PHYSICAL REVIEW E, VOLUME 65, 060102(R)

Lyapunov exponent pairing for a thermostatted hard-sphere gas under shear in the thermodynamic limit

Debabrata Panja[1] and Ramses van Zon[2]
[1]*Instituut Lorentz, Universiteit Leiden, Postbus 9506, 2300 RA Leiden, The Netherlands*
[2]*Chemical Physics Theory Group, Chemistry Department, University of Toronto, 80 St. George Street, Toronto, Ontario M5S 3H6, Canada*

(Received 6 February 2002; published 28 June 2002)

We demonstrate why for a sheared gas of hard spheres, described by the SLLOD equations with an isokinetic 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 isokinetic 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.

DOI: 10.1103/PhysRevE.65.060102 PACS number(s): 05.20.−y, 05.45.−a, 05.60.Cd

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 nonequilibrium 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 γ [4–6]. In these studies, the isokinetic 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 nonequilibrium 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 [5,6], which can be numerically obtained as a function of the shear rate [7]. The analysis of the simulation data [5] 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 interparticle potentials and arbitrary γ [8,9], and later studies and better simulation techniques [10,11] indicated that for systems obeying the SLLOD equations of motion, the CPR is not satisfied exactly under these general conditions [12]. 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 $\mathbf{u}(\mathbf{r})=\gamma y\hat{\mathbf{x}}$. For particles of unit mass, the equations of motion of the ith particle, in terms of its position $\mathbf{r}_i$ and peculiar momentum $\mathbf{p}_i$, is given by

$$\dot{\mathbf{r}}_i=\mathbf{p}_i+\gamma y_i\hat{\mathbf{x}},\quad \dot{\mathbf{p}}_i=\mathbf{F}_i-\gamma p_{iy}\hat{\mathbf{x}}-\alpha\mathbf{p}_i, \tag{1}$$

where $\mathbf{F}_i$ is the force on the ith particle due to the other particles in the system. The value of α, the coefficient of friction representing the isokinetic Gaussian thermostat, is chosen such that the total peculiar kinetic energy of the system, $\Sigma_i p_i^2/2$, 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

$$\dot{\mathbf{r}}_i=\mathbf{v}_i,\quad \dot{\mathbf{v}}_i=\mathbf{F}_i+\alpha\gamma y_i\hat{\mathbf{x}}-\alpha\mathbf{v}_i. \tag{2}$$

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 ith and the jth sphere, the postcollisional positions and laboratory momenta (+ subscripts) are related to their precollisional values (− subscripts) by

$$\mathbf{r}_{i+}=\mathbf{r}_{i-},\quad \mathbf{r}_{j+}=\mathbf{r}_{j-},$$
$$\mathbf{v}_{i+}=\mathbf{v}_{i-}-\{(\mathbf{v}_{i-}-\mathbf{v}_{j-})\cdot\hat{\mathbf{n}}_{ij}\}\hat{\mathbf{n}}_{ij},\quad\text{and}$$
$$\mathbf{v}_{j+}=\mathbf{v}_{j-}+\{(\mathbf{v}_{i-}-\mathbf{v}_{j-})\cdot\hat{\mathbf{n}}_{ij}\}\hat{\mathbf{n}}_{ij}, \tag{3}$$

while the positions and the velocities of the rest of the spheres remain unchanged. Here, $\hat{\mathbf{n}}_{ij}$ is the unit vector along the line joining the center of the ith sphere to the jth sphere at the instant of collision. Note that because we applied the isokinetic Gaussian thermostat only between collisions [13], 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 $\mathbf{R}=(\mathbf{r}_1,\mathbf{r}_2,\ldots,\mathbf{r}_N)$, $\mathbf{V}=(\mathbf{v}_1,\mathbf{v}_2,\ldots,\mathbf{v}_N)$, and $\hat{\mathbf{N}}_{ij}$, whose lth entry is given by $\hat{\mathbf{N}}_{ij}^l=(\delta_{l,i}-\delta_{l,j})\hat{\mathbf{n}}_{ij}/\sqrt{2}$ $(l=1,2,\ldots,N)$, Eqs. (2) and (3) can be compacted to

$$\dot{\mathbf{R}}=\mathbf{V},\quad \dot{\mathbf{V}}=\alpha\gamma\mathsf{C}\mathbf{R}-\alpha\mathbf{V} \tag{4}$$

during a flight segment and

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

at a collision between the ith and the jth sphere [14]. Here, C is a $3N\times 3N$ matrix with $N\times N$ entries, each of which is a 3×3 matrix. In terms of the entry index (l,m), in the xyz basis, $\mathsf{C}_{lm}=\mathsf{c}\delta_{lm}$ $(l,m=1,2,\ldots,N)$ and

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

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

$$\delta\mathbf{X}(t)=\mathsf{L}(t)\,\delta\mathbf{X}(0), \tag{5}$$

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

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

where $\tilde{\mathsf{L}}(t)=[\mathsf{L}(t)]^{\mathrm{T}}\mathsf{L}(t)$.

It can be shown [15] that the *sufficient condition* for the CPR to hold exactly for a dynamical system obeying Eq. (5) is the existence of a *constant nonsingular* matrix K satisfying $\mathsf{K}^2\propto\mathsf{I}$, such that

$$[\mathsf{L}(t)]^{\mathrm{T}}\mathsf{K}\mathsf{L}(t)=\mu\mathsf{K}. \tag{6}$$

Here, μ is a scalar function of t. If $\mathsf{L}(t)$ satisfies Eq. (6), then we call $\mathsf{L}(t)$ to be "generalized μ-symplectic." It is easy to show from Eq. (6) that if $\tilde{L}$ is an eigenvalue of $\tilde{\mathsf{L}}(t)$, then so is $\mu^2/\tilde{L}$; from which the (exact) CPR follows. For the situations where the CPR has been proved to be exact [14,16–18], only the μ-symplecticity case of Eq. (6) (i.e., $\mathsf{K}=\mathsf{J}$, where 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 α, in the nonequilibrium steady state, fluctuates with $1/\sqrt{N}$ fluctuations around a fixed value α_0 in the thermodynamic limit [19]. Thus, to calculate the Lyapunov exponents for large N, to which we confine ourselves henceforth, α can be replaced by α_0 in Eq. (4), except for a beginning transient time. On average, for small γ, $\alpha\propto\gamma^2$ and so is α_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 α_0, and then return to the case where the coefficient of friction represents an isokinetic Gaussian thermostat. The detailed derivation of the following results is given elsewhere [15]. At present, we focus only on the main points.

Once α_0 replaces α in Eq. (4), we find that in the time evolution of $\delta\mathbf{X}$ over a collisionless flight segment between t and $t+\tau$ is given by

$$\delta\mathbf{X}(t+\tau)=\mathsf{H}(\tau)\,\delta\mathbf{X}(t). \tag{7}$$

$\mathsf{H}(\tau)$ can be decomposed into $3N\times 3N$ submatrices as

$$\mathsf{H}(\tau)=\begin{bmatrix}\mathsf{h}^{[1]}(\tau)&\mathsf{h}^{[2]}(\tau)\\\mathsf{h}^{[3]}(\tau)&\mathsf{h}^{[4]}(\tau)\end{bmatrix}. \tag{8}$$

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

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

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

$$\mathsf{h}^{[3]}_{lm}(\tau)=\{\gamma[1-e^{-\alpha_0\tau}]\mathsf{c}\}\delta_{lm},\quad\text{and}$$

$$\mathsf{h}^{[4]}_{lm}(\tau)=e\left\{^{-\alpha_0\tau}\mathsf{I}-\gamma\left[\tau+\frac{1}{\alpha_0}(1-e^{\alpha_0\tau})\right]\mathsf{c}\right\}\delta_{lm}. \tag{9}$$

If we now form a $6N\times 6N$ matrix G [in the notation of Eq. (8)], which looks like $\mathsf{G}^{[1]}_{lm}=\mathsf{G}^{[4]}_{lm}=\emptyset$ and $\mathsf{G}^{[2]}_{lm}=\mathsf{G}^{[3]}_{lm}=\mathsf{g}\delta_{lm}$, where

$$\mathsf{g}=\begin{bmatrix}0&1&0\\1&0&0\\0&0&1\end{bmatrix}. \tag{10}$$

Then $\mathsf{H}(\tau)$ can be easily shown to satisfy [20]

$$[\mathsf{H}(\tau)]^{\mathrm{T}}\mathsf{G}\mathsf{H}(\tau)=e^{-\alpha_0\tau}\mathsf{G}. \tag{11}$$

Thus, $\mathsf{H}(\tau)$ is generalized μ-symplectic with G, but it is not μ-symplectic, i.e., $[\mathsf{H}(\tau)]^{\mathrm{T}}\mathsf{J}\mathsf{H}(\tau)\neq e^{-\alpha_0\tau}\mathsf{J}$. The fact that the same analysis [Eqs. (7)–(10)] can be carried out for any constant coefficient of friction (not necessarily α_0), implies that the CPR is exact for a *collisionless* gas of point particles obeying Eq. (4) 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 ith and the jth 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 postcollisional infinitesimal deviation vector $\delta\mathbf{X}_+$ can be related to its precollisional value $\delta\mathbf{X}_-$ by

$$\delta\mathbf{X}_+=\mathsf{M}_{ij}\delta\mathbf{X}_-,$$

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

$$\mathsf{M}_{ij}=(\mathsf{I}-2\hat{\mathbf{N}}_{ij}\hat{\mathbf{N}}_{ij})\begin{bmatrix}\mathsf{I}&0\\\mathsf{R}&\mathsf{I}\end{bmatrix}.$$

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

$$\mathsf{M}_{ij}^{\mathrm{T}}\mathsf{J}\mathsf{M}_{ij}=\mathsf{J},$$

but not generalized symplectic with G ($\mathsf{M}_{ij}^{\mathrm{T}}\mathsf{G}\mathsf{M}_{ij}\neq\mathsf{G}$).

We can now express the matrix $\mathsf{L}(t)$ 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

$$\mathsf{L}(t)=\mathsf{H}(\Delta t_s)\mathsf{M}_{i_s j_s}\mathsf{H}(\Delta t_{s-1})\cdots\mathsf{M}_{i_1 j_1}\mathsf{H}(\Delta t_0). \tag{12}$$

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. (7)–(12) can be summarized by the following: for a collection of hard spheres obeying the SLLOD equations of motion with constant coefficient of friction α_0, (a) the H matrices are generalized μ-symplectic with G, but not with J, and (b) the M matrices are symplectic but not generalized μ-symplectic with G. Hence, once the H and the M matrices are combined together, as in Eq. (12), $\mathsf{L}(t)$ is seen to be generalized μ-symplectic with neither G nor J. This is consistent with the claim that $\mathsf{L}(t)$ is not generalized μ-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 α_0.

The degree of deviation from an exact CPR must follow from the properties of $\mathsf{L}(t)$, and to estimate this deviation, we can use either $\mathsf{K}=\mathsf{G}$, or $\mathsf{K}=\mathsf{J}$ in Eq. (6). 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 $\hat{\mathbf{N}}_{ij}$'s and the collision angles for different sets of binary collisions in the expression of 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 τ_0. We choose the latter approach, because an estimate of the deviation from the exact CPR can be made at small γ, as a *power series expansion* in γ. It is important to realize at this point that as the density sets a time scale in the form of the mean flight time τ_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 $\mathsf{H}_0(\Delta t)$ by setting $\gamma=0$ but $\alpha_0\neq 0$ in the explicit form of $\mathsf{H}(\Delta t)$ in Eqs. (7)–(9), i.e.,

$$\mathsf{H}_0(\Delta t)=\mathsf{H}(\Delta t)\big|_{\alpha_0\neq 0,\gamma=0}.$$

It is easy to show that $\mathsf{H}_0(\Delta t)$ satisfies the equation,

$$[\mathsf{H}_0(\Delta t)]^{\mathrm{T}}\mathsf{J}\mathsf{H}_0(\Delta t)=e^{-\alpha_0\Delta t}\mathsf{J}.$$

Following Eq. (12), we then form the matrix $\mathsf{L}_0(t)$ as

$$\mathsf{L}_0(t)=\mathsf{H}_0(\Delta t_s)\mathsf{M}_{i_s j_s}\mathsf{H}_0(\Delta t_{s-1})\cdots\mathsf{M}_{i_1 j_1}\mathsf{H}_0(\Delta t_0), \tag{13}$$

such that *all* the M_{ij} matrices in Eqs. (12) and (13) are the same. Since both the M_{ij} and the $\mathsf{H}_0(\Delta t)$ matrices are now μ-symplectic with J, so is $\mathsf{L}_0(t)$. As a consequence, the logarithms of the eigenvalues of $\tilde{\mathsf{L}}_0(t)=[\mathsf{L}_0(t)]^{\mathrm{T}}\mathsf{L}_0(t)$ pair exactly. This implies that if we arrange the corresponding Lyapunov spectrum

$$\mathbf{\Lambda}_0=\lim_{t\to\infty}[\tilde{\mathsf{L}}_0(t)]^{1/(2t)},$$

in the decreasing order of magnitude as $\lambda_1^{(0)}\geqslant\lambda_2^{(0)}\geqslant\cdots\geqslant\lambda_{6N}^{(0)}$, then $\lambda_i^{(0)}+\lambda_{6N-i+1}^{(0)}=-\alpha_0$.

It is a simple exercise to show that $\mathsf{H}(\Delta t)-\mathsf{H}_0(\Delta t)=O(\tilde{\gamma}^3)$, from which we conclude that for $\Delta t=\tau=O(\tau_0)$,

$$\mathsf{L}(\tau)=\mathsf{L}_0(\tau)[\mathsf{I}+\tilde{\gamma}^3\mathsf{B}], \tag{14}$$

where the matrix B is of the order of one in both $\tilde{\gamma}$ and N. Note that B contains higher powers of $\tilde{\gamma}$ as well. Because it involves the matrix c and contributions from collisions between spheres, B is not proportional to I, 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 $\Delta\tilde{\mathsf{L}}(\tau)\equiv\tilde{\mathsf{L}}(\tau)-\tilde{\mathsf{L}}_0(\tau)$,

$$\Delta\tilde{\mathsf{L}}(\tau)=\tilde{\gamma}^3[\mathsf{B}^{\mathrm{T}}\tilde{\mathsf{L}}_0(\tau)+\tilde{\mathsf{L}}_0(\tau)\mathsf{B}]+\tilde{\gamma}^6\mathsf{B}^{\mathrm{T}}\tilde{\mathsf{L}}_0(\tau)\mathsf{B}. \tag{15}$$

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

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 [23] in $\tilde{\gamma}$, the odd powers vanish. Hence, we conclude that the logarithm of the eigenvalues of $\mathsf{L}(\tau)$ and $\mathsf{L}_0(\tau)$ must differ by a term of the order of $\tilde{\gamma}^4$, i.e., the conjugate pairing of $\lambda_i(\tau)$'s must be valid up to corrections of the form $\gamma\tilde{\gamma}^3$.

To explicitly extend this formalism to large t and thereby obtain a relation between λ_is and $\lambda_i^{(0)}$s, we need to sequentially concatenate a lot of $\mathsf{L}(\tau)$'s. In general, these matrices neither commute with each other, nor with the B's, which prevents us from explicitly demonstrating how the deviation $[\mathsf{L}(t)-\mathsf{L}_0(t)]$ is built up. However, we can argue in the following manner: $\tilde{\mathsf{L}}(t)$ and $\tilde{\mathsf{L}}_0(t)$ are positive definite and symmetric. This allows us to express them in the form $\tilde{\mathsf{L}}_0(t)=\exp(\mathsf{A}_0)$ and $\tilde{\mathsf{L}}(t)=\exp(\mathsf{A})$, 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 $\tilde{\mathsf{L}}(t)$ and $\tilde{\mathsf{L}}_0(t)$ is related to $(\mathsf{A}-\mathsf{A}_0)$. Since the difference between $\tilde{\mathsf{L}}(t)$ and $\tilde{\mathsf{L}}_0(t)$ has an explicit prefactor of $\tilde{\gamma}^3$, so does A

$-\mathsf{A}_0$. Using the symmetry argument that the Lyapunov exponents have to be even functions of γ, we obtain

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

For the largest and the most negative Lyapunov exponents, it has been possible to show that they pair to $-\alpha_0$ plus corrections of $O(\gamma\tilde{\gamma}^3)$ by means of a kinetic theory approach [24,25], based on the independence of subsequent collisions of a sphere. Likewise, one expects that in subsequent time intervals of $O(\tau_0)$, the $\mathsf{L}(\tau)$ matrices are not qualitatively much different from each other. Therefore, we expect that the coefficient of the $O(\gamma\tilde{\gamma}^3)$ term in Eq. (16), to be of the same order as that for a flight time $\tau=O(\tau_0)$ [i.e., of the order of $\mathsf{B}=O(1)$], and therefore Eq. (16) to hold.

In summary, for the SLLOD equations with a constant α_0 thermostat, the finite-time Lyapunov exponents obey the CPR up to $O(\gamma\tilde{\gamma}^3)$ 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 isokinetic Gaussian thermostat is equivalent to the constant multiplier thermostat in the thermodynamic limit [19], and hence one expects that with an isokinetic Gaussian thermostat between collisions, the Lyapunov exponent spectrum also exhibits $O(\gamma\tilde{\gamma}^3)$ deviations from the CPR, in the thermodynamic limit. Finally, given that the source of the CPR violation is basically the $\alpha_0\gamma\mathsf{C}\mathbf{R}$ term in Eq. (4), one can argue that when the gas particles interact with each other by means of a short-ranged, repulsive potential with a constant multiplier thermostat, the violation of the CPR would also be at least of $O(\tilde{\gamma}^4)$ (for gas particles interacting with each other by means of a short-ranged, repulsive potential with an isokinetic Gaussian thermostat, the same results are expected) [15].

It is a pleasure to thank Professor J. R. Dorfman and Professor H. van Beijeren for many useful and motivating discussions regarding this subject. D.P. was supported by research grants from ''Fundamenteel Onderzoek der Materie (FOM)'' and that of Professor J. R. Dorfman, NSF-PHY-9600428. R.v.Z. was supported by the research grant of Professor H. van Beijeren, by FOM, SMC, and NWO Priority Program Non-Linear Systems, and by a grant from the Natural Sciences and Engineering Research Council of Canada.

[1] A.W. Lees and S.F. Edwards, J. Phys. C **5**, 1921 (1980).
[2] D.J. Evans and G.P. Morriss, Comput. Phys. Rep. **1**, 297 (1983).
[3] D.J. Evans and G.P. Morriss, Phys. Rev. A **30**, 1528 (1984).
[4] G.P. Morriss, Phys. Rev. A **37**, 2118 (1988).
[5] G.P. Morriss, Phys. Lett. A **134**, 307 (1989).
[6] D.J. Evans and G.P. Morriss, *Statistical Mechanics of Nonequilibrium Liquids* (Academic Press, London, 1990).
[7] With CPR, the viscosity can be computed from two pairing Lyapunov exponents, but numerically it is not very efficient.
[8] D.J. Evans, E.G.D. Cohen, and G.P. Morriss, Phys. Rev. A **42**, 5990 (1990).
[9] S. Sarman, D.J. Evans, and G.P. Morriss, Phys. Rev. A **45**, 2233 (1992).
[10] D.J. Isbister, D.J. Searles, and D.J. Evans, Physica A **240**, 105 (1997).
[11] D.J. Searles, D.J. Evans, and D.J. Isbister, Chaos **8**, 337 (1998).
[12] A recent work by G.P. Morriss, Phys. Rev. E **65**, 017201 (2002) has once again verified that the original results of Ref. [5] were correct, thereby contradicting the simulation results of Refs. [10] and [11].
[13] For the limit $\mathbf{F}_i\to\infty$ with an isokinetic Gaussian thermostat during the collision, see J. Petravic, D.J. Isbister, and D.J. Morriss, J. Stat. Phys. **76**, 1045 (1994).
[14] Debabrata Panja, e-print nlin.CD/0107048.
[15] Debabrata Panja and Ramses van Zon, e-print nlin.CD/0202015.
[16] C.P. Dettmann and G.P. Morriss, Phys. Rev. E **53**, R5545 (1996).
[17] M.P. Wojtkowski and C. Liverani, Commun. Math. Phys. **194**, 47 (1998).
[18] D. Ruelle, J. Stat. Phys. **95**, 393 (1999).
[19] R. van Zon, Phys. Rev. E **60**, 4158 (1999).
[20] There may exist other forms of g satisfying Eq. (11), but Eq. (10) is the simplest one for which $\mathsf{G}^2\propto\mathsf{I}$.
[21] P. Gaspard and J.R. Dorfman, Phys. Rev. E **52**, 3525 (1995).
[22] Ch. Dellago, H.A. Posch, and W.G. Hoover, Phys. Rev. E **53**, 1485 (1996).
[23] Here we assume that such a power series expansion can be carried out for individual Lyapunov exponents. This is not unreasonable, but it might be applicable only to low densities. In any case, it is clear from the previous paragraph that the presence of such nonanalytic terms can only give rise to differences between the finite-time Lyapunov exponents $\lambda_i(\tau)$ and $\lambda_i^{(0)}(\tau)$ (or the actual Lyapunov exponents λ_i and $\lambda_i^{(0)}$) that are *weaker* than $\gamma\tilde{\gamma}^2$.
[24] R. van Zon, Ph.D. thesis, University of Utrecht, The Netherlands, 2000.
[25] R. van Zon and H. van Beijeren (unpublished).