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Lyapunov dimension of two-body planar Couette flow

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The complete set of Lyapunov exponents for a two-dimensional two-body shearing system is calculated using an extension of the method of Hoover and Posch. The Lyapunov dimension is found to be a decreasing function of the shear rate. This implies that the nonequilibrium distribution function is a fractal attractor whose dimension is less than that of the equilibrium phase space.

I. INTRODUCTION

The nonequilibrium molecular dynamics (NEMD) of shear flow in periodic boundary conditions using the "SLLOD" algorithm[1] is a well-defined statistical mechanical system which exhibits a nonequilibrium steady state. The behavior of these systems (of 10^2 to 10^4 atoms) in both two[2] and three[3] dimensions is relatively well understood. The shear liquid exhibits a non-Newtonian viscosity, pressure, and normal stress difference, each varying as a function of shear rate in a nonanalytic way for a significant range of the accessible strain rates ($10^{-2} < \gamma < 2$). Recently the emphasis has shifted towards a better formal understanding of the properties and attainment of nonequilibrium steady states.[4] To test such theories of the nonlinear response directly in computer experiments, the "SLLOD" algorithm for shear flow has proved to be a very useful model system. For example, the transient correlation time function theory[5] was demonstrated to be correct by comparing its predictions directly in NEMD simulations. To be able to characterize a nonequilibrium steady state completely we need to obtain the nonequilibrium phase-space distribution function $f(\Gamma,t)$. We can consider an ensemble of equilibrium systems at time zero, to which we apply a steady shear. The distribution function will change from equilibrium at $t=0$ to the steady state distribution function as $t \to \infty$. Taking a two-dimensional system of N particles $f(\Gamma,t)$ is a function of $2N$ position coordinates and $2N$ momenta, as well as the time. In order to make some progress in this direction we need to reduce the number of degrees of freedom in the system. The smallest nontrivial shearing system is $N=2$, and this is the one we shall investigate here.

The two-body shearing system, with hard core pair interactions, has been simulated using molecular dynamics,[6] while the relaxation time approximation to the Boltzmann equation has been solved in both two and three dimensions.[7] The relaxation-time approximation incorporates the biasing of the angle θ between collisions (due to the combination of the strain rate and the total kinetic energy constraint) but assumes that the coordinate distribution remains uniform. These studies do indeed show that this two-body system retains many of the properties of many-body systems; however, the Boltzmann equation solution predicts analytic behavior of the viscosity, pressure, and normal stress as a function of shear rate. It was also shown[7] that the distribution of velocities in NEMD simulation is biased by the applied shear.

It has been clear that the effect of an applied field must be to deform and distort the initial equilibrium distribution function. However, in a previous paper[8] it was shown that if the initial equilibrium phase-space distribution function exists on a subspace of dimension X, then the Gaussian isokinetic nonequilibrium distribution function exists on a space with a fractal dimension which is less than X. This is a much stronger result and it implies that any phase point in the initial ensemble will move towards a fractal attractor under the influence of a field and that the size of the attractor is determined by the field. The implication of this dimensional contraction for the resolution of Loschmidt's paradox has been emphasized recently.[9]

The information dimension D_I for the two-body shearing system was shown to be a decreasing function of shear rate, initially at $\gamma=0$, $D_I \sim 2.89$, this value falls and eventually approaches 1 at very large shear rates. There are a number of difficulties in the calculation of the information dimension. One must calculate the discrete entropy $S(\varepsilon)$ as a function of discretization length ε and extrapolate $S(\varepsilon)/\ln\varepsilon$ to $\varepsilon \to 0$. Attempts have been made to improve the extrapolation procedure[10] but problems with systematic error still remain. In an attempt to better characterize the system we have calculated the Lyapunov dimension D_L of the two-body shearing system. This requires the complete set of Lyapunov exponents for the system and no subsequent extrapolation procedure is needed. This approach is generally believed[11] to be a more accurate way of estimating the effective fractal dimension.

Two other very recent studies of similar Nosé-Hoover thermostatted nonequilibrium systems have been made but both of these are analogues of diffusion; they are diffusion in a periodic Lorentz gas[12] and conductivity in a one-dimensional periodic potential.[13] In both cases a decrease in the effective dimension is observed.

II. LYAPUNOV EXPONENTS

Consider the trajectory $\Gamma(t)$ of a d-dimensional, N-particle system in phase space. The dimension of the phase space is $2dN$. In general the system trajectory will cover a surface whose dimension is lower than the full phase space. The dimension of the surface is $2dN-N_c$, where N_c is the number of constants of the motion ($2dN-N_c$ is the embedding dimension). If we want to study the convergence or divergence of neighboring trajectories then we consider a set of basis vectors in the $(2dN-N_c)$-dimensional subset of phase space called the tangent space $\{\boldsymbol{\delta}_1,\boldsymbol{\delta}_2,\boldsymbol{\delta}_3,\ldots\}$, where $\boldsymbol{\delta}_i=\boldsymbol{\Gamma}_i-\boldsymbol{\Gamma}_0$. If the equation of motion for the trajectory is of the form

$$\dot{\boldsymbol{\Gamma}}=\mathbf{G}(\boldsymbol{\Gamma}) , \tag{1}$$

then the equation of motion for the tangent vector $\boldsymbol{\delta}_i$ is

$$\dot{\boldsymbol{\delta}}_i=\mathbf{F}_i(\boldsymbol{\Gamma})=\mathbf{T}(\boldsymbol{\Gamma})\cdot\boldsymbol{\delta}_i+O(\boldsymbol{\delta}_i^2) . \tag{2}$$

$\mathbf{T}(\boldsymbol{\Gamma})$ is the Jacobian matrix (or stability matrix $\partial\mathbf{G}/\partial\boldsymbol{\Gamma}$) for the system. If the magnitude of the tangent vector is small enough the nonlinear terms in Eq. (2) can be neglected. The formal solution of Eq. (2) is

$$\boldsymbol{\delta}_i(t)=\exp\left[\int_0^t ds\,\mathbf{T}(s)\right]\boldsymbol{\delta}_i(0) . \tag{3}$$

The mean exponential rate of separation of the ith tangent vector gives the ith Lyapunov exponent

$$\lambda_i(\boldsymbol{\Gamma}(0),\boldsymbol{\delta}_i(0))=\lim_{t\to\infty}\left[\frac{1}{t}\ln\frac{\|\boldsymbol{\delta}_i(t)\|}{\|\boldsymbol{\delta}_i(0)\|}\right] . \tag{4}$$

The Lyapunov exponents can be ordered $\lambda_1>\lambda_2>\cdots>\lambda_M$ and if the system is ergodic, the exponents are independent of the initial phase $\boldsymbol{\Gamma}(0)$ and the initial phase-space separation $\boldsymbol{\delta}_i(0)$.

A new method of calculating Lyapunov exponents has been proposed by Hoover and Posch.[14] It uses Gauss's principle of least constraint to make the length of each tangent vector a constant of the motion, and to maintain the orthogonality of the set of tangent vectors. The method is simplest to describe if we consider its application to the calculation of the largest Lyapunov exponent. Take two trajectories $\boldsymbol{\Gamma}_1$ and $\boldsymbol{\Gamma}_0$, and define the tangent vector $\boldsymbol{\delta}$, where $\boldsymbol{\delta}=\boldsymbol{\Gamma}_1-\boldsymbol{\Gamma}_0$. In the Gaussian method the equations of motion for one trajectory, $\boldsymbol{\Gamma}_1$, are changed to include a constraint force term $-\zeta\boldsymbol{\delta}$. The multiplier ζ is chosen to fix the length of the tangent vector $\|\boldsymbol{\delta}\|=(\boldsymbol{\delta}\cdot\boldsymbol{\delta})^{1/2}$. The constrained equations of motion for the tangent vector are

$$\dot{\boldsymbol{\delta}}=\mathbf{F}-\zeta\boldsymbol{\delta} . \tag{5}$$

If we assume that on average, the magnitude of the unconstrained tangent vector $\boldsymbol{\delta}^u$ diverges exponentially, then

$$\langle \|\boldsymbol{\delta}^u(t)\| \rangle \sim \langle \|\boldsymbol{\delta}^u(0)\| \rangle e^{\lambda t} , \tag{6}$$

and differentiating with respect to time, the Lyapunov exponent λ can be written as

$$\lambda=\frac{\langle \boldsymbol{\delta}^u(t)\cdot\dot{\boldsymbol{\delta}}^u(t)\rangle}{\langle \boldsymbol{\delta}^u(t)\cdot\boldsymbol{\delta}^u(t)\rangle} . \tag{7}$$

It may seem from Eq. (7) that the exponent λ is a function of the length of the tangent vector $(\boldsymbol{\delta}^u)^2$, but as we shall see numerically any such dependence is negligible. For the constrained case the instantaneous multiplier ζ is given by

$$\zeta=\frac{\boldsymbol{\delta}(t)\cdot\mathbf{F}(t)}{\boldsymbol{\delta}(t)\cdot\boldsymbol{\delta}(t)}=\frac{\boldsymbol{\delta}(t)\cdot\dot{\boldsymbol{\delta}}^u(t)}{\boldsymbol{\delta}(t)\cdot\boldsymbol{\delta}(t)} . \tag{8}$$

The second equality follows from the equation of motion for the unconstrained tangent vector. As the magnitude of $\boldsymbol{\delta}(t)$ is fixed, the denominator is a constant and assuming $\langle\zeta\rangle$ to be independent of $\boldsymbol{\delta}^2$,

$$\lambda=\langle\zeta\rangle=\frac{\langle \boldsymbol{\delta}(t)\cdot\dot{\boldsymbol{\delta}}^u(t)\rangle}{\boldsymbol{\delta}(t)\cdot\boldsymbol{\delta}(t)} . \tag{9}$$

This is an example of the application of Gauss's principle of least constraint to constrain a mechanical system. In molecular dynamics simulations it has become commonplace to use Gauss's principle to change from one ensemble to another.[15] Typically a fixed external field ensemble is changed to the ensemble conjugate to it, the fixed flux ensemble. The application to Gauss's principle to the calculation of Lyapunov exponents exactly parallels this situation. In the past it has been usual to monitor the divergence of a pair of trajectories. Here we monitor the force required to keep those two trajectories a fixed distance apart in phase space.

As an example of the Hoover-Posch technique to a particular problem, consider the Lorenz model.[16] The equations of motion are

$$\begin{bmatrix}\dot{x}\\ \dot{y}\\ \dot{z}\end{bmatrix}=\begin{bmatrix}-\sigma(x-y)\\ (r-z)x-y\\ xy-bz\end{bmatrix} , \tag{10}$$

where σ, r, and b are predetermined positive parameters. To calculate the Lyapunov exponents we use a method which is very similar to the Gaussian method of fixing bond lengths and bond angles in simulations of alkanes.[17] The principal difference is that, rather than applying the constraint symmetrically to both trajectories (or sites), we leave one trajectory $\boldsymbol{\Gamma}_0(t)$ unconstrained. This ensures that the origin of the set of tangent vectors is a real physical trajectory. We then constrain trajectory $\boldsymbol{\Gamma}_1(t)$ to be a fixed distance from $\boldsymbol{\Gamma}_0(t)$. Trajectory $\boldsymbol{\Gamma}_2(t)$ is constrained to be a fixed separation from $\boldsymbol{\Gamma}_0(t)$, and orthogonal to the first tangent vector $\boldsymbol{\delta}_1(t)=\boldsymbol{\Gamma}_1(t)-\boldsymbol{\Gamma}_0(t)$. Introducing the double script notation $\boldsymbol{\delta}_{ij}=\boldsymbol{\delta}_j-\boldsymbol{\delta}_i$, we have that the ith tangent vector is $\boldsymbol{\delta}_i=\boldsymbol{\delta}_{0i}$, and $\boldsymbol{\delta}_{ij}$ where $i\neq0$ is an orthogonality condition; for example, fixing the distance $\boldsymbol{\delta}_{12}$ maintains the orthogonality of the first two tangent vectors. Trajectory $\boldsymbol{\Gamma}_3(t)$ is constrained to be a fixed separation from $\boldsymbol{\Gamma}_0(t)$, and $\boldsymbol{\delta}_{03}$ orthogonal to both $\boldsymbol{\delta}_{01}$ and $\boldsymbol{\delta}_{02}$. The equations of motion for the individual constrained trajectories are

$$\begin{bmatrix}\dot{\mathbf{\Gamma}}_0\\ \dot{\mathbf{\Gamma}}_1\\ \dot{\mathbf{\Gamma}}_2\\ \dot{\mathbf{\Gamma}}_3\end{bmatrix}=\begin{bmatrix}\mathbf{F}_0\\ \mathbf{F}_1\\ \mathbf{F}_2\\ \mathbf{F}_3\end{bmatrix}-\begin{bmatrix}0&0&0&0&0&0\\1&0&0&0&0&0\\0&1&1&0&0&0\\0&0&0&1&1&1\end{bmatrix}\begin{bmatrix}\zeta_1\boldsymbol{\delta}_{01}\\ \zeta_2\boldsymbol{\delta}_{02}\\ \zeta_3\boldsymbol{\delta}_{12}\\ \zeta_4\boldsymbol{\delta}_{03}\\ \zeta_5\boldsymbol{\delta}_{13}\\ \zeta_6\boldsymbol{\delta}_{23}\end{bmatrix}. \quad (11)$$

The equations of motion for the separation vector $\boldsymbol{\delta}_{ij}$ can be obtained from the equations of motion for the trajectories. For $\boldsymbol{\delta}_{ij}^2$ to be a constant of the motion,

$$\dot{\boldsymbol{\delta}}_{ij}\cdot\boldsymbol{\delta}_{ij}=0 . \quad (12)$$

Substituting the equations of motion for $\boldsymbol{\delta}_{ij}$ into Eq. (12) gives a set of six coupled linear equations, of the form $\mathbf{AX}=\mathbf{B}$, to solve for the multipliers ζ_i, where

$$\mathbf{A}=\begin{bmatrix}\boldsymbol{\delta}_{01}^2&0&0&0&0&0\\0&\boldsymbol{\delta}_{02}^2&\boldsymbol{\delta}_{02}\cdot\boldsymbol{\delta}_{12}&0&0&0\\-\boldsymbol{\delta}_{12}\cdot\boldsymbol{\delta}_{01}&\boldsymbol{\delta}_{12}\cdot\boldsymbol{\delta}_{02}&\boldsymbol{\delta}_{12}^2&0&0&0\\0&0&0&\boldsymbol{\delta}_{03}^2&\boldsymbol{\delta}_{03}\cdot\boldsymbol{\delta}_{13}&\boldsymbol{\delta}_{03}\cdot\boldsymbol{\delta}_{23}\\-\boldsymbol{\delta}_{13}\cdot\boldsymbol{\delta}_{01}&0&0&\boldsymbol{\delta}_{13}\cdot\boldsymbol{\delta}_{03}&\boldsymbol{\delta}_{13}^2&\boldsymbol{\delta}_{13}\cdot\boldsymbol{\delta}_{23}\\0&-\boldsymbol{\delta}_{23}\cdot\boldsymbol{\delta}_{02}&-\boldsymbol{\delta}_{23}\cdot\boldsymbol{\delta}_{12}&\boldsymbol{\delta}_{23}\cdot\boldsymbol{\delta}_{03}&\boldsymbol{\delta}_{23}\cdot\boldsymbol{\delta}_{13}&\boldsymbol{\delta}_{23}^2\end{bmatrix}, \quad (13)$$

$$\mathbf{B}=\begin{bmatrix}\boldsymbol{\delta}_{01}\cdot\mathbf{F}_{01}\\ \boldsymbol{\delta}_{02}\cdot\mathbf{F}_{02}\\ \boldsymbol{\delta}_{12}\cdot\mathbf{F}_{12}\\ \boldsymbol{\delta}_{03}\cdot\mathbf{F}_{03}\\ \boldsymbol{\delta}_{13}\cdot\mathbf{F}_{13}\\ \boldsymbol{\delta}_{23}\cdot\mathbf{F}_{23}\end{bmatrix},\ \text{and}\ \mathbf{X}=\begin{bmatrix}\zeta_1\\ \zeta_2\\ \zeta_3\\ \zeta_4\\ \zeta_5\\ \zeta_6\end{bmatrix}. \quad (14)$$

We have seen from Eq. (9) that the largest Lyapunov exponent is simply the average of the multiplier ζ_i. To relate the second and third Lyapunov exponents to the set of Gaussian multipliers ζ_i, consider the equation of motion for tangent vector $\boldsymbol{\delta}_{02}$ derived from Eq. (11), substituted into Eq. (12),

$$\begin{aligned}\boldsymbol{\delta}_{02}\cdot\dot{\boldsymbol{\delta}}_{02}&=\boldsymbol{\delta}_{02}\cdot\dot{\boldsymbol{\delta}}_{02}^{u}-\boldsymbol{\delta}_{02}\cdot[\zeta_2\boldsymbol{\delta}_{02}+\zeta_3(\boldsymbol{\delta}_{02}-\boldsymbol{\delta}_{01})]\\&=\boldsymbol{\delta}_{02}\cdot\dot{\boldsymbol{\delta}}_{02}^{u}-(\zeta_2+\zeta_3)\boldsymbol{\delta}_{02}^2+\zeta_3\boldsymbol{\delta}_{02}\cdot\boldsymbol{\delta}_{01}\\&=0 .\end{aligned} \quad (15)$$

As $\boldsymbol{\delta}_{01}$ is orthogonal to $\boldsymbol{\delta}_{02}$, the third term on the right-hand side is zero. From Eq. (7) we see that the ith Lyapunov exponent is defined by

$$\langle \boldsymbol{\delta}_{0i}\cdot\dot{\boldsymbol{\delta}}_{0i}^{u}\rangle=\lambda_i\boldsymbol{\delta}_{0i}^2 . \quad (16)$$

Combining Eqs. (15) and (16), the second Lyapunov exponent is given by

$$\lambda_2=\langle\zeta_2+\zeta_3\rangle . \quad (17)$$

Similarly, the third Lyapunov exponent can be calculated by considering the equation of motion for $\boldsymbol{\delta}_{03}$, substituted into Eq. (12)

$$\begin{aligned}\boldsymbol{\delta}_{03}\cdot\dot{\boldsymbol{\delta}}_{03}=&\ \boldsymbol{\delta}_{03}\cdot\dot{\boldsymbol{\delta}}_{03}^{u}-(\zeta_4+\zeta_5+\zeta_6)\boldsymbol{\delta}_{03}^2\\&+\zeta_5\boldsymbol{\delta}_{03}\cdot\boldsymbol{\delta}_{01}+\zeta_6\boldsymbol{\delta}_{03}\cdot\boldsymbol{\delta}_{02}=0 .\end{aligned} \quad (18)$$

As $\boldsymbol{\delta}_{01}$, $\boldsymbol{\delta}_{02}$, and $\boldsymbol{\delta}_{03}$ are all orthogonal, the last two terms on the right-hand size are zero, and using Eq. (16), we find that

$$\lambda_3=\langle\zeta_4+\zeta_5+\zeta_6\rangle . \quad (19)$$

The observation that the Lyapunov exponent depends on both the length multiplier *and* the orthogonality multipliers is a little counter-intuitive. Hoover *et al.*[13] have formulated a similar method using orthogonal forces, and in that case the Lyapunov exponent is related to a single multiplier.

The scheme developed above was used to calculate the Lyapunov exponents for the Lorenz model, which are shown in Table I. The equations of motion were solved using the 4th-order Runge-Kutta scheme in double precision (64 bit) arithmetic, with a timestep of 0.01. A typical simulation run length was 2×10^5 timesteps. The tangent vectors were periodically rescaled and reorthogonalized using the Gram-Schmidt procedure, to remove accumulated error in the differential equation solver. For most simulations we used $\sigma=16$, $r=40$, and $b=4$. The initial phase point was $(x,y,z)=(10,0,30)$ and the initial tangent vector directions were (1,0,0), (0,1,0), and (0,0,1). These were chosen to allow direct comparison with the previous results.[18–21] It appears that the optimal value of the tangent vector for 64-bit arithmetic is in the range $10^{-2}\sim10^{-6}$. At this level the error estimates are small-

TABLE I. Lyapunov exponents for the Lorenz model.

Tangent vector length δ_i^2	λ_1	λ_2	λ_3	Ref.
10^0	1.373(3)	−0.001(5)	−22.373(5)	
10^{-2}	1.375(1)	−0.003(3)	−22.372(3)	
10^{-4}	1.375(1)	−0.003(3)	−22.372(3)	
10^{-6}	1.375(1)	−0.003(3)	−22.372(3)	
10^{-8}	1.375(1)	−0.003(3)	−22.372(3)	
10^{-10}	1.375(1)	−0.003(4)	−22.372(4)	
	1.36			18
	1.37	0.00	−22.37	19
	1.37(8)	−0.02(9)	−15.2(21)	21
	$\sigma=10$, $r=28$, and $b=\frac{8}{3}$			
10^{-6}	0.905(5)	0.000(1)	−14.571(1)	
	0.91	0	−14.6	20

est. The Lyapunov exponents do not show any dependence upon the tangent vector length.

III. TWO-BODY PLANAR COUETTE FLOW

Gaussian thermostatted planar Couette flow which can be driven by the following set of first-order equations of motion:[1]

$$\dot{\mathbf{q}}_i=\frac{\mathbf{p}_i}{m}+\mathbf{n}_x\gamma y_i\ ,$$
$$\dot{\mathbf{p}}_i=\mathbf{F}_i-\mathbf{n}_x\gamma p_{yi}-\alpha\mathbf{p}_i\ , \tag{20}$$

$$\alpha=\frac{\sum_{i=1}^{N}(\mathbf{F}_i\cdot\mathbf{p}_i-\gamma p_{xi}p_{yi})}{\sum_{i=1}^{N}\mathbf{p}_i^2}\ , \tag{21}$$

where $\mathbf{n}_x$ is the unit vector in the x direction, and γ is the strain rate. We consider an infinite system made up of periodic replications of the central two-particle square, constructed using the usual *sliding brick* periodic boundary conditions. The dissipative flux $J(\Gamma)$ due to the applied field is given by the adiabatic time derivative of the internal energy H_0. Here this is the shear stress $P_{xy}(\Gamma)$ times the volume V,

$$P_{xy}(\Gamma)V=\sum_{i=1}^{N}\left[\frac{p_{xi}p_{yi}}{m}+y_iF_{xi}\right]. \tag{22}$$

The shear rate dependent viscosity $\eta(\gamma)$ is related to the shear stress by the constitutive relation

$$\eta(\gamma)=\frac{-\langle P_{xy}\rangle}{\gamma}\ . \tag{23}$$

For two-body planar Couette flow in two-dimensions we find the total phase space reduces from eight degrees of freedom to three.[7,8] These three variables are the relative separation of the two particles $(x_{12},y_{12})=(x_2-x_1,y_2-y_1)$, and the direction of the momentum vector of particle 1 (p_{x1},p_{y1}) with respect to the x axis, which we call θ. The magnitude of the momentum p is fixed by the total kinetic energy constraint and the fact that the total momentum is zero.

In this paper we present the Lyapunov exponents for the two-body shearing system with Lennard-Jones pair interactions (with the pair potential cutoff at its minimum), at a reduced temperature $T^*=kT/\varepsilon_{LJ}=1.0$ and a reduced density of $\rho^*=\rho\sigma^2=0.4$. The simulations were performed using the 4th-order Runge-Kutta method to integrate the equations of motion, with reduced time step 0.002. A typical simulation length was 5×10^6 timesteps and the length of each tangent vector was 10^{-4}.

A useful characterization of the system is given by the effective dimension. This may be calculated from a covering of the attractor,[11] or from a scaling relation for the discrete entropy,[11] or from a knowledge of the Lyapunov exponents. Kaplan and Yorke[22] have conjectured that the effective dimension of an attractor can be related to the set of Lyapunov exponents by

$$D_L^{KY}=n+\frac{\sum_{i=1}^{n}\lambda_i}{|\lambda_{n+1}|}\ , \tag{24}$$

where n is the largest integer for which $\sum_{i=1}^{n}\lambda_i>0$. There is a second postulated relation between Lyapunov exponents and dimension due to Mori,[23]

$$D_L^M=m_0+m^+\left[1+\frac{|\lambda^+|}{|\lambda^-|}\right], \tag{25}$$

where m_0 and m^+ are the number of zero and positive exponents, respectively, and $\lambda^\pm$ is the mean value of the positive or negative exponents (depending upon the superscript). Farmer[24] gives a modified form of the Mori dimension which is found to give integer dimensions for systems of an infinite number of degrees of freedom. Farmer's version of the Mori dimension gives values which are worse than the standard form, so the values we report in Table II are those obtained using Mori's original prescription.

TABLE II. Lyapunov exponents for two-body planar Couette flow.

Shear rate γ	λ_1	λ_2	λ_3	Dimension D_L Kaplan-Yorke	Mori
0	2.047(2)	0.002(2)	−2.043(2)	3.003	3.00
0.25	2.063(3)	−0.046(2)	−2.1192(3)	2.952	2.90
0.5	1.995(3)	−0.187(4)	−2.242(3)	2.81	2.64
0.75	1.922(4)	−0.388(3)	−2.442(3)	2.62	2.36
1.0	1.849(5)	−0.63(1)	−2.74(1)	2.445	2.10
1.25	1.807(4)	−0.873(5)	−3.17(1)	2.295	1.89
1.5	1.800(5)	−1.121(2)	−4.12(5)	2.14	1.68
1.75	1.733(4)	−1.424(3)	−5.63(6)	2.058	1.49
2.0	1.649(9)	−1.54(1)	−7.36(8)	2.015	1.37
2.25	1.575(3)	−1.60(1)	−9.25(9)	1.981	1.29
2.5	1.61(2)	−2.14(1)	−11.5(1)	1.75	1.24
2.75	0.2616(8)	−2.12(1)	−19.84(3)	1.123	1.02
3.0	0.678(5)	−2.69(1)	−19.85(2)	1.252	1.06
3.5	−0.111(4)	−2.62(1)	−17.49(4)	0	0
4.0	0.427(4)	−4.25(1)	−14.43(5)	1.10	1.05
4.5	−0.674(5)	−2.96(1)	−10.78(3)	0	0
5.0	−0.132(2)	−1.97(1)	−8.152(3)	0	0

When the shear rate γ is zero, both methods of calculating the Lyapunov dimension agree. However, as soon as the shear rate changes from zero, differences appear. In the Kaplan-Yorke formula the value of n is 2 from $\gamma=0$, until the magnitude of λ_2 exceeds that of λ_1 (somewhere between $\gamma=2$ and 2.5). This means that $2<D_L<3$ in this range. For $\gamma>2$ the dimension is between 1 and 2 as long as λ_1 remains positive. The value of λ_3 is irrelevant as soon as $|\lambda_2|>\lambda_1$. When λ_1 becomes negative the dimension is equal to zero. The Kaplan-Yorke formula can never give fractional values between 0 and 1.

In the Mori formula the value of λ_3 always contributes to the dimension and its large negative value tends to dominate the denominator, reducing D_L. The transition from dimension greater than 2 to dimension less than 2 is somewhere between $\gamma=1$ and 1.25. Indeed, the Mori dimension is systematically less than the Kaplan-Yorke dimension. Of the two routes to the dimension the Kaplan-Yorke method agrees qualitatively with the information dimension results,[8] whereas the Mori method does not. In particular the Kaplan-Yorke method and the information dimension both give a change from values greater than 2 to values less than 2 at about $\gamma=2.5$.

The sliding brick periodic boundary conditions in the Couette flow algorithm induce an explicit time dependence into the two-body shear flow system. This is most easily seen by removing the potential cutoff. The force on particle 1 due to particle 2 is then given by a lattice sum where the positions of the lattice points are functions of time. The three equations of motion are then nonautonomous and hence do not have a zero Lyapunov exponent.[25] These three equations can be transformed to four autonomous equations by the introduction of a trivial extra variable whose time derivative is the velocity of the lattice points. In this form there is a zero Lyapunov exponent associated with this extra variable.

IV. SUM RULES FOR LYAPUNOV EXPONENTS

The largest Lyapunov exponent indicates the rate of growth of trajectory separation in phase space. The largest two exponents, λ_1 and λ_2, give the rate of growth in two orthogonal directions. We can use these two directions to define an area element $V_2(t)$, and growth in this two-dimensional volume element is given by

$$V_2(t)=V_2(0)\exp[(\lambda_1+\lambda_2)t] . \tag{26}$$

Similarly, the three-dimensional volume element is related to the three largest exponents by

$$V_3(t)=V_3(0)\exp[(\lambda_1+\lambda_2+\lambda_3)t] . \tag{27}$$

This type of construction has been used[19,26] to calculate the Lyapunov exponents. It is also possible to use this idea to show that the Gaussian orthogonality multipliers contribute to the Lyapunov exponents. We illustrate this here by considering the area element defined by the tangent vectors $\boldsymbol{\delta}_{01}$ and $\boldsymbol{\delta}_{02}$. Let $l_1=(\boldsymbol{\delta}_{01})^2$, $l_2=(\boldsymbol{\delta}_{02})^2$, and $l_{12}=(\boldsymbol{\delta}_{12})^2$; then using the cosine rule, the area V_2 is given by

$$V_2=\tfrac{1}{2}[2(l_1l_2+l_1l_{12}+l_2l_{12})-(l_1^2+l_2^2+l_{12}^2)]^{1/2} . \tag{28}$$

Using Eq. (11) to construct the time derivatives of l_1, l_2, and l_{12}, it can be shown that

$$\dot{V}_2=\dot{V}_2^u-\langle\zeta_1+\zeta_2+\zeta_3\rangle V_2 , \tag{29}$$

where the u superscript refers to the unconstrained time derivative. As the constrained time derivative of V_2 is zero, combining Eqs. (29) and (26) yields Eq. (17).

If we consider the volume element V_N, where N is the dimension of the initial system, then we have that the phase-space compression factor gives the rate of change of phase-space volume,

TABLE III. Lyapunov exponents for two-body planar Couette flow.

Shear rate γ	Viscosity η	$\sum_i \lambda_i$	$\langle -\alpha+\gamma \sin\theta \cos\theta \rangle$
0.5	0.30	−0.434(10)	−0.438
1.0	0.263	−1.521(6)	−1.50
1.5	0.285	−3.53(3)	−3.48
2.0	0.333	−7.36(1)	−7.36
2.5	0.366	−12.03(4)	−12.03
3.0	0.460	−21.85(2)	−21.85
5.0	0.072	−10.25(1)	−10.26

$$\dot{V}_N=\left\langle \frac{\partial}{\partial \Gamma}\cdot\dot{\Gamma}\right\rangle V_N=\left[\sum_{i=1}^{N}\lambda_i\right]V_N \ , \tag{30}$$

so the average of the divergence is equal to the sum of the Lyapunov exponents. The divergence is easiest to calculate if we write the equations of motion, Eqs. (20), in terms of the minimum number of variables, that is x_{12}, y_{12}, and θ. Dropping the subscripts, the equations of motion are

$$\dot{x}=\frac{2p}{m}\cos\theta+\gamma y \ ,$$
$$\dot{y}=\frac{2p}{m}\sin\theta \ , \tag{31}$$
$$\dot{\theta}=-\frac{F_x}{p}\sin\theta+\frac{F_y}{p}\cos\theta+\gamma\sin^2\theta \ ,$$

where p is the magnitude of the momentum of particle 1, F_x and F_y are the components of the force on particle 1 due to particle 2. Although we have eliminated the thermostatting variable α from the dynamics, its value can be obtained from

$$\alpha=\frac{F_x}{p}\cos\theta+\frac{F_y}{p}\sin\theta-\gamma\sin\theta\cos\theta \ , \tag{32}$$

and the phase-space compression factor is given by

$$\frac{\partial\dot{\theta}}{\partial\theta}=-\alpha+\gamma\sin\theta\cos\theta \ . \tag{33}$$

In Table III we compare the result obtained from Eq. (33) with the sum of the Lyapunov exponents.

V. CONCLUSIONS

In summary, the results presented here confirm the fact that an ensemble of two-dimensional two-body shearing systems whose initial distribution has dimension 3, contracts with increasing shear rate, onto an attractor of dimension less than 3. This change in dimension was first observed[8] by calculating the information dimension. Although the results obtained here do not agree precisely with the information dimension calculations, the trends are similar. The Kaplan-Yorke Lyapunov dimension is 3 at equilibrium; drops steadily towards 2 at approximately $\gamma=2.5$, approaching 1 at $\gamma=3$. As the calculation of the information dimension is beset with systematic errors, we believe that the results presented here are the best characterization of the attractor to date.

It has been firmly established that the behavior of the simplest nontrivial NEMD simulation of planar Couette flow is dominated by a fractal attractor. This behavior must now be expected in NEMD simulations of any size. The calculation of mechanical averages in NEMD simulations is well understood, but a workable predictive thermodynamics has yet to be obtained. Critical to such a theory will be an understanding of the nonequilibrium entropy. The existence of a fractal attractor is a vital clue in this direction, but as yet we only have information concerning the rate of approach to the attractor, and conjectures about its effective dimension. To proceed further we need to know more about the structure of the attractor itself and how frequently each part of the attractor is visited by a steady state trajectory. If the whole initial phase space forms the basin for the attractor we expect the system to come to a unique steady state. However, at high shear rates, $\gamma>2.5$, this is almost certainly not the case, and the final steady state will depend upon the initial phase point. The two-dimensional two-body system considered here is an ideal model system for such studies.

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