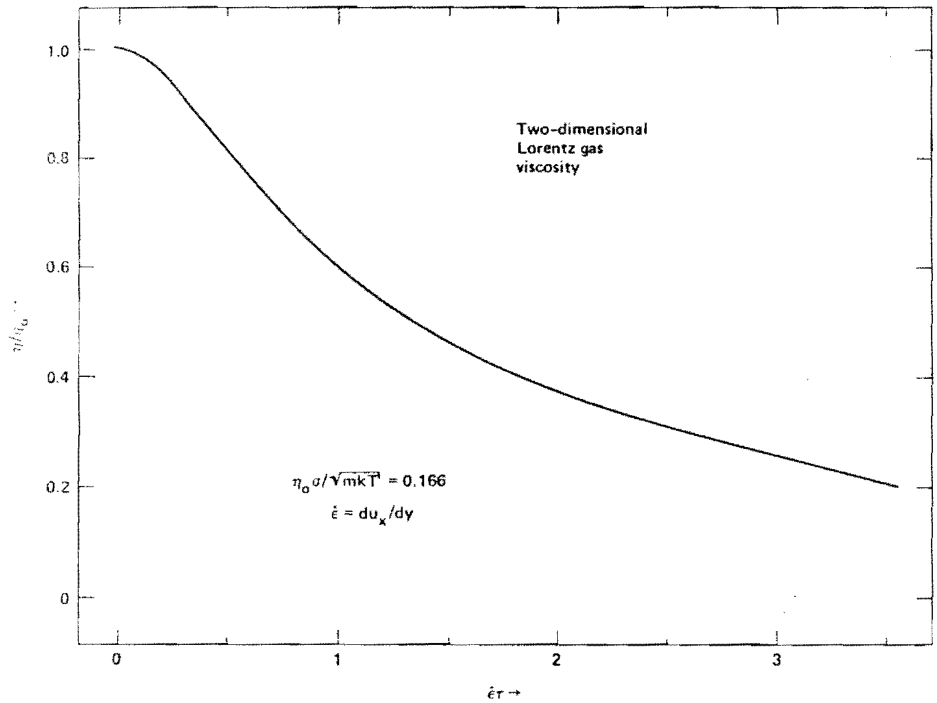

Fig. 2. Shear viscosity for two hard disks, as calculated from the corresponding Boltzmann equation. Here $1/\tau$ is the collision rate. For the range of strain rates $\dot{\epsilon}$ shown, shear stress is an increasing function of strain rate, but the increase is less rapid than linear.

atomic mass. Then the flow field (1) can be obtained from a microscopic Hamiltonian which depends explicitly upon the strain rate $\dot{\epsilon}$:

$$H = H_0 + \dot{\epsilon} \sum y p_x; \qquad H_0 = \Phi + \sum (p^2/2m). \tag{2}$$

In (2) Φ is the potential energy, typically including $N(N-1)/2$ pair terms, and the sum includes all N particles in the system. The equilibrium Hamiltonian H_0 corresponds to the hydrodynamic internal energy. To see that the rate-dependent nonequilibrium Hamiltonian (2) does properly reproduce the macroscopic flow field, apply Hamilton's

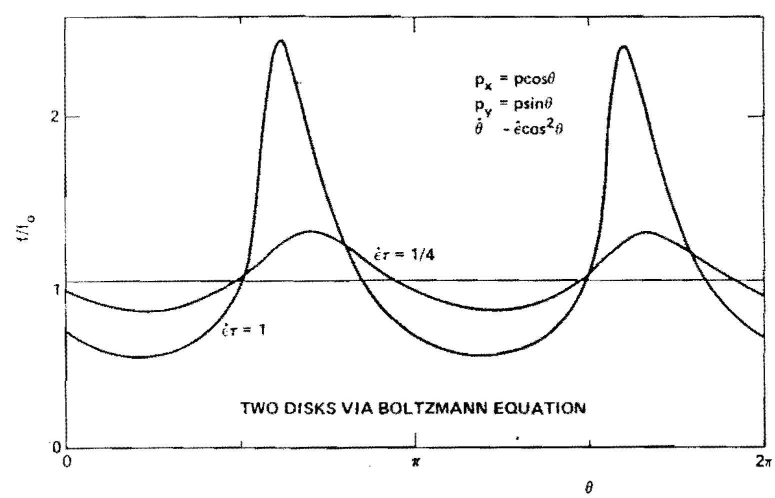

Fig. 3. Distribution function for the momentum in the nonequilibrium steady state. The distribution results from the balance of the circulation in the equations of motion with the randomizing effect of collisions.

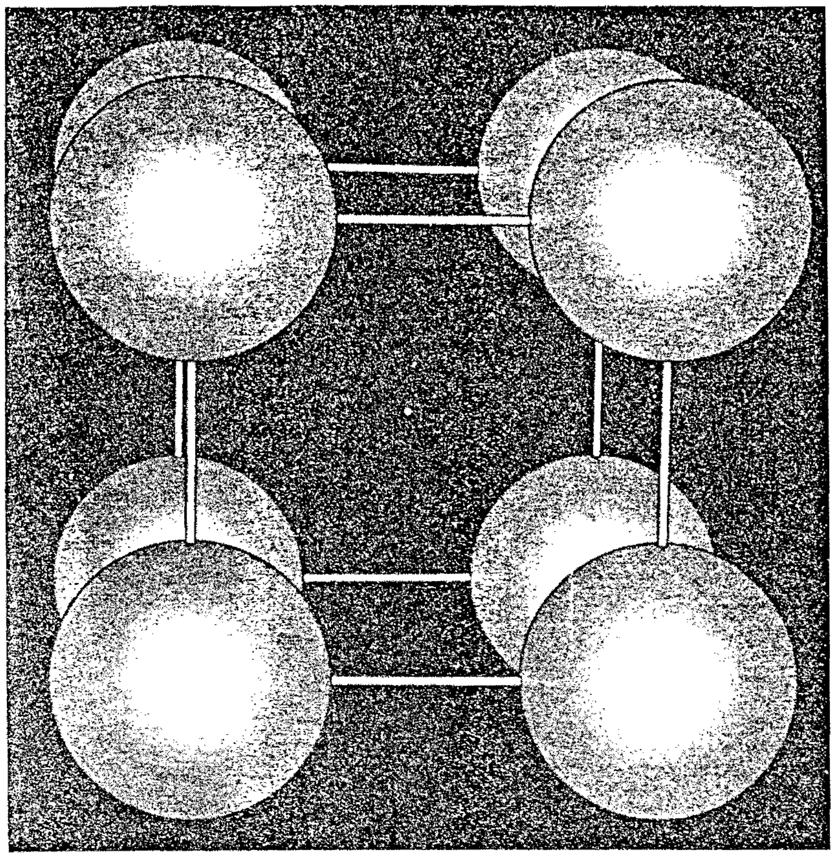

Fig. 4. Three successive views showing the divergence of neighboring configuration-space trajectories for two three-dimensional hard spheres of diameter σ, mass m, and speed l. The equivalent Lorentz-gas problem, in which a point particle, with mass $m/2$ and speed 2, scatters from an infinitely-massive particle with *radius* σ is shown. The periodic cell has volume $10^{3/2}\sigma^3$. The points shown represent 125 separate numerical solutions of the equations of motion, with slightly different initial coordinates. The second and third views show the trajectory positions after shear strains of four and eight, so that the periodic lattice of larger particles is again a simple cubic lattice in each view. Figure generated using the Nelson Max "ATOMLLL" computer program.

equations of motion, $\dot{q} = \partial H/\partial p$ and $\dot{p} = -\partial H/\partial q$. For the two-dimensional shear flow described by (1) and (2), the following microscopic equations result:

$$\dot{x} = \partial H/\partial p_x = (p_x/m) + \dot{\epsilon}y; \qquad \dot{y} = \partial H/\partial p_y = (p_y/m); \tag{3}$$

$$\dot{p}_x = -\partial H/\partial x = F_x; \qquad \dot{p}_y = -H/\partial y = F_y - \dot{\epsilon}p_x. \tag{4}$$

In order to implement these equations boundary conditions must be specified. Periodic boundaries work best because they eliminate the stratification associated with flat physical boundaries. To avoid discontinuities in the flow field it is necessary to generalize the periodic boundaries to include shear, as is illustrated in Fig. 1. From the figure it can be seen that the "system"—that is, a unit cell of the periodic structure—is undergoing shear imposed by moving images above and below. One might expect, and calculation confirms, that such a system would tend to heat up, so that the eqns (3) and (4) do not lead to a steady state. A steady state can be obtained by adding the further restriction that a thermodynamic state variable, such as pressure, energy or temperature, be a constant of the motion. Such a restriction can be implemented in several ways [6] and it is not obvious, on physical grounds, which choice is best. Gauss suggested that the best way to impose constraints on a mechanical system is to use the minimum constraint forces possible. We can apply this suggestion to the shear flow problem. Consider the possibility

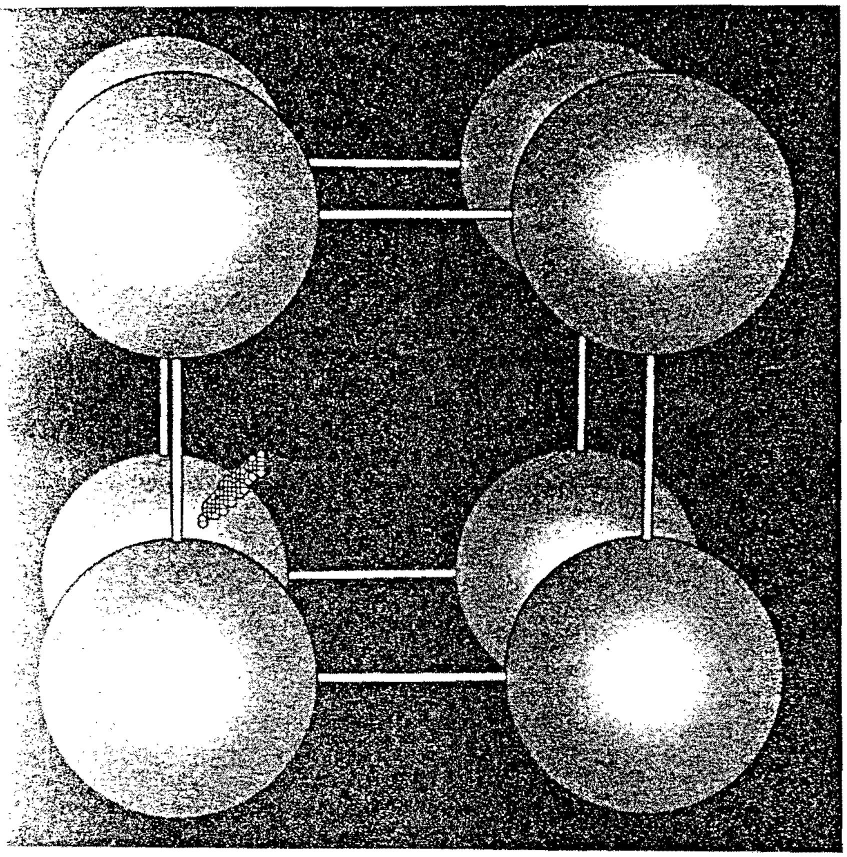

Fig. 4 (*Continued*). Second view.

of making the flow isothermal, with the (internal part of the) kinetic energy $\sum (p^2/2m)$ fixed, where again the sum runs over all N particles in the system. In this case Gauss' suggestion leads to the addition forces of constraint:

$$\Delta\dot{p} = -\zeta p; \qquad \zeta = \sum [(F \cdot p/m) - \dot{\epsilon}(p_x p_y/m)]/\sum (p^2/m). \qquad (5)$$

Calculations, described in more detail in the following sections, show that the system of eqns (3)–(5) does result in a steady, homogeneous isothermal shear flow.

It should be noted that these equations, just like Newton's, are time reversible. We mean by this that a movie of the motion, run backwards, would still satisfy the same motion equations. In the reversed version of the movie the variables x, y, $\dot{p}_x$, $\dot{p}_y$, F_x and F_y have the same numerical values as in the forward version. The variables $\dot{x}$, $\dot{y}$, p_x, p_y and ζ, on the other hand, change sign relative to their forward-version values. It is easy to verify that eqns (3)–(5) are satisfied equally well in either direction. This establishes that the shear-flow equations are formally reversible. As we will see in the following sections, this apparent reversibility is illusory, just as it is for Newton's equations. In fact the set of eqns (3)–(5) exhibits thermodynamic irreversibility.

3. SOLUTIONS OF THE NONEQUILIBRIUM EQUATIONS OF MOTION

A straightforward solution of the equations of motion (3)–(5) can be obtained using any one of several numerical schemes. Such methods replace the differential equations by difference equations giving particle coordinates and momenta at discrete times 0, dt, 2 dt, 3 dt, ... Typically, the errors in such a method vary as $(\mathrm{d}t)^4$ or $(\mathrm{d}t)^6$ and can therefore be made small by an appropriate choice of dt. The simplest force law, an elastic

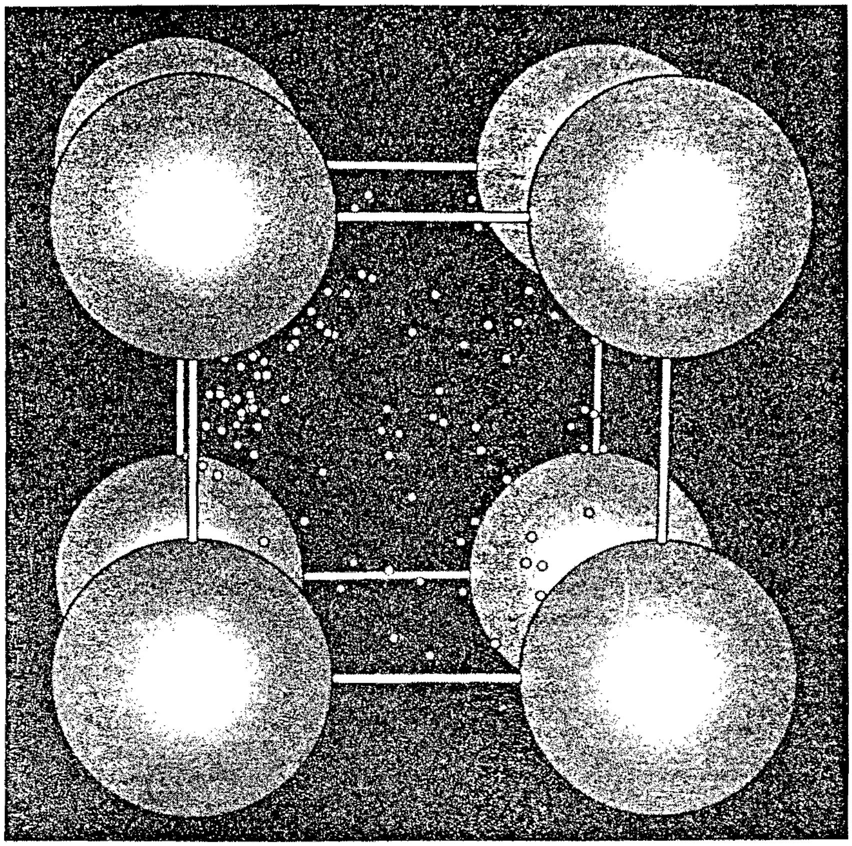

Fig. 4 (*Continued*). Third view.

hard-disk repulsion, which prevents two particles from interpenetrating, requires special methods [7] because the impulsive hard-disk forces are singular at collision. An adequate approximation is to smooth out this interaction by using a truncated Hooke's Law repulsive force, with the force constant chosen large enough that a well-defined collision diameter results. Calculations of this kind have been carried out for small two- and three-disk systems. They are stable and provide values of the viscosity coefficient (stress/strain rate) close to Senger's prediction for hard disks [8]. The two-body problem is formally equivalent to the scattering of a reduced-mass disk from a shearing periodic lattice. This is a "Lorentz gas" problem.

The problem can also be solved in the spirit of the Boltzmann equation, finding the probability density $f(p)$ for the momentum by taking two-body collisions into account statistically. In this case a partial differential equation for the time development of $f(p, t)$ replaces the coupled ordinary differential equations of motion for discrete particles. But the numerical approach is similar. The differential equation describing the problem can be represented as a difference equation and iterated to find a steady state solution. Both approaches lead to similar results [9]. A steady value of the shear stress is found. The shear stress increases less rapidly than linearly with strain rate so that viscosity (stress/strain rate) is a decreasing function of strain rate. Figure 2 indicates this dependence.

4. IRREVERSIBILITY FROM REVERSIBLE EQUATIONS

The irreversibility found from the reversible equations of motion (3)–(5) can be understood very directly. If we define a polar angle θ to describe the momenta, with $p_x = p \cos \theta$ and $p_y = p \sin \theta$, then, in the absence of collisions, the equations of motion reduce to

$$d\theta/dt = -\dot{\epsilon}\cos^2\theta. \tag{6}$$

The kinetic part of the shear stress $-\langle p_x p_y/(mV)\rangle$ would be zero for the (equilibrium) distribution $f_0 = 1/(2\pi)$. But the equation of motion (6) introduces a clockwise drift, into the second and fourth quadrants of momentum space. In these quadrants $p_x p_y$ is negative so that the corresponding shear stress is positive. The free-streaming equation of motion (6) can be integrated analytically, establishing that a particle with an initial velocity corresponding to θ_0 (in the first or third quadrants of momentum space) enters the second or fourth quadrants at a time $\tan(\theta_0)/\dot{\epsilon}$. Thus, after one mean collision time τ, the particles with positive shear stress contributions exceed those making negative contributions by a term of order $\dot{\epsilon}t$. The shear viscosity which results is of order $P\tau$, where P is the equilibrium pressure.

The presence of collisions complicates the calculation. Superimposed on the clockwise drift is a redistribution of $f(p, t)$ over the circle, weighted strongly toward head-on collisions. For hard disks, as opposed to hard spheres, the probability of glancing collisions is relatively small. Taking collisions into account, the momentum distribution which results—see Fig. 3—is relatively complicated. For small strain rates the perturbation is proportional to $\sin\theta\cos\theta$. For greater strain rates the distribution approaches delta functions at $\theta = \pm\pi/2$. At any strain rate the probability peaks lie in the second and fourth quadrants of momentum space. The implication of these Boltzmann-equation results, that away from equilibrium there is a preponderance of positive shear stress states, is borne out by the numerical two-body calculations.

What about the arguments of Poincare and Zermelo? Recurrence is no longer a problem, because here we are describing a nonequilibrium steady state. But the reversal properties of the equations of motion are still paradoxical. The virial-theorem expression for the shear stress is, according to the equations of motion, unchanged by reversing the particle trajectories. In the reversed motion the strain rate changes sign. Thus, formal reversibility implies that the viscosity (stress/strain rate) must change sign in a reversed solution of the equations of motion. The Boltzmann equation, on the other hand, correctly predicts a positive viscosity. In order for the viscosity actually to change sign (as required for a reversed trajectory) it would be necessary for the collisions to be computed with sufficient accuracy so they occur in precisely the reverse order. This can be done for one, two, three, . . . collisions with increasing difficulty. More precision is required in the trajectory to reverse it accurately after a longer time. The error grows exponentially in the time so that the number of digits kept must be proportional to the time over which reversal is desired. In practice finite computer precision would limit the reversibility. A caricature of the exponential error growth is shown in Fig. 4. In that figure the points reached by particles originally arranged in a small $5 \times 5 \times 5$ cube in physical space and with identical velocities are shown after shear strains of four and eight. The same rapid growth of phase-space separation persists at all scales, and will eventually dominate any finite-precision calculation.

There is still another source of irreversibility, beyond the randomizing effects of collisions and the finite precision of calculations. That is the interaction of any system with its surroundings. Very weak interactions would be sufficient to destroy the reversibility of a system. For instance, consider the time reversal of a terrestrial shear-flow experiment. If the motion were reversed, but without taking the earth's rotation into account, the exact reversibility of trajectories would be destroyed. The Coriolis acceleration, applied over a mean free time of 1 nanosecond, would change the angle at which two molecules collide by about a nanoradian. This small error would completely destroy the reversed sequence of collisions after about nine collisions per particle.

Thus we conclude that Boltzmann's description of irreversibility in terms of a drift in phase space is essentially correct, and, that if this drift is somehow prevented by choosing special initial conditions, that irreversibility will still prevail at a time determined either by the precision of the initial conditions or by the presence of irreversible interactions with the system's surroundings.

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REFERENCES

[1] S. G. BRUSH, *Kinetic Theory*, Vols. 1–3 (Pergamon, New York, 1956–72). For a current view of irreversibility see I. PRIGOGINE, *From Being to Becoming* (W. H. Freeman, San Francisco, 1980).

[2] *Molecular-Based Study of Fluids* (Edited by J. M. Haile and G. A. Mansoori), *Adv. Chem. Series* Vol. 204 (American Chemical Society, Washington, 1983).

[3] C. TROZZI and G. CICCOTTI, *Stationary Nonequilibrium States by Molecular Dynamics. II. Newton's Law*, *Phys. Rev.* A, **29**, 916 (1984) and references cited therein.

[4] A. J. C. LADD and W. G. HOOVER, *Phys. Rev.* B **28**, 1756 (1983).

[5] W. G. HOOVER, *Physica* **118A**, 111 (1983).

[6] D. J. EVANS, W. G. HOOVER, B. FAILOR and B. MORAN, *Phys. Rev.* A **28**, 1016 (1983).

[7] B. J. ALDER and T. E. WAINWRIGHT, *J. Chem. Phys.* **31**, 459 (1959); **33**, 1439 (1960).

[8] D. M. GASS, *J. Chem. Phys.* **54**, 1898 (1971).

[9] A. J. C. LADD and W. G. HOOVER *J. Stat. Phys.* (1985), in press.