Conjugate pairing of Lyapunov exponents for isokinetic shear flow algorithms

G. P. Morriss
School of Physics, The University of New South Wales, UNSW Sydney, New South Wales 2052, Australia
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Previous numerical calculations of the Lyapunov exponents for the eight particle isokinetic SLLOD algorithm for shear viscosity are extended to higher shear rates and a more careful error analysis presented. These calculations imply that within error bars, the conjugate pairing rule is satisfied for this system. The shift in the unpaired exponent appears to be unconnected with the shift in the other conjugate pairs. This distinguishes one degree of freedom from all others in the system.

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The numerical calculation of Lyapunov exponents began with the work of Benettin *et al*. [1] and Shimada and Nagashima [2] where a set of tangent vectors (or the volume elements constructed from them) was allowed to grow (with periodic rescaling) to calculate the exponents. Later methods using a set of basis vectors with the tangent vector lengths and the orthogonality maintained by constraints was pioneered by Hoover and Posch [3] and by Morriss [4]. These constraint algorithms were used to calculate the Lyapunov spectrum of systems of particles in a nonequilibrium stationary state under the action of an external field and thermostat [9]. The Lyapunov spectrum of a Hamiltonian (or equilibrium) system has exponents that occur in positive and negative pairs with the sum of each pair equal to zero, that is $\lambda_i+\lambda_{-i}=0$. For symplectic systems this is a consequence of the symplectic eigenvalue theorem [6], but for equilibrium nonsymplectic systems time reversibility is sufficient. A numerical result of particular interest for thermostatted nonequilibrium stationary states is the conjugate pairing rule $\lambda_i+\lambda_{-i}=C(F_e)$, where C depends on the value of the external field. This result first appeared in Ref. [5] based on the simulation results of Morriss [7] for the isokinetic thermostatted SLLOD algorithm [5] in two-dimensional systems of four and eight particles. Later work by Sarman, Evans and Morriss [8] supported these results but also found that the Evans algorithm for thermal conductivity does not obey conjugate pairing. A number of analytic results have also been obtained. The conjugate pairing rule for Gaussian isokinetic color conductivity and for Nose-Hoover isokinetic color diffusion has been proved by Dettmann and Morriss [9,10], but the status of the original numerically observed result for Gaussian isokinetic SLLOD has not been proved. Indeed recent results have casted some doubt on its validity [11].

The conjugate pairing rule is not a generic property of all thermostatted nonequilibrium stationary states and many situations where it is violated have been reported. The Evans thermal conductivity algorithm does not satisfy conjugate pairing but it has been argued that it is possible to construct a different algorithm that does [8]. Conjugate pairing has only been observed for isokinetic thermostats and does not appear to hold for isoenergetic thermostats [8]. However, for thermostatted Hamiltonian systems with constant thermostatting multiplier pairing is observed, but for this constant α thermostat SLLOD does not pair. All of these numerical observations are for systems with a small number of particles, and the departures from conjugate pairing may disappear in the large system limit, as the differences between thermodynamic averages in the isokinetic and isoenergetic ensemble. Indeed, Ruelle has shown the equivalence of isokinetic and isoenergetic thermostats as the system size becomes large [12].

In this work, we have simulated the Lyapunov spectrum for a two dimensional, eight particle, Gaussian isokinetic SLLOD system at a number of reduced shear rates γ. The method used is based on the construction of a set of basis vectors in the 27-dimensional phase space formed by a central trajectory and 27 nearby trajectories (the phase-space dimension after the elimination of conserved quantities). A Gaussian constraint method is used to maintain tangent vector lengths and orthogonality. The constraint method has the advantage that the length and orthogonality can be checked continuously as the simulation proceeds, as well as the usual energy balance checks that can be done for individual trajectories in nonequilibrium steady states. Further, the sum of the Lyapunov exponents is related to the average thermostatting multiplier $\langle\alpha\rangle$ and the kinetic shear stress $\langle P_{xy}^K\rangle$ by

$$\sum_{i=1}^{2dN-2d-1}\lambda_i=(dN-d-1)\langle\alpha\rangle-\frac{\gamma\langle P_{xy}^K\rangle V}{(dN-d-1)kT}. \quad (1)$$

This provides a further consistency check on the quality of the Lyapunov spectrum (calculated in tangent space) while the right hand side is determined by properties of the central trajectory alone. This system of differential equations is nonautonomous due to the time dependence in the SLLOD *sliding brick* periodic boundary conditions. For this type of simple time dependence, we can obtain a set of autonomous differential equations by introducing a new variable, thus enlarging the phase space by one. However, this new autonomous system must then have a Lyapunov exponent that is equal to zero [13].

The state point details are as follows: a WCA potential (that is, soft disk Lennard-Jones with the potential cutoff at $r=2^{1/6}\sigma$) was used for $\gamma\leqslant 2.5$; a reduced density of 0.4, temperature of 1.0, with a total simulation length of 10^6 time steps of size 0.002. For higher shear rates a potential that has four derivatives that are continuous at the cutoff was used: that is,

$$\phi(r) = 600\left[1 - \left(\frac{r}{r_c}\right)^2\right]^4; \quad r \leqslant r_c, \tag{2}$$

where the coefficients have been chosen so that the thermodynamic state matches the WCA potential as closely as possible. For higher shear rates time steps as small as 0.0008 were needed. A fourth order Runge-Kutta scheme was used to solve the SLLOD equations of motion with the tangent vector lengths constrained to 10^{-6} with a maximum deviation of 10^{-9}. The length and orthogonality of the basis vectors was checked every ten time steps and on average their lengths needed to be rescaled by the Gram-Schmidt procedure on typically two of these occasions.

It is difficult to determine accurate error estimates for the Lyapunov exponents because, for example, the raw values for the largest exponent (or largest constraint multiplier) are numbers of order one, with a standard deviation of order ten, and the time record is correlated. The source of the large variations is easy to understand as the Lyapunov exponents are the multipliers needed to maintain the basis set constraints. In phase space the coordinates vary smoothly, but the momenta vary wildly at collisions. For a hard core interaction the momentum variation is actually discontinuous at collision, while for smooth potentials the discontinuity is removed, but the variation is still very rapid.

To produce reliable error bar estimates, we adopted a procedure where the simulation was separated into N equal blocks of time steps, and the average Lyapunov exponent for the block and standard deviation of the block averages was calculated. If $\sigma(N)$ is the standard deviation for N blocks of equal size, then the standard deviation of the whole data set is $\sigma(1) = \lim_{N\to 1} \sigma(N)/\sqrt{N}$. Here we used typically 10 and 100 blocks. This method is correct if the block averages are independent and we can use this scaling relation to check that the block data is independent. The resulting error quoted is the average plus or minus two standard deviations (as this gives 95% confidence that the true value lies within the error bars, that is, typically one point in 20 is outside the error bars).

The Lyapunov exponents calculated here are presented in Fig. 1. The largest Lyapunov exponent is almost independent of the shear rate, whereas increasingly smaller exponents are more and more shifted in a negative direction. The sums of individual conjugate pairs in all cases, we have studied, satisfy the conjugate pairing rule within numerical errors, as shown in Fig. 2. The only exception to this is the unpaired exponent, which for $\gamma = 1$ shifts the same amount as the other conjugate pairs. However, as the shear rate is increased the shift in the unpaired exponent becomes less than that of the other pairs. This suggests a preferred direction in phase space, and the possibility that removing this direction will give a reduced phase space for which conjugate pairing may be proved.

The numerical results for the Lyapunov exponents obtained here agree with the original results of Morriss [4], and those of Sarman *et al.* [8], and with the newer results of Searles *et al.* [11] at $\gamma = 2$. However, from the error estimates reported by Searles *et al.*, it was concluded that the conjugate pairing rule was not satisfied. A more careful estimation of the error bars in this study shows that the conjugate pairing rule is satisfied. Thus the status of the original observation of conjugate pairing for the isokinetic SLLOD

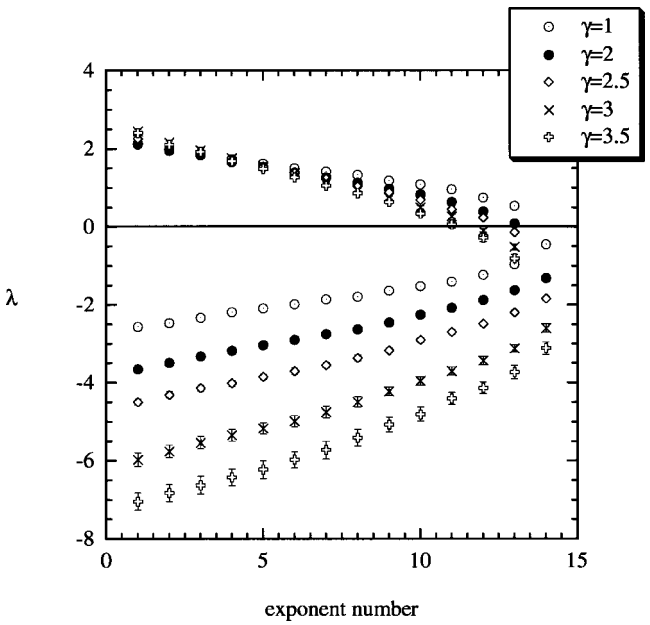

FIG. 1. The Lyapunov spectrum for two-dimensional, Gaussian isokinetic, eight particle SLLOD, at a density of 0.4 and a temperature of 1. The largest exponents are almost independent of the shear rate, but the smaller exponents (and the negative branch in particular) show a systematic dependence upon shear rate.

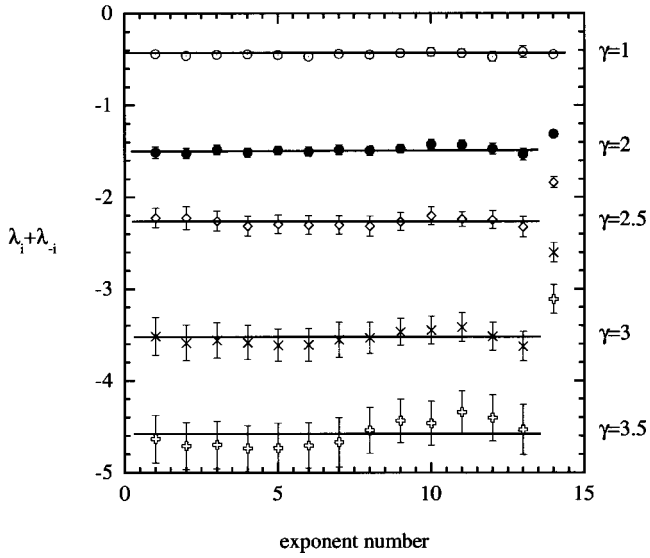

FIG. 2. The sums of conjugate pairs of Lyapunov exponents. Notice that within error bars the conjugate pairing rule is obeyed for all exponents except the unpaired exponent. There is some indication of an oscillatory variation about the conjugate pairing result, particularly at $\gamma = 3.5$. For $\gamma \geqslant 2$ the unpaired exponent differs significantly for the sum of the conjugate pairs.

equations remains. The simulations by Searles *et al.*, do include an extra degree of freedom, but they conclude that the extra Lyapunov exponent (at $\gamma=2$) is 0.067 ± 0.024, rather than zero. This again highlights the fact that the error estimates in their work are too optimistic by about a factor of 3 for this exponent.

If the conjugate pairing is observed then this implies that the phase-space contraction is applied democratically by the thermostat to all degrees of freedom, and then the isokinetic thermostat can be considered to be the optimal thermostat for systems of a few hundred or a few thousand particles (and isokinetic SLLOD the optimal algorithm). It is easy to imagine changing the thermostat so that it is nondemocratic or nonoptimal. Applying the thermostat to only a subset of the particles would be sufficient. We have proved the conjugate pairing theorem for Gaussian (or Nose-Hoover) isokinetic color conductivity [9,10] and there the result is, in fact, stronger in that it holds exactly for an arbitrary piece of trajectory in the comoving coordinate frame. For isokinetic SLLOD, the result can at best be considered to hold on average in the phase space that excludes the unpaired exponent.

In the large system limit, we would expect the fluctuations in α to decrease and, therefore, expect any departures from CPR to disappear regardless of the details of the thermostat. However, at constant field, increasing the system size eventually leads to a hydrodynamic instability such as turbulent or stringy phases, or even color separation in the color diffusion algorithm. For homogeneous systems away from hydrodynamic instabilities, we would expect that the conjugate pairing rule would be true on average, but the strong form of conjugate pairing would not be valid.

Recent numerical studies of the Lyapunov spectrum of 1024 hard disks at equilibrium has shown that the smallest exponents appear in discrete degenerate groups [14]. It has been argued that these exponents are connected with the time scales associated with hydrodynamic modes in a combined tangent space and coordinate space, and a simplified random matrix model proposed to provide justification of this idea [15]. In the results presented here, there is no evidence of these modes, but this is a consequence of the small system size. Even if hydrodynamic modes do exist in nonequilibrium steady states of color diffusion, the conjugate pairing rule must hold for all exponents.

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