Lyapunov Exponent Pairing for a Thermostatted Hard-Sphere Gas under Shear in the Thermodynamic Limit

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We demonstrate why for a sheared gas of hard spheres, described by the SLLOD equations with an iso-kinetic Gaussian thermostat in between collisions, deviations of the conjugate pairing rule for the Lyapunov spectrum are to be expected, employing a previous result that for a large number of particles $N$, the iso-kinetic Gaussian thermostat is equivalent to a constant friction thermostat, up to $1/\sqrt{N}$ fluctuations. We also show that these deviations are at most of the order of the fourth power in the shear rate.

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The SLLOD equations of motion, combined with Lees-Edwards boundary condition [1], were originally proposed in Refs. [2,3], and since then they have been convenient tools to calculate the shear viscosity of gases in the bulk by means of non-equilibrium molecular dynamics simulations for many years. These studies consider systems with a large number of mutually interacting particles that are driven by an external shear rate $\gamma$. In these studies, the iso-kinetic Gaussian thermostat is an artificial way to continuously remove the energy generated inside the system due to the work done on it by the external shear field, such that a non-equilibrium steady state, homogeneous in space, can be reached. The Lyapunov spectrum of such systems is of interest since it has been shown that the shear viscosity can be related to the spectrum [3], which can be numerically obtained as a function of the shear rate [3]. The analysis of the simulation data [2,3] indicated that the sum of the largest and the smallest, the sum of the second largest and the second smallest and so on, were the same. The phenomenon of such pairing of the Lyapunov exponents is known as the Conjugate Pairing Rule, or the CPR. Based on this observation, an attempt to prove an exact CPR was made for arbitrary inter-particle potentials and arbitrary $\gamma$ [4,5], and later studies and better simulation techniques [6,7,8] indicated that for systems obeying the SLLOD equations of motion, the CPR is not satisfied exactly under these general conditions [9]. However, any conclusive theoretical proof regarding the status of an approximate CPR for systems under SLLOD equations of motion is absent in the literature till now, leaving the problem open for a long time.

The SLLOD equations of motion describe the dynamics of a collection of $N$ particles constituting a fluid with a macroscopic velocity field $\mathbf{u}(\mathbf{r}) = \gamma \mathbf{x}$. For particles of unit mass, the equations of motion of the $i$-th particle, in terms of its position $\mathbf{r}_i$ and peculiar momentum $\mathbf{p}_i$, is given by

$$
\dot{\mathbf{r}}_i = \mathbf{p}_i + \gamma y_\mathbf{x}, \quad \dot{\mathbf{p}}_i = F_i - \gamma p_{iy} \mathbf{x} - \alpha \mathbf{p}_i, \quad (1)
$$

where $\mathbf{F}_i$ is the force on the $i$-th particle due to the other particles in the system. The value of $\alpha$, the coefficient of friction representing the iso-kinetic Gaussian thermostat, is chosen such that the total peculiar kinetic energy of the system, $\sum p_i^2/2$, is a constant of motion in between collisions. In terms of the positions $\mathbf{r}_i$ and the laboratory momenta $\mathbf{v}_i$ of the particles, Eq. (1) reads

$$
\dot{\mathbf{r}}_i = \mathbf{v}_i, \quad \dot{\mathbf{v}}_i = \mathbf{F}_i + \alpha \gamma y_\mathbf{x} - \alpha \mathbf{v}_i. \quad (2)
$$

In the present context, the gas particles are hard spheres, which for simplicity are assumed to have unit radius. The dynamics of the gas particles consists of an alternating sequence of flight segments and instantaneous binary collisions. During a flight, the dynamics of the gas particles is described by Eqs. (2) with $\mathbf{F}_i = 0$. At an instantaneous collision between the $i$-th and the $j$-th sphere, the post-collisional positions and laboratory momenta (+ subscripts) are related to their pre-collisional values (− subscripts) by

$$
r_{i+} = r_{i-}, \quad r_{j+} = r_{j-},
$$

$$
v_{i+} = v_{i-} - \{(v_{i-} - v_{j-}) \cdot \hat{n}_{ij}\} \hat{n}_{ij} \quad \text{and}
$$

$$
v_{j+} = v_{j-} + \{(v_{i-} - v_{j-}) \cdot \hat{n}_{ij}\} \hat{n}_{ij}, \quad (3)
$$

while the positions and the velocities of the rest of the spheres remain unchanged. Here, $\hat{n}_{ij}$ is the unit vector along the line joining the center of the $i$-th sphere to the $j$-th sphere at the instant of collision. Note that because we applied the iso-kinetic Gaussian thermostat only between collisions [3], the peculiar kinetic energy changes in individual collisions. These changes are random, both in magnitude and sign, due to the randomness of the collision parameters, and hence it is quite likely that the system would reach a steady state, where the average change of peculiar kinetic energy would be zero.
In terms of the $3N$-dimensional vectors $\mathbf{R} = (r_1, r_2, ..., r_N)$, $\mathbf{V} = (v_1, v_2, ..., v_N)$ and $\mathbf{N}_{ij}$, whose $l$-th entry is given by $\mathbf{N}_{lj}^l = (\delta_{l,i} - \delta_{l,j})\hat{n}_{ij}/\sqrt{2}$ ($l = 1, 2, ..., N$), Eqs. (3) can be compacted to

$$\dot{\mathbf{R}} = \mathbf{V}, \quad \dot{\mathbf{V}} = \alpha \gamma \mathbf{CR} - \alpha \mathbf{V}$$

(4)
during a flight segment and

$$\mathbf{R}_+ = \mathbf{R}_-, \quad \mathbf{V}_+ = \mathbf{V}_- - 2(\mathbf{V}_- \cdot \mathbf{N}_{ij})\hat{n}_{ij}$$

at a collision between the $i$-th and the $j$-th sphere \[14\]. Here, $\mathbf{C}$ is a $3N \times 3N$ matrix with $N \times N$ entries, each of which is a $3 \times 3$ matrix. In terms of the entry index $(l, m)$, in the $xyz$-basis, $C_{lm} = c \delta_{lm} (l, m = 1, 2, ..., N)$ and

$$c = \hat{x}\hat{y} = \begin{bmatrix} 0 & 1 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}.$$

Having described the dynamics of the infinitesimal deviation $\delta \mathbf{X} = (\delta \mathbf{R}, \delta \mathbf{V})$ between two typical trajectories in the $6N$-dimensional phase space for a time $t$ as

$$\delta \mathbf{X}(t) = \mathbf{L}(t) \delta \mathbf{X}(0),$$

(5)

the Lyapunov exponents for this system are the logarithms of the eigenvalues of the matrix $\Lambda$, defined by

$$\Lambda = \lim_{t \to \infty} \left[ \mathbf{L}(t) \right]^{1/(2t)} ,$$

where $\mathbf{L}(t) = [\mathbf{L}(t)^T \mathbf{L}(t)]$.

It can be shown \[13\] that the sufficient condition for the CPR to hold exactly for a dynamical system obeying Eq. (3) is the existence of a constant non-singular matrix $K$ satisfying $K^2 = \mathcal{I}$, such that

$$[\mathbf{L}(t)^T \mathbf{K} \mathbf{L}(t)] = \mu \mathcal{K}.$$  

(6)

Here, $\mu$ is a scalar function of $t$. If $\mathbf{L}(t)$ satisfies Eq. (3), then we call $\mathbf{L}(t)$ to be “generalized $\mu$-symplectic”. It is easy to show from Eq. (3) that if $\mathbf{L}$ is an eigenvalue of $\tilde{\mathbf{L}}(t)$, then so is $\mu^2 / \tilde{\mathbf{L}}$; from which the (exact) CPR follows. For the situations where the CPR has been proved to be exact \[14\], only the $\mu$-symplecticity case of Eq. (3) (i.e., $K = \mathcal{J}$, where $\mathcal{J}$ is the usual symplectic matrix) has been exploited. In this context, we note that despite the similarity between the present problem and the one discussed in Ref. \[14\], the elaborate formalism developed therein is not applicable here.

A significant simplification can be achieved by noticing that the coefficient of friction $\alpha$, in the non-equilibrium steady state, fluctuates with $1/\sqrt{N}$ fluctuations around a fixed value $\alpha_0$ in the thermodynamic limit \[13\]. Thus, to calculate the Lyapunov exponents for large $N$, to which we confine ourselves henceforth, $\alpha$ can be replaced by $\alpha_0$ in Eq. (3), except for a beginning transient time. On average, for small $\gamma$, $\alpha \propto \gamma^2$ and so is $\alpha_0$. Higher order corrections play a role for larger shear rates.

In the following analysis, we first explore the status of the CPR when the coefficient of friction is a constant, $\alpha_0$, and then return to the case where the coefficient of friction represents an iso-kinetic Gaussian thermostat. The detailed derivation of the following results is given elsewhere \[18\]. At present, we focus only on the main points.

Once $\alpha_0$ replaces $\alpha$ in Eq. (3), we find that in the time evolution of $\delta \mathbf{X}$ over a collision-less flight segment between $t$ and $t + \tau$ is given by

$$\delta \mathbf{X}(t + \tau) = \mathbf{H}(\tau) \delta \mathbf{X}(t).$$

(7)

$\mathbf{H}(\tau)$ can be decomposed into $3N \times 3N$ sub-matrices as

$$\mathbf{H}(\tau) = \left[ \begin{array}{c|c|c} h^{[1]}(\tau) & h^{[2]}(\tau) & \vline \ \hline h^{[3]}(\tau) & h^{[4]}(\tau) \end{array} \right].$$

(8)

Having further decomposed each of the $\mathbf{h}^{[l]}(\tau)$ matrices ($l = 1, 2, 3, 4$) into $N \times N$ entries of $3 \times 3$ matrices as $h^{[lm]}(\tau)$ ($l$ and $m$ are counted along the row and the column respectively), we have (with $I$ as the identity matrix)

$$h^{[1]}_{lm}(\tau) = \left\{ \begin{array}{c} 1 + \gamma \tau - \frac{\gamma}{\alpha_0} (1 - e^{-\alpha_0 \tau}) \\ \frac{1 - e^{-\alpha_0 \tau}}{\alpha_0} \end{array} \right\} \delta_{lm},$$

$$h^{[2]}_{lm}(\tau) = \left\{ \begin{array}{c} 1 - e^{-\alpha_0 \tau} \\ \frac{\gamma}{\alpha_0} \left( 1 + e^{-\alpha_0 \tau} - 2 + 2e^{-\alpha_0 \tau} \right) \end{array} \right\} \delta_{lm},$$

$$h^{[3]}_{lm}(\tau) = \left\{ \begin{array}{c} \gamma (1 - e^{-\alpha_0 \tau}) \\ 0 \end{array} \right\} \delta_{lm} \text{ and}$$

$$h^{[4]}_{lm}(\tau) = \left\{ \begin{array}{c} e^{-\alpha_0 \tau} I - \gamma \tau + \frac{1}{\alpha_0} (1 - e^{-\alpha_0 \tau}) \\ 0 \end{array} \right\} \delta_{lm},$$

(9)

If we now form a $6N \times 6N$ matrix $G$, \[13\] in the notation of Eq. (3) which looks like $G^{[1]}_{lm} = G^{[4]}_{lm} = 0$ and $G^{[2]}_{lm} = G^{[3]}_{lm} = g \delta_{lm}$, where

$$g = \begin{bmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{bmatrix}.$$  

(10)

Then $\mathbf{H}(\tau)$ can be easily shown to satisfy \[13\]

$$[\mathbf{H}(\tau)]^T \mathbf{G} \mathbf{H}(\tau) = e^{-\alpha_0 \tau} \mathbf{G}.$$  

(11)

Thus, $\mathbf{H}(\tau)$ is generalized $\mu$-symplectic with $\mathbf{G}$, but it is not $\mu$-symplectic, i.e., $[\mathbf{H}(\tau)]^T \mathbf{J} \mathbf{H}(\tau) \neq e^{-\alpha_0 \tau} \mathbf{J}$. The fact that the same analysis \[Eqs. (3)\] can be carried out for any constant coefficient of friction (not necessarily $\alpha_0$), implies that the CPR is exact for a collision-less gas of point particles obeying Eq. (3) with a constant coefficient of friction. This has been found previously in simulation data \[11\].

For the transformation of $\delta \mathbf{X}$ over a binary collision between the $i$-th and the $j$-th sphere, we follow the explicit derivation in Ref. \[14\], which in turn is based on
the formalism developed simultaneously by Gaspard and Dorfman [21], and by Dellago and co-workers [22]. The post-collisional infinitesimal deviation vector \( \delta \mathbf{X}_+ \) can be related to its pre-collisional value \( \delta \mathbf{X}_- \) by

\[
\delta \mathbf{X}_+ = M_{ij} \delta \mathbf{X}_- ,
\]

where the \( 6N \times 6N \) matrix \( M_{ij} \) can be decomposed into four \( 3N \times 3N \) blocks, having the following structure

\[
M_{ij} = (1 - 2N_{ij} \mathbf{N}_{ij}) \begin{bmatrix} 1 & 0 \\ R & 1 \end{bmatrix} .
\]

Here, \( R \) is a symmetric matrix. The above expression for \( M \) implies that the collisions are symplectic, i.e.,

\[
M_{ij}^{T} J M_{ij} = J ,
\]

but not generalized symplectic with \( G \) (\( M_{ij}^{T} G M_{ij} \neq G \)).

We can now express the matrix \( L(t) \) in terms of the \( H \) and \( M \) matrices in the following way: if the dynamics involves free flight segments separated by \( s \) instantaneous binary collisions at \( t_1, t_2, \ldots, t_s \) such that \( 0 < t_1 < t_2 < \cdots < t_s < t \), then

\[
L(t) = H(\Delta t_s) M_{i_{s-1}j_{s}}, H(\Delta t_{s-1}) \cdots M_{i_1j_1}, H(\Delta t_0) . \tag{12}
\]

Here, \( \Delta t_s = t - t_s \) and \( \Delta t_i = t_{i+1} - t_i \) for \( i = 1, \ldots, (s-1) \).

The consequences of Eqs. (12) can be summarized by the following: for a collection of hard spheres obeying the SLLOD equations of motion with constant coefficient of friction \( \alpha_0 \), (a) the \( H \) matrices are generalized \( \mu \)-symplectic with \( G \), but not with \( J \), and (b) the \( M \) matrices are symplectic but not generalized \( \mu \)-symplectic with \( G \). Hence, once the \( H \) and the \( M \) matrices are combined together, as in Eq. (12), \( L(t) \) is seen to be generalized \( \mu \)-symplectic with neither \( G \) nor \( J \). This is consistent with the claim that \( L(t) \) is not generalized \( \mu \)-symplectic (and consequently, the CPR does not hold exactly) for a collection of hard spheres obeying the SLLOD equations of motion with constant coefficient of friction \( \alpha_0 \).

The degree of deviation from an exact CPR must follow from the properties of \( L(t) \), and to estimate this deviation, we can use either \( K = G \), or \( K = J \) in Eq. (1). While the former choice implies that one has to try to estimate the deviation from an exact CPR from the distribution of the unit vectors \( \mathbf{N}_{ij} \)'s and the collision angles for different sets of binary collisions in the expression of \( \mathbf{M}_{ij} \)'s, the latter choice means that one can make the estimate by using the typical magnitude of a free flight time, i.e., the mean free time \( \tau_0 \). We choose the latter approach, because an estimate of the deviation from the exact CPR can be made at small \( \gamma \), as a power series expansion in \( \gamma \). It is important to realize at this point that as the density sets a time scale in the form of the mean flight time \( \tau_0 \) between collisions, the actual dimensionless small parameter corresponding to the shear rate is \( \tilde{\gamma} = \gamma \tau_0 \).

We begin by constructing another matrix \( H_0(\Delta t) \) by setting \( \gamma = 0 \) but \( \alpha_0 \neq 0 \) in the explicit form of \( H(\Delta t) \) in Eqs. (4), i.e.,

\[
H_0(\Delta t) = H(\Delta t)|_{\alpha_0 \neq 0, \gamma = 0} .
\]

It is easy to show that \( H_0(\Delta t) \) satisfies the equation

\[
[H_0(\Delta t)]^T J H_0(\Delta t) = e^{-\alpha_0 \Delta t} J .
\]

Following Eq. (12), we then form the matrix \( L_0(t) \) as

\[
L_0(t) = H_0(\Delta t_s) M_{i_{s-1}j_{s}}, H_0(\Delta t_{s-1}) \cdots M_{i_1j_1}, H_0(\Delta t_0) , \tag{13}
\]

such that all the \( M_{ij} \) matrices in Eqs. (12) and (13) are the same. Since both the \( M_{ij} \) and the \( H_0(\Delta t) \) matrices are now \( \mu \)-symplectic with \( J \), so is \( L_0(t) \). As a consequence, the logarithms of the eigenvalues of \( \lambda_0(t) = [L_0(t)]^T L_0(t) \) pair exactly. This implies that if we arrange the corresponding Lyapunov spectrum

\[
\lambda_0 = \lim_{t \to \infty} \{ \lambda_0(t) \}^{1/(2n)} ,
\]

in the decreasing order of magnitude as \( \lambda_0^{(0)} \geq \lambda_0^{(1)} \geq \cdots \geq \lambda_0^{(N)} \), then \( \lambda_0^{(i)} + \lambda_0^{(i-1)} = -\alpha_0 \).

It is a simple exercise to show that \( H(\Delta t) - H_0(\Delta t) = O(\gamma^3) \), from which we conclude that for \( \Delta t = \tau = O(\tau_0) \)

\[
L(\tau) = L_0(\tau)[1 + \gamma^3 B] , \tag{14}
\]

where the matrix \( B \) is of order 1 in \( \gamma \) and order 1 in \( N \). Note that \( B \) contains higher powers of \( \gamma \) as well. Because it involves the matrix \( c \) and contributions from collisions between spheres, \( B \) is not proportional to 1, and hence, we cannot regard it simply as a scalar factor (in which case the exact conjugate pairing would be easy to obtain again). Equation (14) implies that for \( \Delta \lambda(\tau) = \tilde{\lambda}(\tau) - \tilde{\lambda}(0) \)

\[
\Delta \tilde{\lambda}(\tau) = \gamma^3 \{ \tilde{B}^T \tilde{\lambda}(0) + \tilde{\lambda}(0) B \} + \gamma^6 \tilde{B}^T \tilde{\lambda}(0) B . \tag{15}
\]

From Eqs. (14) and (15), we can now see that the differences between \( L(\tau) \) and \( L_0(\tau) \), and between \( \tilde{\lambda}(\tau) \) and \( \tilde{\lambda}_0(\tau) \) are small, by a relative order \( \gamma^3 \). Therefore the logarithm of the eigenvalues of \( L(\tau) \) and \( \tilde{\lambda}(\tau) \) also differ by a term of order \( \gamma^3 \) in an absolute sense. If we now divide the logarithms of these eigenvalues by the time \( \tau \), we see that the finite time (for time \( \tau \) Lyapunov exponents, calculated from \( \tilde{\lambda}_0(\tau) \) and from \( \tilde{\lambda}(\tau) \) (which we denote as \( \lambda_i^{(0)}(\tau) \) and \( \lambda_i(\tau) \) respectively, for \( i = 1, 2, \ldots, 6N \)), differ by a term \( O(\gamma^3/\tau) = O(\gamma^{2}) \).

We make one further observation at this stage. The Lyapunov exponents (even the finite time ones) are invariant under \( \gamma \to -\gamma \), so in a power series expansion in \( \gamma \) [24], the odd powers vanish. Hence, we conclude that the logarithm of the eigenvalues of \( L(\tau) \) and \( \tilde{\lambda}(\tau) \) must differ by a term of order \( \gamma^4 \), i.e., the conjugate pairing of \( \lambda_i(\tau) \)'s must be valid up to corrections of the form \( \gamma^{2.5} \).
To explicitly extend this formalism to large $t$ and thereby obtain a relation between $\lambda_i$ and $\lambda_i^{(0)}$, we need to sequentially concatenate a lot of $L(\tau)$'s. In general, these matrices neither commute with each other, nor with the $B$'s, which prevents us from explicitly demonstrating how the deviation $|\hat{L}(t) - \bar{L}(t)|$ is built up. However, we can argue in the following manner: $\hat{L}(t)$ and $\bar{L}(t)$ are positive definite and symmetric. This allows us to express them in the form $\hat{L}(t) = \exp(A_0)$ and $\bar{L}(t) = \exp(A)$, where for large $t$, both the eigenvalues of $A_0$ and $A$ must behave $\sim t$. From this perspective, the difference between the Lyapunov exponents for $\hat{L}(t)$ and $\bar{L}(t)$ is related to $(A - A_0)$. Since the difference between $\hat{L}(t)$ and $\bar{L}(t)$ has an explicit prefactor of $\tilde{\gamma}^3$, so does $A - A_0$. Using the symmetry argument that the Lyapunov exponents have to be even functions of $\gamma$, we obtain

$$\lambda_i + \lambda_{6N-i+1} = -\alpha_0 + O(\gamma^3) \quad i = 1, \ldots, 6N \quad (16)$$

For the largest and the most negative Lyapunov exponents, it has been possible to show that they pair to $-\alpha_0$ plus corrections of $O(\gamma^3)$ by means of a kinetic theory approach [23,24], based on the independence of subsequent collisions of a sphere. Likewise, one expects that in subsequent time-intervals of $O(\tau_0)$, the $L(\tau)$ matrices are not qualitatively much different from each other. Therefore, we expect that the coefficient of the $O(\gamma^3)$ term in Eq. (14), to be of the same order as that for a flight time $\tau = O(\tau_0)$ [i.e. of the order of $B = O(1)$], and therefore Eq. (14) to hold.

In summary, for the SLLOD equations with a constant thermostat, the finite time Lyapunov exponents obey the CPR up to $O(\gamma^3)$ when that time is of the order of the mean flight time, and this is expected to hold for the infinite time Lyapunov exponents too. Moreover, the iso-kinetic Gaussian thermostat is equivalent to the constant multiplier thermostat in the thermodynamic limit [19], and hence one expects that with an iso-kinetic Gaussian thermostat between collisions, the Lyapunov exponent spectrum also exhibits $O(\gamma^3)$ deviations from the CPR, in the thermodynamic limit. Finally, given that the source of the CPR violation is basically the repulsive potential with a constant multiplier thermostat, the violation of the CPR would also be at least of $O(\gamma^4)$ (for gas particles interacting with each other by means of a short-ranged, repulsive potential with an iso-kinetic Gaussian thermostat, the same results are expected) [20].

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