Front Propagation Techniques to Calculate the Largest Lyapunov Exponent of Dilute Hard Disk Gases

R. van Zon[1] **and Henk van Beijeren**[2]

A kinetic approach is adopted to describe the exponential growth of a small deviation of the initial phase space point, measured by the largest Lyapunov exponent, for a dilute system of hard disks, both in equilibrium and in a uniform shear flow. We derive a generalized Boltzmann equation for an extended one-particle distribution that includes deviations from the reference phase space point. The equation is valid for very low densities n, and requires an unusual expansion in powers of $1/|\ln n|$. It reproduces and extends results from the earlier, more heuristic clock model and may be interpreted as describing a front propagating into an unstable state. The asymptotic speed of propagation of the front is proportional to the largest Lyapunov exponent of the system. Its value may be found by applying the standard front speed selection mechanism for pulled fronts to the case at hand. For the equilibrium case, an explicit expression for the largest Lyapunov exponent is given and for sheared systems we give explicit expressions that may be evaluated numerically to obtain the shear rate dependence of the largest Lyapunov exponent.

1. INTRODUCTION

Often, familiar models from statistical mechanics exhibit the strong dependence on the initial phase space point that we know as chaos.[1]

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[1] Chemical Physics Theory Group, Department of Chemistry, University of Toronto, Toronto, Ontario, Canada M5S 3H6; and Institute for Theoretical Physics, Utrecht University, Leuvenlaan 4, 3584 CE Utrecht, The Netherlands.

[2] Institute for Theoretical Physics, University of Utrecht, Leuvenlaan 4, 3584 CE Utrecht, The Netherlands; and Center for Nonlinear Phenomena and Complex Systems, Université Libre de Bruxelles, Campus Plaine, Code Postal 231, 1050 Brussels, Belgium; e-mail: H.van Beijeren@phys.uu.nl

Examples are the Lorentz gas, the hard disk and the hard sphere gas.[2] We call a system *chaotic* if the growth of a deviation from a reference trajectory in phase space is exponential, $\propto \exp(\lambda^+ t)$, in the limit that the initial deviation becomes infinitesimally small. λ^+ is called the largest Lyapunov exponent.

The systems we discuss in this paper, consist of N hard disks with equal mass m and equal diameters a, in a two dimensional volume V. The density is $n = N/V$, and a (dimensionless) reduced density is defined as $\tilde{n} = na^2$. The position and velocity of disk l are denoted by $\mathbf{r}_l$ and $\mathbf{v}_l$ respectively. We define a temperature in equilibrium by $Nk_BT = \langle \sum_{l=1}^{N} \frac{1}{2} m |\mathbf{v}_l|^2 \rangle$, where the brackets denote an ensemble average. For non-equilibrium stationary states, a generalization of this is used for the temperature. A typical velocity v_0 is defined as $v_0 = \sqrt{k_BT/m}$.

Considering a point in phase space $\{\mathbf{r}_h, \mathbf{v}_h\}$ ($h = 1 \cdots N$) and an adjacent point $\{\mathbf{r}_h^*, \mathbf{v}_h^*\}$ with $\mathbf{r}_h^* = \mathbf{r}_h + \delta\mathbf{r}_h$ and $\mathbf{v}_h^* = \mathbf{v}_h + \delta\mathbf{v}_h$, one may obtain the largest Lyapunov exponent by studying the exponential growth of the deviations $\delta\mathbf{r}_h$ and $\delta\mathbf{v}_h$. Other Lyapunov exponents exist, measuring growth rates of deviations in carefully selected different directions. Typical deviations have a component in the most rapidly expanding direction, so they grow with the largest Lyapunov exponent.

Of this chaotic behavior, little is seen on a macroscopic level, especially when we consider systems in or near equilibrium, but surprisingly, from numerical simulations, one found relations between Lyapunov exponents in stationary non-equilibrium systems, and linear transport coefficients.[3–5] Even if the generality of such relations can be questioned,[6] it is still interesting to consider models in which they hold. Among these are particle systems subject to a velocity independent external force and kept at a constant kinetic energy by means of a Gaussian thermostat.[7, 8]

For the last six years, efforts have been made to get an analytic grasp on the Lyapunov exponents. For the Lorentz gas at low density in two and three dimensions, Van Beijeren, Dorfman and co-workers have set up a kinetic theory in which all Lyapunov exponents could be calculated and relations with transport coefficients could be verified.[9–18] The hard disk and the hard sphere gas, which were next in line for kinetic investigation, proved harder to deal with. It is possible to obtain estimates for the largest Lyapunov exponent in equilibrium for these systems, based on heuristic effective dynamics of deviations.[19–21] Some results also have been obtained for the sum of all positive Lyapunov exponents, the KS-entropy.[21, 22]

In these approaches, one uses the linear dependence of the deviations after a collision on their values before, together with the linear growth of position deviations during the times between collisions. From this, it was

argued in refs. 19 and 21 that *at low densities*, it is enough to look at the *clock value*

$$k_l = \frac{\ln(|\boldsymbol{\delta}\mathbf{v}_l|/\delta v_0)}{|\ln \tilde{n}|}, \tag{1}$$

where δv_0 is an arbitrary unit of infinitesimal velocity. These clock values approximately change in a collision between particle i and j according to

$$k_i' = k_j' = \max(k_i, k_j) + 1 + \mathcal{O}(1/\ln \tilde{n}), \tag{2}$$

which is valid to leading order in $\tilde{n}$. The clock values k could therefore be restricted to integer values. In a chaotic system, each deviation $\boldsymbol{\delta}\mathbf{v}_l$ is expected to grow exponentially and the clock value k_l to grow linearly with time. Because not all deviations of the particles are identical, there is a distribution of clock values. The dynamics described by Eq. (2) tends to bring clock values far below average at any given time back towards the mean. As a result of this the distribution of all clock values with respect to the instantaneous average for long times approaches a stationary mean profile, about which the actual distribution keeps fluctuating. It then follows that the average clock value increases by 1 plus half the average difference between clock values per unit time (the mean free time between collisions for a single particle). In an abstract sense, this is equivalent to the situation of a propagating front, where a stable phase propagates into an unstable phase. The propagation occurs along a k-axis. One of the phases for a given "position" k is to have the clock distribution concentrated to its left, i.e., around lower clock values. This distribution will shift to the right and go beyond k. So this phase is unstable. The stable phase for a "position" k is to have the distribution concentrated to its right. On a technical note, it turns out that this problem falls into the class of pulled fronts,[24] which is fortunate as it is known how to obtain the front propagation speed w for such systems. Using those techiques, for long times the average clock values was found to behave as

$$\bar{k} = N^{-1} \sum_{l=1}^{N} k_l(t) = k_0 + w\bar{v}t,$$

with $\bar{v}$ the average collision frequency and w a constant of order $\tilde{n}^0$. As a consequence of Eq. (1) the largest Lyapunov exponent is

$$\lambda^+ = -w\bar{v} \ln \tilde{n}. \tag{3}$$

to leading order in the density. In ref. 21 this analysis was refined further. It was recognized that the distribution of clock values depends explicitly on the speed of the particles and the equations describing its time evolution were adjusted accordingly. Nonetheless the pulled front analogy remains fully valid.

The purpose of this paper is to give a firmer basis to the heuristic arguments leading to equation (3), and to extend the methods so as to be applicable to higher densities and to non-equilibrium cases.

A typical example of a non-equilibrium case is the hard disk gas in a uniform shearing state, described by the so-called SLLOD equations.[23] The gas is confined between two infinite (one-dimensional) parallel plates a distance $2L$ apart, moving in opposite directions with velocities $\pm\gamma L$ (see Fig. 1). We look at the limit of large L and infinite extension in the x-direction, with fixed shear rate γ and density $n = N/V$. For small shear rate, a linear velocity profile develops in the system, so that the fluid velocity at y is $\mathbf{u} = \gamma y\hat{x}$. We remark that, although we want the volume V to be macroscopic, L should not be too large, otherwise the Reynolds number would become so high that the system becomes turbulent and the assumed linear velocity profile breaks down.

The paper is set up as follows. In Section 2 we discuss the dynamics of deviations. In Section 3 we consider the velocity distribution function and the distribution of the duration of intercollisional flights for the hard disk gas under shear. In Section 4 we set up a generalized Boltzmann equation for a one particle distribution function that includes the deviations, and expand that in powers of $1/\ln \tilde{n}$. In Section 5, this equation is reinterpreted as describing a propagating front. The largest Lyapunov exponent is proportional to the front velocity w, which we can determine using a standard method for pulled fronts.[24] The perturbation expansion in the density is further developed in Section 6. In Section 7 we calculate the first two terms in the density expansion of the largest Lyapunov exponent for the two-dimensional hard disk gas in equilibrium. The results are formally extended to the shear case in Section 8. We conclude with a discussion in Section 9.
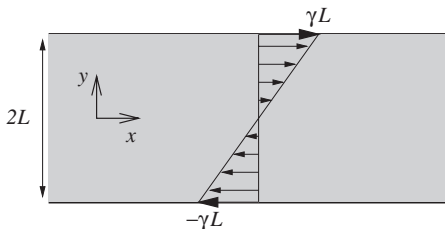

Fig. 1.   Velocity profile in a gas under shear.

2. CHAOS IN HARD DISK GASES

The dynamics of the hard disk system is defined as follows. When disks i and j hit each other, they collide elastically. We define $\mathbf{r}_{ij} = \mathbf{r}_i - \mathbf{r}_j$ and $\mathbf{v}_{ij} = \mathbf{v}_i - \mathbf{v}_j$, and get

$$
\begin{aligned}
\mathbf{v}'_i &= \mathbf{v}_i - (\hat{\boldsymbol{\sigma}} \cdot \mathbf{v}_{ij})\, \hat{\boldsymbol{\sigma}}, \\
\mathbf{v}'_j &= \mathbf{v}_j + (\hat{\boldsymbol{\sigma}} \cdot \mathbf{v}_{ij})\, \hat{\boldsymbol{\sigma}},
\end{aligned}
\tag{4}
$$

with $\hat{\boldsymbol{\sigma}}$ the unit vector in the direction of the line connecting the center of the two disks at contact, i.e., $\hat{\boldsymbol{\sigma}} = a^{-1}\mathbf{r}_{ij}$. Primed quantities denote post-collisional values throughout this paper. The positions remain unchanged, $\mathbf{r}'_i = \mathbf{r}_i$, $\mathbf{r}'_j = \mathbf{r}_j$.

In between collisions, the coordinates of disk l satisfy

$$
\dot{\mathbf{r}}_l = \mathbf{v}_l; \qquad \dot{\mathbf{v}}_l = \frac{1}{m}\, \mathbf{F}_l(\{\mathbf{r}_h, \mathbf{v}_h\}),
\tag{5}
$$

The forces $\mathbf{F}_l$ are smooth functions of the coordinates $\{\mathbf{r}_h, \mathbf{v}_h\}$, $h = 1 \cdots N$. In an instantaneous collision between disks i and j, the smooth forces $\mathbf{F}_i$ and $\mathbf{F}_j$ cannot perform any action, therefore Eq. (4) describing the collision, holds for any $\mathbf{F}_l$.

The dynamics of the deviations $\delta\mathbf{r}_l$ and $\delta\mathbf{v}_l$ in collisionless flight are given by the linearized version of Eq. (5),

$$
\begin{aligned}
\dot{\delta}\mathbf{r}_l &= \delta\mathbf{v}_l \\
\dot{\delta}\mathbf{v}_l &= \frac{1}{m} \sum_{h=1}^{N} \sum_{a=1}^{2} \left(\frac{\partial \mathbf{F}_l}{\partial r_{h,a}}\, \delta r_{h,a} + \frac{\partial \mathbf{F}_l}{\partial v_{h,a}}\, \delta v_{h,a} \right),
\end{aligned}
\tag{6}
$$

where $\delta r_{h,a}$ and $\delta v_{h,a}$ denote the ath component of $\delta\mathbf{r}_h$ and $\delta\mathbf{v}_h$, respectively.

To find the collision dynamics, we use a method developed both by Gaspard and Dorfman[25] and by Dellago et al.[26] Here, we work out the dynamics for the general system of Eqs. (4) and (5). For the equilibrium case this was done in refs. 21 and 26. The reference trajectory and the adjacent trajectory are infinitesimally close so we can assume that they have the same collision sequence. The most subtle ingredient in the derivation of the collision dynamics of deviations, is the time difference δt between the (i, j) collision on the two adjacent trajectories. We set the time of the (i, j) collision equal to zero for the reference trajectory, so that of the adjacent trajectory equals δt. We consider here the case that δt is

positive, but one easily checks that the final results are equally valid for negative δt. We define

$$\delta\mathbf{r}_l = \mathbf{r}_l^*(0^-) - \mathbf{r}_l(0^-), \qquad \delta\mathbf{v}_l = \mathbf{v}_l^*(0^-) - \mathbf{v}_l(0^-),$$

$$\delta\mathbf{r}_l' = \mathbf{r}_l^*(\delta t^+) - \mathbf{r}_l(\delta t^+), \qquad \delta\mathbf{v}_l' = \mathbf{v}_l^*(\delta t^+) - \mathbf{v}_l(\delta t^+),$$

where $l = i$ or j, the superscript * denotes values on the adjacent trajectory and $+$ and $-$ indicate after and before collision, respectively.

The time shift δt can be found from the requirement that at the instant of collision, the two disks are a distance a apart, i.e., $|\mathbf{r}_{ij}(0)| = a$ and $|\mathbf{r}_{ij}^*(\delta t)| = a$. Because the time difference δt is infinitesimal, we only have to express the $\mathbf{r}_l^*(\delta t)$ to linear order in δt, yielding $\mathbf{r}_l^*(\delta t) = \mathbf{r}_l + \delta\mathbf{r}_l + \mathbf{v}_l \, \delta t$. Note that here (and in the rest of this section) unprimed quantities without time specification are assumed to carry their value at $t = 0$ before the collision, e.g., $\mathbf{v}_l = \mathbf{v}_l(0^-)$. From the requirement $|\mathbf{r}_{ij}^*(\delta t)|^2 - |\mathbf{r}_{ij}|^2 = 0$, we get

$$2\mathbf{r}_{ij} \cdot (\delta\mathbf{r}_{ij} + \mathbf{v}_{ij} \, \delta t) = 0$$

to linear order in the deviations, so

$$\delta t = -\frac{\mathbf{r}_{ij} \cdot \delta\mathbf{r}_{ij}}{\mathbf{r}_{ij} \cdot \mathbf{v}_{ij}} = -\frac{\hat{\boldsymbol{\sigma}} \cdot \delta\mathbf{r}_{ij}}{\hat{\boldsymbol{\sigma}} \cdot \mathbf{v}_{ij}}. \tag{7}$$

The difference in collision normal $\delta\hat{\boldsymbol{\sigma}} = \hat{\boldsymbol{\sigma}}^* - \hat{\boldsymbol{\sigma}}$ follows from

$$\delta\hat{\boldsymbol{\sigma}} = \frac{\mathbf{r}_{ij}^*(\delta t) - \mathbf{r}_{ij}}{a} = \frac{\delta\mathbf{r}_{ij} + \mathbf{v}_{ij} \, \delta t}{a} = \frac{(\hat{\boldsymbol{\sigma}} \cdot \mathbf{v}_{ij}) \, \mathbb{1} - \mathbf{v}_{ij}\hat{\boldsymbol{\sigma}}}{a(\hat{\boldsymbol{\sigma}} \cdot \mathbf{v}_{ij})} \, \delta\mathbf{r}_{ij},$$

where we used Eq. (7) in the last equality. $\mathbb{1}$ is the identity matrix and we use the conventions that non-dotted products of two vectors are dyadic products, and a product of matrices always implies matrix multiplication, as does the product of a matrix with a vector.

Consider first the position deviations. For the reference trajectory we have, for $l = i$ or j,

$$\mathbf{r}_l(\delta t) = \mathbf{r}_l + \mathbf{v}_l' \, \delta t,$$

because the trajectory is determined by the velocity $\mathbf{v}_l(0^+)$ after the collision at $t = 0$. For the adjacent trajectory we have

$$\mathbf{r}_l^*(\delta t) = \mathbf{r}_l^* + \mathbf{v}_l^*(0^-) \, \delta t,$$

because this trajectory has velocity $\mathbf{v}_i^*(0^-)$, before colliding at time δt. We write $\delta\mathbf{r}_i' = \mathbf{r}_i^* + \mathbf{v}_i^* \, \delta t - \mathbf{r}_l - \mathbf{v}_l' \, \delta t$ and insert the expressions for $\mathbf{v}_l'$ from Eq. (4) and the one for δt from Eq. (7), to find

$$\begin{aligned}
\delta\mathbf{r}_i' &= \delta\mathbf{r}_i - (\delta\mathbf{r}_{ij} \cdot \hat{\boldsymbol{\sigma}}) \, \hat{\boldsymbol{\sigma}}, \\
\delta\mathbf{r}_j' &= \delta\mathbf{r}_j + (\delta\mathbf{r}_{ij} \cdot \hat{\boldsymbol{\sigma}}) \, \hat{\boldsymbol{\sigma}}
\end{aligned} \tag{8}$$

(neglecting again expressions quadratic in deviations). For the velocity deviation vectors on the reference trajectory, one finds for $l = i$ or j,

$$\mathbf{v}_l(\delta t^+) = \mathbf{v}_l(0^+) + \frac{1}{m} \mathbf{F}_l(\{\mathbf{r}_h, \mathbf{v}_h'\}) \, \delta t,$$

Of course, only the velocities of the colliding disks, $\mathbf{v}_i$ and $\mathbf{v}_j$, have really changed. We abbreviate $\mathbf{F}_l(\{\mathbf{r}_h, \mathbf{v}_h'\})$ by $\mathbf{F}_l'$ and $\mathbf{F}_l(\{\mathbf{r}_h, \mathbf{v}_h\})$ by $\mathbf{F}_l$ from now on. For the adjacent trajectory,

$$\mathbf{v}_l^*(\delta t^+) = \left[\mathbf{v}_l^* + \frac{1}{m} \mathbf{F}_l(\{\mathbf{r}_h^*, \mathbf{v}_h^*\}) \, \delta t \right]' = \left[\mathbf{v}_l^* + \frac{1}{m} \mathbf{F}_l \, \delta t \right]'$$

where in the last equation, the difference between $\mathbf{F}_l^* \, \delta t$ and $\mathbf{F}_l \, \delta t$ has been neglected (second order in the deviations). The prime means that the collision rule for velocities should be applied. For the adjacent trajectory, this is a collision with collision normal $\hat{\boldsymbol{\sigma}}^*$, so, for disk i,

$$\begin{aligned}
\mathbf{v}_i^*(\delta t^+) &= [\mathbf{v}_i^*(\delta t^-) - \hat{\boldsymbol{\sigma}}^*(\hat{\boldsymbol{\sigma}}^* \cdot \mathbf{v}_{ij}^*(\delta t^-))] \\
&= \mathbf{v}_i(\delta t^+) + \delta\mathbf{v}_i - \hat{\boldsymbol{\sigma}}(\hat{\boldsymbol{\sigma}} \cdot \delta\mathbf{v}_{ij}) - [(\hat{\boldsymbol{\sigma}} \cdot \mathbf{v}_{ij}) \, \mathbb{1} + \hat{\boldsymbol{\sigma}}\mathbf{v}_{ij}] \, \delta\hat{\boldsymbol{\sigma}} \\
&\quad + \frac{1}{m} (\mathbf{F}_i - \mathbf{F}_i') \, \delta t - \frac{1}{m} (\hat{\boldsymbol{\sigma}} \cdot \{\mathbf{F}_i - \mathbf{F}_j\}) \, \hat{\boldsymbol{\sigma}} \, \delta t.
\end{aligned}$$

Inserting the expressions for $\delta\hat{\boldsymbol{\sigma}}$ and δt, we obtain

$$\delta\mathbf{v}_i' = \delta\mathbf{v}_i - \hat{\boldsymbol{\sigma}}(\hat{\boldsymbol{\sigma}} \cdot \delta\mathbf{v}_{ij}) - (\mathbf{Q}_{\hat{\boldsymbol{\sigma}}} - \mathscr{E}_1) \, \delta\mathbf{r}_{ij}$$

where

$$\begin{aligned}
\mathbf{Q}_{\hat{\boldsymbol{\sigma}}} &= \frac{[(\hat{\boldsymbol{\sigma}} \cdot \mathbf{v}_{ij}) \, \mathbb{1} + \hat{\boldsymbol{\sigma}}\mathbf{v}_{ij}][(\hat{\boldsymbol{\sigma}} \cdot \mathbf{v}_{ij}) \, \mathbb{1} - \mathbf{v}_{ij}\hat{\boldsymbol{\sigma}}]}{a(\hat{\boldsymbol{\sigma}} \cdot \mathbf{v}_{ij})}, \\
\mathscr{E}_1 &= \frac{[\hat{\boldsymbol{\sigma}} \cdot (\mathbf{F}_i - \mathbf{F}_j)] \, \hat{\boldsymbol{\sigma}} + \mathbf{F}_i' - \mathbf{F}_i}{m} \frac{\hat{\boldsymbol{\sigma}}}{\hat{\boldsymbol{\sigma}} \cdot \mathbf{v}_{ij}}.
\end{aligned} \tag{9}$$

Similarly, for disk j, we find

$$\delta\mathbf{v}'_j = \delta\mathbf{v}_j + \hat{\boldsymbol{\sigma}}(\hat{\boldsymbol{\sigma}} \cdot \delta\mathbf{v}_{ij}) + (\mathbf{Q}_{\hat{\boldsymbol{\sigma}}} - \mathscr{E}_1)\,\delta\mathbf{r}_{ij} \tag{10}$$

Thus when the dynamics of a point in phase space is determined by Eqs. (5) and (4), the dynamics of the deviation vectors is given by Eqs. (6) and (8)–(10).

3. SHEARED SYSTEM

In the sheared hard sphere gas, it is convenient to transform to the peculiar velocities of the particles,

$$\mathbf{V}_l = \mathbf{v}_l - \mathbf{u}(\mathbf{r}_l) = \mathbf{v}_l - \gamma y_l \hat{\mathbf{x}}. \tag{11}$$

The equations of motion in collisionless flight ($\dot{\mathbf{r}}_l = \mathbf{v}_l$, $\dot{\mathbf{v}}_l = 0$) are transformed to

$$\dot{\mathbf{r}}_l = \mathbf{V}_l + \gamma y_l \hat{\mathbf{x}}, \tag{12}$$

$$\dot{\mathbf{V}}_l = -\gamma V_{l,y} \hat{\mathbf{x}} \tag{13}$$

These equations are called the SLLOD equations of motion.[23] The pseudo-force $-m\gamma V_{l,y}\hat{\mathbf{x}}$ is called the shear force. Due to Eq. (11), in a collision between disks i and j, the peculiar velocities transform as

$$\begin{aligned}
\mathbf{V}'_i &= \mathbf{V}_i - (\hat{\boldsymbol{\sigma}} \cdot \mathbf{V}_{ij})\,\hat{\boldsymbol{\sigma}} - a\gamma\hat{\boldsymbol{\sigma}}(\hat{\mathbf{x}} \cdot \hat{\boldsymbol{\sigma}})(\hat{\mathbf{y}} \cdot \hat{\boldsymbol{\sigma}}), \\
\mathbf{V}'_j &= \mathbf{V}_j + (\hat{\boldsymbol{\sigma}} \cdot \mathbf{V}_{ij})\,\hat{\boldsymbol{\sigma}} + a\gamma\hat{\boldsymbol{\sigma}}(\hat{\mathbf{x}} \cdot \hat{\boldsymbol{\sigma}})(\hat{\mathbf{y}} \cdot \hat{\boldsymbol{\sigma}}),
\end{aligned} \tag{14}$$

In simulations, boundary effects can be minimized by a special kind of periodic boundary conditions, Lees–Edwards boundary conditions, in which case the periodic copies in the y-direction are moving with respect to another. When a particle crosses the boundary, it is put back at the other end but with a corrected position and unchanged *peculiar* velocity.[4, 23, 27]

The system as defined above does not have a steady state. The reason is that the shear force continuously converts macroscopic kinetic energy of flow into heat, i.e., internal kinetic energy. In realistic Couette-flow situations the work required for this is performed by the shearing walls of the system. In the present situation this work is a consequence of the boundary conditions. Because the location of the y-coordinate of the Lees–Edwards boundary is arbitrary, the system develops no temperature gradient, in contrast to a system with realistic boundaries. In such a realistic system a stationary state is usually reached by the establishment of a stationary heat

flow towards the boundaries, which absorb the heat and transmit it to a thermostat. If one doesn't want to include the environment explicitly, as is usually the case when one performs MD-simulations, one needs to put in a mechanism by hand to extract heat from the system. Such a mechanism commonly is also called a *thermostat*. Several thermostats are around for non-equilibrium systems, but we focus on one in particular. An extra term is added to the equations of motion for the velocities during collisionless flight, which become

$$\dot{\mathbf{V}}_i = -\gamma V_{yi}\hat{\mathbf{x}} - \alpha \mathbf{V}_i. \tag{15}$$

We choose for α a constant positive value, so that the extra terms can be interpreted as standard friction forces. In molecular dynamics simulations it is more common to use an isokinetic Gaussian thermostat,[23] which keeps the (peculiar) kinetic energy $\sum_i \frac{1}{2} m |\mathbf{V}_i|^2$ strictly constant. In that case, α depends on the positions and velocities of all the particles and can be chosen such that the equations of motion are time-reversible, i.e., form invariant under a time reversal operation. α then may take both positive and negative values and only on average will it be positive in the stationary state. In the thermodynamical limit, this thermostat is equivalent to the one with a constant α,[28, 29] and we choose the latter one, as it is simpler. The value of α determines the average peculiar kinetic energy, which is identified with the steady state temperature through

$$\left\langle \sum_i \frac{1}{2} m |\mathbf{V}_i|^2 \right\rangle = N k_{\mathrm{B}} T. \tag{16}$$

The brackets here denote a time average, which, when the system is ergodic, is also the average over an appropriate steady state distribution. Our thermostat suppresses turbulence[23] in regimes where it is expected physically. So the model is representative for an actual physical system only for low enough Reynolds number.

In the low density regime we can use the Boltzmann equation for the one-particle distribution function.[16, 30] We only consider stationary flows of uniform shear, so we can focus on the velocity distribution function of the form $f(\mathbf{V})$, which is normalized to unity. The Boltzmann equation for this distribution is

$$-\partial_{\mathbf{V}_1} \cdot [(\gamma V_{1y}\hat{\mathbf{x}} + \alpha \mathbf{V}_1) f_1] = \int \cdots \int' na |\hat{\boldsymbol{\sigma}} \cdot \mathbf{v}_{12}| (f_1' f_2' - f_1 f_2) \, d\mathbf{V}_2 \, d\hat{\boldsymbol{\sigma}}, \tag{17}$$

with the short hand notation $f_i = f(\mathbf{V}_i)$ and $f_i' = f(\mathbf{V}_i')$. The prime on the integration denotes the condition $\hat{\boldsymbol{\sigma}} \cdot \mathbf{v}_{12} < 0$.

We want to discuss briefly how one can solve this Boltzmann equation for small shear rates. In equilibrium, $\gamma = \alpha = 0$, and the right-hand side vanishes if f is a Maxwell velocity distribution. To allow for treating the left-hand side as a perturbation, γ has to be small compared to $na\langle|\mathbf{v}_{12}|\rangle$. Hence, the small parameter proportional to the shear rate is $\tilde{\gamma} = \gamma a/(\tilde{n}v_0)$. A Chapman–Enskog expansion of Eq. (17) can now be made by expanding in powers of this parameter. The expansion of f has the form

$$f(\mathbf{V}) = \varphi(\mathbf{V})[1 + \tilde{\gamma}g_1(\mathbf{V}) + \tilde{\gamma}^2 g_2(\mathbf{V}) + \cdots], \tag{18}$$

where φ is the Maxwell distribution

$$\varphi(\mathbf{V}) = \frac{m}{2\pi k_B T} e^{-m|\mathbf{V}|^2/(2k_B T)}. \tag{19}$$

In the rest of the paper, we use $\tilde{\gamma}$ as an independent variable, separate from the density $\tilde{n}$. In this spirit, higher density corrections are terms which vanish (relatively) when the density is lowered while $\tilde{\gamma}$ is kept fixed. Thus we neglect the last terms $\pm a\varphi(\hat{\boldsymbol{\sigma}} \cdot \hat{\mathbf{x}})(\hat{\boldsymbol{\sigma}} \cdot \hat{\mathbf{y}})$ in Eq. (14), as they are $\mathcal{O}(\tilde{\gamma}\tilde{n}v_0)$, i.e., one order in density higher than the other terms, which are of $\mathcal{O}(v_0)$. Likewise, the restriction on the integral in Eq. (17) is replaced by $\mathbf{V}_{12} \cdot \hat{\boldsymbol{\sigma}} < 0$ and $\mathbf{u}(a\hat{\boldsymbol{\sigma}})$ is neglected in $|\hat{\boldsymbol{\sigma}} \cdot \mathbf{v}_{12}| = |\hat{\boldsymbol{\sigma}} \cdot (\mathbf{V}_{12} + \mathbf{u}(a\hat{\boldsymbol{\sigma}}))|$. Finally, $\mathbf{v}_{ij}$ is replaced by $\mathbf{V}_{ij}$ in the matrix $\mathbf{Q}_{\hat{\boldsymbol{\sigma}}}$ in Eq. (9).

Within the framework of the Chapman–Enskog expansion the zeroth order solution, φ, entirely determines the temperature T; higher orders should not change the second moment of f. For fixed γ and T the friction coefficient α has to be expanded as $\alpha = \gamma[\alpha_1 + \tilde{\gamma}\alpha_2 + \cdots]$. To determine the coefficients, we note that $\langle \partial_t \sum_i |\mathbf{V}_i|^2 \rangle = 0$ in the stationary state and that $\sum_i |\mathbf{V}_i|^2$ is conserved in a collision, so that for the time derivative we can insert Eq. (15). In this way, we see that

$$\alpha = \gamma\langle V_x V_y \rangle/\langle|\mathbf{V}|^2\rangle = \frac{\gamma m}{k_B T} \int V_x V_y f(\mathbf{V}) \, d\mathbf{V}. \tag{20}$$

Thus, if we know f up to order $\tilde{\gamma}^{n-1}$, we can calculate α up to order $\tilde{\gamma}^n$, which we need to calculate f up to order $\tilde{\gamma}^n$. One also immediately sees that $\alpha_1 = 0$, because the average of the odd function $V_x V_y$ with the even distribution φ is zero. This is no surprise, as α gives the dissipation and this should be an even function of γ.

We will need the distribution $s(\mathbf{V}, \tau; t)$ of particles at time t with velocity $\mathbf{V}$ and time τ passed since their last collision. In the stationary state this satisfies the equation

$$\partial_\mathbf{V} \cdot [\dot{\mathbf{V}} s(\mathbf{V}, \tau)] + \partial_\tau s(\mathbf{V}, \tau) = -\nu(\mathbf{V}) \, s(\mathbf{V}, \tau),$$

for $\tau > 0$. The collision frequency v is given by

$$v(\mathbf{V}_1) = \int \cdots \int' na \, |\hat{\boldsymbol{\sigma}} \cdot \mathbf{V}_{12}| \, f_2 \, d\mathbf{V}_2 \, d\hat{\boldsymbol{\sigma}}. \tag{21}$$

We rewrite the density s in terms of a conditional distribution function: $s(\mathbf{V}, \tau) = f(\mathbf{V}) \, S(\tau \mid \mathbf{V})$. With

$$v^*(\mathbf{V}) \equiv v(\mathbf{V}) + \partial_{\mathbf{V}} \cdot \dot{\mathbf{V}} + \dot{\mathbf{V}} \cdot \partial_{\mathbf{V}} \ln f, \tag{22}$$

we find the following equation for $S(\tau \mid \mathbf{V})$,

$$\partial_\tau S(\tau \mid \mathbf{V}) + \dot{\mathbf{V}} \cdot \partial_{\mathbf{V}} S(\tau \mid \mathbf{V}) = -v^*(\mathbf{V}) \, S(\tau \mid \mathbf{V}),$$

with the initial condition to be determined by normalization. The general solution of this equation is

$$S(\tau \mid \mathbf{V}) = S_0(\mathbf{V}(-\tau)) \exp\left[-\int_{-\tau}^0 v^*(\mathbf{V}(t')) \, dt' \right]$$

where $\mathbf{V}(t)$ is the solution of the equations of motion, Eq. (15), with initial condition $\mathbf{V}(0) = \mathbf{V}$, i.e., $\mathbf{V}(t) = e^{-\alpha t}[\mathbf{V} - \hat{\mathbf{x}}\gamma t V_y]$. It is simple to show that for $\int_0^\infty S(\tau \mid \mathbf{V}) \, d\tau$ to be equal to 1, we need $S_0(\mathbf{V}) = v^*(\mathbf{V})$, so

$$S(\tau \mid \mathbf{V}) = v^*(\mathbf{V}(-\tau)) \exp\left[-\int_{-\tau}^0 v^*(\mathbf{V}(t')) \, dt' \right]. \tag{23}$$

4. GENERALIZED BOLTZMANN EQUATION

In this section we derive a generalized Boltzmann equation for the distribution function of $\mathbf{V}$ and $\delta\mathbf{V}$. But first of all, we make the dynamics of the deviations explicit for the case of the SLLOD equations (12)–(15) that we are investigating. In terms of $\mathbf{r}_i$ and $\mathbf{v}_i$, we have $\dot{\mathbf{v}}_i = \alpha\gamma y_i \hat{\mathbf{x}} - \alpha\mathbf{v}_i$. For this case, we get

$$\mathscr{E}_1 = \alpha\gamma a \, \frac{\hat{\boldsymbol{\sigma}} \cdot \hat{\mathbf{x}} \, \hat{\boldsymbol{\sigma}} \cdot \hat{\mathbf{y}}}{\hat{\boldsymbol{\sigma}} \cdot \mathbf{v}_{ij}} \, \hat{\boldsymbol{\sigma}}\hat{\boldsymbol{\sigma}},$$

(see Eq. (9)). The $\delta\mathbf{V}$ then change in a collision according to

$$\begin{aligned}
\delta\mathbf{V}'_i &= \delta\mathbf{V}_i - \hat{\boldsymbol{\sigma}}(\hat{\boldsymbol{\sigma}} \cdot \delta\mathbf{V}_{ij}) - (\mathbf{Q}_{\hat{\boldsymbol{\sigma}}} - \mathscr{E}_1 - \mathscr{E}_2) \, \delta\mathbf{r}_{ij} \\
\delta\mathbf{V}'_j &= \delta\mathbf{V}_j + \hat{\boldsymbol{\sigma}}(\hat{\boldsymbol{\sigma}} \cdot \delta\mathbf{V}_{ij}) + (\mathbf{Q}_{\hat{\boldsymbol{\sigma}}} - \mathscr{E}_1 - \mathscr{E}_2) \, \delta\mathbf{r}_{ij}
\end{aligned} \tag{24}$$

where $\mathscr{E}_2 = \gamma[\hat{\mathbf{x}}(\hat{\boldsymbol{\sigma}} \cdot \hat{\mathbf{y}}) \, \hat{\boldsymbol{\sigma}} - \hat{\boldsymbol{\sigma}}(\hat{\mathbf{x}} \cdot \hat{\boldsymbol{\sigma}}) \, \hat{\mathbf{y}}]$. The terms $\mathscr{E}_1$ and $\mathscr{E}_2$ are of higher order in the density than $\mathbf{Q}_{\hat{\boldsymbol{\sigma}}}$, which is of order (v_0/a), as one sees when expressing these quantities in terms of $\tilde{\gamma}$ and $\tilde{n}$; $\mathscr{E}_1 = \mathcal{O}(v_0 \tilde{\gamma}^3 \tilde{n}^2/a)$ and $\mathscr{E}_2 = \mathcal{O}(v_0 \tilde{\gamma} \tilde{n}/a)$. As we are restricting ourselves to the leading powers in density, with at most correction terms of relative order $1/|\ln \tilde{n}|$, we neglect $\mathscr{E}_1$ and $\mathscr{E}_2$ in the sequel.

In collisionless flight, the dynamics of deviations is,

$$\delta \dot{x}_i = \gamma \, \delta y_i + \delta V_{i,x}; \qquad\qquad \delta \dot{y}_i = \delta V_{i,y};$$

$$\delta \dot{V}_{i,x} = -\gamma \, \delta V_{i,y} - \alpha \, \delta V_{i,x}; \qquad \delta \dot{V}_{i,y} = -\alpha \, \delta V_{i,y}.$$

The solutions of these equations are:

$$\boldsymbol{\delta V}_i(t) = e^{-\alpha t}[\boldsymbol{\delta V}_i(0) - \hat{\mathbf{x}} \gamma t \, \delta V_{y,i}(0)] \tag{25}$$

$$\boldsymbol{\delta r}_i(t) = \boldsymbol{\delta r}_i(0) + \delta y_i(0) \, \gamma t \hat{\mathbf{x}} + \frac{1 - e^{-\alpha t}}{\alpha} \, \boldsymbol{\delta V}_i(0)$$

$$+ \frac{\alpha t(1 + e^{-\alpha t}) - 2 + 2e^{-\alpha t}}{\alpha^2} \, \gamma \, \delta V_{i,y}(0) \, \hat{\mathbf{x}}$$

$$\equiv t \mathbf{S}_t \, \boldsymbol{\delta V}_i(0) + \boldsymbol{\delta r}_i(0) + \delta y_i \, \gamma t \hat{\mathbf{x}}. \tag{26}$$

We follow the deviation dynamics from collision to collision. So we are interested in the case where the time t in the equations above is of the order of a mean intercollisional flight time, $t = \mathcal{O}(a/(v_0 \tilde{n}))$. Then $\alpha t = \mathcal{O}(\tilde{\gamma}^2)$, and $\gamma t = \mathcal{O}(\tilde{\gamma})$, and both are of zeroth order in the density. We *assume* that

$$\mathcal{O}(\boldsymbol{\delta V}_i) = \mathcal{O}(\boldsymbol{\delta r}_i) \times v_0/a, \tag{27}$$

just after a collision. Then, at the next collision, the terms with a factor $t \boldsymbol{\delta V}_i(0)$ in Eq. (26) typically are one order in $1/\tilde{n}$ larger than the corresponding terms proportional to $\boldsymbol{\delta r}_i(0)$, which therefore may be neglected. The $\boldsymbol{\delta r}_i$ deviations just before a collision then are $\boldsymbol{\delta r}_i(\tau_i) = \tau_i \mathbf{S}_{\tau_i} \, \boldsymbol{\delta V}_i(0)$, where τ_i is the time from the previous collision of particle i. The effective equation linking the $\boldsymbol{\delta V}_i$ just after collision to their values just after the previous collisions of the two particles, is found from Eqs. (24) and (26):

$$\boldsymbol{\delta V}'_i \approx -\boldsymbol{\delta V}'_j \approx -\mathbf{Q}_{\hat{\boldsymbol{\sigma}}}(\tau_i \mathbf{S}_{\tau_i} \, \boldsymbol{\delta V}_i - \tau_j \mathbf{S}_{\tau_j} \, \boldsymbol{\delta V}_j), \tag{28}$$

where we neglected terms of higher order in $\tilde{n}$ coming from the center-of-mass contribution. To check for the consistency of our assumption about

the relative order of velocity and position deviations just after a collision, we consider also $\delta\mathbf{r}_i$ and $\delta\mathbf{r}_j$ after the next collision:

$$\delta\mathbf{r}'_i \approx -\delta\mathbf{r}'_j \approx (\tfrac{1}{2}\mathbb{1} - \hat{\boldsymbol{\sigma}}\hat{\boldsymbol{\sigma}})(\tau_i\mathbf{S}_{\tau_i}\,\delta\mathbf{V}_i - \tau_j\mathbf{S}_{\tau_j}\,\delta\mathbf{V}_j),$$

and we see that if Eq. (27) holds for $\delta\mathbf{r}_i$, $\delta\mathbf{V}_i$ and $\delta\mathbf{r}_j$, $\delta\mathbf{V}_j$ just after the previous collision, it also holds for $\delta\mathbf{r}'_i$, $\delta\mathbf{V}'_i$ and $\delta\mathbf{r}'_j$, $\delta\mathbf{V}'_j$.

In two dimensions, the matrix $\mathbf{Q}_{\hat{\boldsymbol{\sigma}}}$ in Eq. (28) is

$$\mathbf{Q}_{\hat{\boldsymbol{\sigma}}} = \frac{(\mathbf{R}\mathbf{v}'_{ij})(\mathbf{R}\mathbf{v}_{ij})}{a(\hat{\boldsymbol{\sigma}}\cdot\mathbf{v}_{ij})}$$

where $\mathbf{R}$ denotes a rotation over 90 degrees counterclockwise. To leading order in the density we may replace $\mathbf{v}_{ij}$ by $\mathbf{V}_{ij}$. Neglecting further $\mathscr{E}_1$ and $\mathscr{E}_2$ in Eq. (24) we obtain as effective equations of change for the velocity deviation vectors in a collision,

$$\delta\mathbf{V}'_i = \frac{\mathbf{R}\mathbf{V}'_{ij}[\mathbf{R}\mathbf{V}_{ij}\cdot(\tau_j\mathbf{S}_{\tau_j}\,\delta\mathbf{V}_j - \tau_i\mathbf{S}_{\tau_i}\,\delta\mathbf{V}_i)]}{a(\hat{\boldsymbol{\sigma}}\cdot\mathbf{V}_{ij})}, \tag{29}$$

$$\delta\mathbf{V}'_j = -\delta\mathbf{V}'_i.$$

To compare different contributions to $\delta\mathbf{V}'_i$ and $\delta\mathbf{V}'_j$, we want to know the order of $\delta\mathbf{V}_i$ and $\delta\mathbf{V}_j$. We write the value of $\delta\mathbf{V}_i$ *just after the previous collision* as

$$\delta\mathbf{V}_i \equiv v_0\left(\frac{1}{\tilde{n}}\right)^{k_i}\hat{\mathbf{e}}_i = v_0 e^{k_i/\vartheta}\hat{\mathbf{e}}_i, \tag{30}$$

where $\hat{\mathbf{e}}_i$ is a unit vector and ϑ is defined as

$$\vartheta \equiv \frac{1}{|\ln\tilde{n}|}$$

The clock values and unit vectors thus defined do not change during collisionless flight, only in collisions. In contrast to earlier work in refs. 19 and 21, the clock values k_i are real numbers here, not integers.

We obtain k'_1 from Eqs. (29) and (30):

$$k'_1 = \vartheta\ln\left|\frac{\mathbf{R}\mathbf{V}_{12}\cdot\mathbf{S}_{\tau_2}\hat{\mathbf{e}}_2\tau_2 e^{k_2/\vartheta} - \mathbf{R}\mathbf{V}_{12}\cdot\mathbf{S}_{\tau_1}\hat{\mathbf{e}}_1\tau_1 e^{k_1/\vartheta}}{a\,|\hat{\boldsymbol{\sigma}}\cdot\hat{\mathbf{V}}_{21}|}\right|$$

and distinguish two cases, telling us which of the two terms inside the logarithm is the largest, and hence, the most important. We define

$$b(\mathbf{V}, \tau, \hat{\mathbf{e}}, \hat{\boldsymbol{\sigma}}) = \ln \left| \frac{\tau \tilde{n} \mathbf{R} \mathbf{V} \cdot \mathbf{S}_\tau \hat{\mathbf{e}}}{a \hat{\mathbf{V}} \cdot \hat{\boldsymbol{\sigma}}} \right|, \tag{31}$$

and say that

(I)   disk 1 dominates disk 2 if

$$k_1 + \vartheta b(\mathbf{V}_{12}, \tau_1, \hat{\mathbf{e}}_1, \hat{\boldsymbol{\sigma}}) > k_2 + \vartheta b(\mathbf{V}_{12}, \tau_2, \hat{\mathbf{e}}_2, \hat{\boldsymbol{\sigma}}) \tag{32}$$

and that

(II)   disk 2 dominates disk 1 otherwise.

We also define an "alignment" criterion:

(+)   The unit vectors $\hat{\mathbf{e}}_1$ and $\hat{\mathbf{e}}_2$ are said to be aligned if $\mathbf{R} \mathbf{V}_{12} \cdot \mathbf{S}_{\tau_1} \hat{\mathbf{e}}_1$ has the same sign as $\mathbf{R} \mathbf{V}_{12} \cdot \mathbf{S}_{\tau_2} \hat{\mathbf{e}}_2$,

(−)   and anti-aligned if they have opposite signs.

From now on, when a $\pm$ or $\mp$ occurs in an equation, the upper sign corresponds to the aligned case, the lower one to the anti-aligned case. With these definitions, we write for the case (I):

$$\begin{aligned} k_1' = k_1 + 1 + \vartheta b(\mathbf{V}_{12}, \tau_1, \hat{\mathbf{e}}_1, \hat{\boldsymbol{\sigma}}) \\ + \vartheta \ln \left[1 \mp e^{(k_2 - k_1)/\vartheta} \frac{\exp[b(\mathbf{V}_{12}, \tau_2, \hat{\mathbf{e}}_2, \hat{\boldsymbol{\sigma}})]}{\exp[b(\mathbf{V}_{12}, \tau_1, \hat{\mathbf{e}}_1, \hat{\boldsymbol{\sigma}})]} \right] \end{aligned} \tag{33}$$

and for case (II):

$$\begin{aligned} k_1' = k_2 + 1 + \vartheta b(\mathbf{V}_{12}, \tau_2, \hat{\mathbf{e}}_2, \hat{\boldsymbol{\sigma}}) \\ + \vartheta \ln \left[1 \mp e^{(k_1 - k_2)/\vartheta} \frac{\exp[b(\mathbf{V}_{12}, \tau_1, \hat{\mathbf{e}}_1, \hat{\boldsymbol{\sigma}})]}{\exp[b(\mathbf{V}_{12}, \tau_2, \hat{\mathbf{e}}_2, \hat{\boldsymbol{\sigma}})]} \right] \end{aligned} \tag{34}$$

At this point it can be made clear why the distinction of one disk dominating over another was made. Consider Eq. (33). Because ϑ is small for low densities, and because Eq. (32) holds, the term after "$1 \mp$" inside the logarithm tends to be small, at least if k_1 and k_2 differ by an amount of $O(1)$. Consequently, this whole term is small, or, more precisely, it is appreciable only for $|k_2 - k_1| = O(\vartheta)$. Also the term ϑb is typically small. Hence $k_1' = k_1 + 1$ almost always, in the limit that $\vartheta \to 0$ (the infinitely

dilute gas). The same limit in case (II) yields $k'_1 = k_2 + 1$. We see that indeed, the "dominant" particle determines the value of the clocks after collision, at least if the density is low enough. This limiting dynamics for low density, expressed in Eq. (2), was derived before in refs. 19 and 21 and proved sufficient for obtaining the leading term in the density expansion of the largest Lyapunov exponent.

We consider the conditional probability distribution function for having clock value k and unit vector $\hat{\mathbf{e}}$ just after a collision at time t, given that the post-collisional velocity is $\mathbf{V}$. This function is denoted by $\hat{f}(k, \hat{\mathbf{e}} \mid \mathbf{V}; t)$ and it obeys

$$\omega(k, \hat{\mathbf{e}}, \mathbf{V}; t) = \omega(\mathbf{V}) \, \hat{f}(k, \hat{\mathbf{e}} \mid \mathbf{V}; t), \tag{35}$$

where $\omega(X; t)$ stands for the rate at which particles with attributes X are produced in collisions at time t. The production rate $\omega(\mathbf{V})$ of $\mathbf{V}$ in the stationary state is independent of time and satisfies

$$\omega(\mathbf{V}_1) = \iint{}' an \, |\hat{\boldsymbol{\sigma}} \cdot \mathbf{V}_{12}| \, f'_1 f'_2 \, d\mathbf{V}_2 d\hat{\boldsymbol{\sigma}} = v^*(\mathbf{V}_1) \, f_1, \tag{36}$$

where we used Eqs. (15), (17), (21) and (22). By considering the rate of restituting collisions that produce the right $(k, \hat{\mathbf{e}}, \mathbf{V}; t)$, we find that $\omega(k, \hat{\mathbf{e}}, \mathbf{V}; t)$ satisfies the equation

$$\omega(k, \hat{\mathbf{e}}, \mathbf{V}; t) = \int \cdots \int{}' an \, |\hat{\boldsymbol{\sigma}} \cdot \mathbf{V}_{12}| \, f_1 f_2 S(\tau_1 \mid \mathbf{V}_1) \, S(\tau_2 \mid \mathbf{V}_2)$$

$$\times \hat{f}(k_1, \hat{\mathbf{e}}_1 \mid \mathbf{V}_1(-\tau_1); t - \tau_1)$$

$$\times \hat{f}(k_2, \hat{\mathbf{e}}_2 \mid \mathbf{V}_2(-\tau_2); t - \tau_2)$$

$$\times \delta(\mathbf{V}'_1 - \mathbf{V}) \, \delta(k'_1 - k) \, \delta(\hat{\mathbf{e}}'_1 - \hat{\mathbf{e}})$$

$$\times d\mathbf{V}_1 \, d\mathbf{V}_2 \, dk_1 \, dk_2 \, d\hat{\mathbf{e}}_1 \, d\hat{\mathbf{e}}_2 \, d\tau_1 \, d\tau_2 \, d\hat{\boldsymbol{\sigma}}. \tag{37}$$

In the arguments of $\hat{f}$ the velocities need to be traced back to the previous collision, because $\hat{f}$ was defined in terms of the variables at that instant of time. Hence the appearance of $\mathbf{V}(-\tau)$. The clock values and unit vectors do not need such a correction, as they do not change in between collisions. We symmetrize the equation with respect to $\hat{\mathbf{e}}$, because $\hat{\mathbf{e}} \to -\hat{\mathbf{e}}$ only means interchanging the reference and the adjacent trajectory, and this cannot affect their rate of separation. Hence we can replace $\delta(\hat{\mathbf{e}}'_1 - \hat{\mathbf{e}}) = \delta(\mathbf{R}\hat{\mathbf{V}}'_{12} - \hat{\mathbf{e}})$ by $[\delta(\mathbf{R}\hat{\mathbf{V}}'_{12} - \hat{\mathbf{e}}) + \delta(\mathbf{R}\hat{\mathbf{V}}'_{12} + \hat{\mathbf{e}})]/2 = \frac{1}{2}\delta(\hat{\mathbf{e}} \cdot \hat{\mathbf{V}}'_{12})$.

Through linear order in ϑ the logarithmic terms in the expressions (33) and (34) for k_1' may be ignored in Eq. (37); their inclusion merely gives rise to corrections of $O(\vartheta^2)$. With this approximation Eq. (37) may be rewritten as

$$
\omega(k, \hat{\mathbf{e}}, \mathbf{V}; t) = \frac{\partial}{\partial k} \int \cdots \int' S(\tau_1 \mid \mathbf{V}_1) \, S(\tau_2 \mid \mathbf{V}_2) \, f_1 f_2
$$

$$
\times an \, |\hat{\boldsymbol{\sigma}} \cdot \mathbf{V}_{12}| \, \delta(\mathbf{V}_1' - \mathbf{V}) \, \frac{1}{2} \delta(\hat{\mathbf{e}} \cdot \hat{\mathbf{V}}_{12}')
$$

$$
\times C(k - 1 - \vartheta b(\mathbf{V}_{12}, \tau_1, \hat{\mathbf{e}}_1, \hat{\boldsymbol{\sigma}}), \hat{\mathbf{e}}_1 \mid \mathbf{V}_1(-\tau_1); t - \tau_1)
$$

$$
\times C(k - 1 - \vartheta b(\mathbf{V}_{12}, \tau_2, \hat{\mathbf{e}}_2, \hat{\boldsymbol{\sigma}}), \hat{\mathbf{e}}_2 \mid \mathbf{V}_2(-\tau_2); t - \tau_2)
$$

$$
\times d\mathbf{V}_1 \, d\mathbf{V}_2 \, d\hat{\mathbf{e}}_1 \, d\hat{\mathbf{e}}_2 \, d\tau_1 \, d\tau_2 \, d\hat{\boldsymbol{\sigma}} + \mathcal{O}(\vartheta^2). \tag{38}
$$

Here, we introduced a cumulative distribution, defined as

$$
C(k, \hat{\mathbf{e}} \mid \mathbf{V}; t) = \int_{-\infty}^{k} \hat{f}(k^*, \hat{\mathbf{e}} \mid \mathbf{V}; t) \, dk^*. \tag{39}
$$

Integrating Eq. (38) from $-\infty$ to k, using Eqs. (35), (36) and (39) for the left hand side, and changing integration variables from precollisional velocities to post-collisional ones, we arrive at

$$
v^*(\mathbf{V}_1) \, C(k, \hat{\mathbf{e}} \mid \mathbf{V}_1; t)
$$

$$
= \int \cdots \int' S(\tau_1 \mid \mathbf{V}_1') \, S(\tau_2 \mid \mathbf{V}_2') \, f_1^{-1} f_1' f_2'
$$

$$
\times C(k - 1 - \vartheta b(\mathbf{V}_{21}', \tau_1, \hat{\mathbf{e}}_1, \hat{\boldsymbol{\sigma}}), \hat{\mathbf{e}}_1 \mid \mathbf{V}_1'(-\tau_1); t - \tau_1)
$$

$$
\times C(k - 1 - \vartheta b(\mathbf{V}_{12}', \tau_2, \hat{\mathbf{e}}_2, \hat{\boldsymbol{\sigma}}), \hat{\mathbf{e}}_2 \mid \mathbf{V}_2'(-\tau_2); t - \tau_2)
$$

$$
\times an \, |\hat{\boldsymbol{\sigma}} \cdot \mathbf{V}_{12}| \, \frac{1}{2} \delta(\hat{\mathbf{e}} \cdot \hat{\mathbf{V}}_{12}) \, d\mathbf{V}_2 \, d\hat{\mathbf{e}}_1 \, d\hat{\mathbf{e}}_2 \, d\tau_1 \, d\tau_2 \, d\hat{\boldsymbol{\sigma}}. \tag{40}
$$

This is the generalized Boltzmann equation for the cumulative distribution function C, up to $\mathcal{O}(\vartheta^2)$, which will be the starting point for our calculations of the maximal Lyapunov exponent.

5. FRONT PROPAGATION

The generalized Boltzmann equation (40) can be interpreted as describing a propagating front. The propagation here occurs on the real line of clock values k: As clock values tend to grow there is a movement

towards higher clock values. The two ''phases'' that are separated by the front are the stationary solutions $C(k, \hat{\mathbf{e}} \mid \mathbf{V}; t) \equiv 0$ on the left (no particles have a clock value smaller than the k-values in this region) and $C(k, \hat{\mathbf{e}} \mid \mathbf{V}; t) = P(\hat{\mathbf{e}} \mid \mathbf{V})$ on the right (all particles have a clock value smaller than the k-values in this region). $P(\hat{\mathbf{e}} \mid \mathbf{V})$ is the conditional probability for a particle to have unit vector $\hat{\mathbf{e}}$ given that its velocity is $\mathbf{V}$, i.e.,

$$P(\hat{\mathbf{e}} \mid \mathbf{V}_1) = \iint' \frac{f_1' f_2'}{v^*(\mathbf{V}_1)\, f_1}\, na\, |\hat{\boldsymbol{\sigma}} \cdot \mathbf{V}_{12}| \frac{1}{2}\, \delta(\hat{\mathbf{e}} \cdot \hat{\mathbf{V}}_{12})\, d\mathbf{V}_2\, d\hat{\boldsymbol{\sigma}}.$$

It is easy to see that $C \equiv 0$ is stable, whereas $C \equiv P(\hat{\mathbf{e}} \mid \mathbf{V})$ is unstable. In the simplest situation, the front has a fixed shape and moves to the right with a constant velocity:

$$C(k, \hat{\mathbf{e}} \mid \mathbf{V}, t) = F(x, \hat{\mathbf{e}} \mid \mathbf{V}) \tag{41}$$

where $x = k - w\bar{v}t$ with $\bar{v}$ the average collision frequency as mentioned already in the introduction. The constant w is called the *clock speed*. For the simpler clock model where each particle is fully characterized by a single clock variable which increases with time according to Eq. (2), it turned out[19] that the front falls in the class of so-called pulled fronts, as opposed to pushed fronts.[24] We will assume that in the present model this is also the case.

In short, the asymptotic front speed of pulled fronts is determined as follows. Insert a propagating front solution like Eq. (41) into the front equation (40), and linearize around the unstable phase. The resulting linear equation has solutions which are linear superpositions of exponential functions of the form e^{-sx} (multiplied by a polynomial in x in case of degeneracies). For fixed w, there are a number of possible values of s (typically infinite but countable). The dominant term in the superposition is the one where $s = s_d$ has the smallest real part. Since C has to be monotonic in x, the asymptotic large x behavior $\sim e^{-s_d x}$ has to be so too, hence s_d has to be real. This turns out to be possible only for w larger than some critical value w^*. So the asymptotic speed, if it exists, is greater than or equal to w^*. In fact, for a large class of initial conditions, the asymptotic clock speed is exactly w^*. Especially, this is true for localized initial conditions, implying that all initial k-values fall within a finite range (or in fact, are smaller than some value k_{max}; localization on the small-k side is not important). The same speed is also selected by initial distributions that fall off sufficiently rapidly (typically faster than any exponential of type $\exp[-cx]$) at the large-k side. For systems with finite numbers of particles, which we are typically

interested in, the initial distribution is always localized, leading to automatic selection of the minimal clock speed w^*. The additional effects of finite particle numbers only reduce the clock speed further, because correlations between particles tend to reduce their clock speed differences and thereby the boost a "slow" particle receives from colliding with a "fast" one.[21] A more detailed exposition of the velocity selection and other aspects of pulled and pushed fronts can be found in ref. 24.

Applying this scheme to the generalized Boltzmann equation (40), we first insert the Ansatz (41) and consider the resulting equation. We find

$$
v^*(\mathbf{V}_1) \, F(x, \hat{\mathbf{e}} \mid \mathbf{V}_1) = \int \cdots \int' S(\tau_1 \mid \mathbf{V}_1') \, S(\tau_2 \mid \mathbf{V}_2') \, f_1^{-1} f_1' f_2'
$$

$$
\times F(x - 1 - \vartheta b(\mathbf{V}_{12}', \tau_1, \hat{\mathbf{e}}_1, \hat{\boldsymbol{\sigma}}) + w\bar{v}\tau_1, \hat{\mathbf{e}}_1 \mid \mathbf{V}_1'(-\tau_1))
$$

$$
\times F(x - 1 - \vartheta b(\mathbf{V}_{12}', \tau_2, \hat{\mathbf{e}}_2, \hat{\boldsymbol{\sigma}}) + w\bar{v}\tau_2, \hat{\mathbf{e}}_2 \mid \mathbf{V}_2'(-\tau_2))
$$

$$
\times an \, |\hat{\boldsymbol{\sigma}} \cdot \mathbf{V}_{12}| \, \tfrac{1}{2} \, \delta(\hat{\mathbf{e}} \cdot \hat{\mathbf{V}}_{12}) \, d\mathbf{V}_2 \, d\hat{\mathbf{e}}_1 \, d\hat{\mathbf{e}}_2 \, d\tau_1 \, d\tau_2 \, d\hat{\boldsymbol{\sigma}}.
$$

We linearize this equation writing $F(x, \hat{\mathbf{e}} \mid \mathbf{V}) = P(\hat{\mathbf{e}} \mid \mathbf{V}_1) - \Delta(x, \hat{\mathbf{e}} \mid \mathbf{V})$. The resulting linear equation for Δ has superpositions of exponentials as solutions. It turns out convenient to represent these as

$$
\Delta(x, \hat{\mathbf{e}} \mid \mathbf{V}) = \sum_i a_i \frac{v^*(\mathbf{V}) + s_i \bar{v}}{v^*(\mathbf{V})} \, \hat{A}_i(\hat{\mathbf{e}}, \mathbf{V}) \, e^{-s_i x/w}. \tag{42}
$$

The characteristic values s_i and corresponding characteristic functions $\hat{A}_i$ are solutions of the linearized equation with Δ taking the form

$$
\Delta(x, \hat{\mathbf{e}} \mid \mathbf{V}) = \frac{v^*(\mathbf{V}) + s\bar{v}}{v^*(\mathbf{V})} \, \hat{A}(\hat{\mathbf{e}}, \mathbf{V}) \, e^{-sx/w},
$$

This gives the following characteristic equation

$$
\Lambda(v^*(\mathbf{V}_1) + s\bar{v}) \, \hat{A}(\hat{\mathbf{e}}, \mathbf{V}_1)
$$

$$
= \int \cdots \int' f_1^{-1} f_1' f_2' \, an \, |\hat{\boldsymbol{\sigma}} \cdot \mathbf{V}_{12}| \, \tfrac{1}{2} \, \delta(\hat{\mathbf{e}} \cdot \hat{\mathbf{V}}_{12})
$$

$$
\times \sum_{k=1,2} P_s(\tau \mid \mathbf{V}_k') \exp[-(\ln \Lambda) \, \vartheta b(\mathbf{V}_{21}', \tau, \hat{\mathbf{e}}^*, \hat{\boldsymbol{\sigma}})]
$$

$$
\times \hat{A}(\hat{\mathbf{e}}^*, \mathbf{V}_k'(-\tau)) \, d\mathbf{V}_2 \, d\hat{\mathbf{e}}^* \, d\tau \, d\hat{\boldsymbol{\sigma}},
$$

where we defined the eigenvalue $\Lambda = e^{-s/w}$ and

$$P_s(\tau \mid \mathbf{V}) \equiv (v^*(\mathbf{V}(-\tau)) + s\bar{v}) \exp\left[-\int_{-\tau}^{0} (v^*(\mathbf{V}(t)) + s\bar{v})\, dt\right]. \tag{43}$$

We make one more expansion in ϑ:

$$\Lambda(v^* + s\bar{v})\,\hat{A} = \hat{\mathbf{L}}^0\hat{A} - \vartheta \ln \Lambda \hat{\mathbf{L}}^1\hat{A}, \tag{44}$$

where we left out the argument of v^*. The operators $\hat{\mathbf{L}}^0$ and $\hat{\mathbf{L}}^1$ are defined by

$$[\hat{\mathbf{L}}^0\hat{A}](\hat{\mathbf{e}}, \mathbf{V}_1) = \int \cdots \int' f_1' f_2' f_1^{-1} na\, |\hat{\boldsymbol{\sigma}} \cdot \mathbf{V}_{12}| \tfrac{1}{2} \delta(\hat{\mathbf{e}} \cdot \hat{\mathbf{V}}_{12})$$

$$\times \sum_{k=1,2} P_s(\tau \mid \mathbf{V}_k')\,\hat{A}(\hat{\mathbf{e}}^*, \mathbf{V}_k'(-\tau))\, d\tau^*\, d\hat{\mathbf{e}}^*\, d\mathbf{V}_2\, d\tau\, d\hat{\boldsymbol{\sigma}}, \tag{45}$$

$$[\hat{\mathbf{L}}^1\hat{A}](\hat{\mathbf{e}}, \mathbf{V}_1) = \int \cdots \int' f_1' f_2' f_1^{-1} na\, |\hat{\boldsymbol{\sigma}} \cdot \mathbf{V}_{12}| \tfrac{1}{2} \delta(\hat{\mathbf{e}} \cdot \hat{\mathbf{V}}_{12})$$

$$\times \sum_{k=1,2} P_s(\tau \mid \mathbf{V}_k')\, b(\mathbf{V}_{21}', \tau, \hat{\mathbf{e}}^*, \hat{\boldsymbol{\sigma}})$$

$$\times \hat{A}(\hat{\mathbf{e}}^*, \mathbf{V}_k'(-\tau))\, d\tau^*\, d\mathbf{V}_2\, d\hat{\mathbf{e}}^*\, d\tau\, d\hat{\boldsymbol{\sigma}}. \tag{46}$$

Finally, Eq. (44) can be transformed into an equation in which only the integrated function over $\hat{\mathbf{e}}$ enters, i.e., $A(\mathbf{V}) \equiv [\bar{\mathbf{P}}\hat{A}](\mathbf{V}) \equiv (2\pi)^{-1} \int d\hat{\mathbf{e}}\, \hat{A}(\hat{\mathbf{e}}, \mathbf{V})$. Defining

$$[\bar{\mathbf{L}}^0 A](\hat{\mathbf{e}}, \mathbf{V}_1) \equiv \int \cdots \int' f_1' f_2' f_1^{-1} na\, |\hat{\boldsymbol{\sigma}} \cdot \mathbf{V}_{12}|\, \pi\delta(\hat{\mathbf{e}} \cdot \hat{\mathbf{V}}_{12})$$

$$\times \sum_{k=1,2} P_s(\tau \mid \mathbf{V}_k')\, A(\mathbf{V}_k'(-\tau))\, d\mathbf{V}_2\, d\tau\, d\hat{\boldsymbol{\sigma}},$$

we see from Eq. (45) that we can write

$$\hat{\mathbf{L}}^0 = \bar{\mathbf{L}}^0 \bar{\mathbf{P}}. \tag{47}$$

We see from Eqs. (44) and (47) that $\hat{A} = \Lambda^{-1}(v^* + s\bar{v})^{-1}\, \bar{\mathbf{L}}^0 A$ up to first order in ϑ, so Eq. (44) can be written as

$$\Lambda(v^* + s\bar{v})\,\hat{A} = \bar{\mathbf{L}}^0 A - \vartheta\, \frac{\ln \Lambda}{\Lambda}\, \hat{\mathbf{L}}(v^* + s\bar{v})^{-1}\, \bar{\mathbf{L}}^0 A + O(\vartheta^2).$$

Applying $\bar{\mathbf{P}}$ yields a closed equation for A:

$$\Lambda(v^* + s\bar{v})\, A = \mathbf{L}^0 A - \vartheta \Lambda^{-1} \ln \Lambda \mathbf{L}^1 A, \tag{48}$$

where

$$\mathbf{L}^0 = \bar{\mathbf{P}} \bar{\mathbf{L}}^0,$$

and

$$\mathbf{L}^1 = \bar{\mathbf{P}} \hat{\mathbf{L}}^1 (v^* + s\bar{v})^{-1}\, \bar{\mathbf{L}}^0. \tag{49}$$

These are just the first few operators that appear in an expansion in ϑ, each still containing all orders of the shear rate $\tilde{\gamma}$. We use Eq. (48) to find Λ as a function of s through linear order in ϑ. As Λ will be equated to $e^{-s/w}$, we are interested in the largest eigenvalue $\Lambda(s)$ for which Eq. (48) can be satisfied, because this corresponds to the most slowly decaying mode in Eq. (42). There are real solutions to $\Lambda(s) = e^{-s/w}$ for s if $w > w^*$, for $w < w^*$ only complex solutions exist, leading to undesirable oscillations. To find w^* we look at the function

$$\tilde{w}(s) = -\frac{s}{\ln \Lambda(s)} \tag{50}$$

There are no real solutions of $\tilde{w}(s) = w$ if w is smaller than the minimum of the function $\tilde{w}$, hence this minimum is w^*.

6. PERTURBATION IN THE DENSITY

This section will be devoted to finding the solution of Eq. (48) in a perturbation expansion in ϑ, that is we will find $\Lambda(s)$ and with that determine the minimum of $-s/\ln \Lambda(s)$, which is the clock speed w.

We consider Eq. (48) for the largest eigenvalue $\Lambda(s)$. Let us assume that Eq. (48) is solved to zeroth order by A^0 and $\Lambda^0(s)$, i.e.,

$$\Lambda^0(s)(v^* + s\bar{v})\, A^0 = \mathbf{L}^0 A^0. \tag{51}$$

A^0 depends on s, although we will not denote this explicitly. We remark that this zeroth order equation was solved in ref. 21 for the equilibrium case. In the general case, $\mathbf{L}^0$ is not self-adjoint, so we need the left eigenfunction too. We denote this function by $\bar{A}^0$. An inner product is defined as

$$(A, B) = \int A(\mathbf{V})\, B(\mathbf{V})\, \varphi(\mathbf{V})\, d\mathbf{V}, \tag{52}$$

where the Maxwell distribution φ was given in Eq. (19). The function $\bar{A}^0$ may be chosen such that under this inner product $(\bar{A}^0, A^0) = 1$. Inserting the expansions $A = A^0 + \vartheta A^1 + O(\vartheta^2)$ and $\Lambda(s) = \Lambda^0(s) + \vartheta \Lambda^1(s) + O(\vartheta^2)$ into Eq. (48) and considering the $O(\vartheta)$ terms, we get

$$\Lambda^0(s)(v^* + s\bar{v}) A^1 + \Lambda^1(s)(v^* + s\bar{v}) A^0 = \mathbf{L}^0(s) A^1 - \frac{\ln \Lambda^0(s)}{\Lambda^0(s)} \mathbf{L}^1 A^0.$$

The inner product of this equation with $\bar{A}^0$ yields

$$\Lambda^1(s) = -\frac{\ln \Lambda^0(s)}{\Lambda^0(s)} \frac{(\bar{A}^0, \mathbf{L}^1 A^0)}{(\bar{A}^0, (v^* + s\bar{v}) A^0)}, \tag{53}$$

where we used Eq. (51). The critical value w is found from $(d\tilde{w}/ds)(s^*) = 0$ and $w = \tilde{w}(s^*)$ (where s^* is the location of the minimum). Using Eq. (53) for $\Lambda^1(s)$ and Eq. (50) we find $\tilde{w}(s) = \tilde{w}^0(s) + \vartheta \tilde{w}^1(s) + \mathcal{O}(\vartheta^2)$, where

$$\begin{aligned} \tilde{w}^0(s) &= -\frac{s}{\ln \Lambda^0(s)}, \\ \tilde{w}^1(s) &= \frac{\tilde{w}^0(s)}{\Lambda^0(s)^2} \frac{(\bar{A}^0, \mathbf{L}^1 A^0)}{(\bar{A}^0, (v^* + s\bar{v}) A^0)}. \end{aligned} \tag{54}$$

Note that $\bar{A}^0$, A^0 and $\mathbf{L}^1$ depend on s as well. Again we assume the minimum of $\tilde{w}^0$ to be known, and to be located at s^0, with a value of $w^0 = \tilde{w}^0(s^0)$. The first order value of the minimum, which to first order is located at $s^* = s^0 + \vartheta s^1$, is (up to that order)

$$\tilde{w}^0(s^0) + \frac{d\tilde{w}^0}{ds^0} \vartheta s^1 + \vartheta \tilde{w}^1(s^0) = \tilde{w}^0(s^0) + \vartheta \tilde{w}^1(s^0),$$

where we used that the derivative of $\tilde{w}^0$ at s^0 is zero. From Eq. (54) and the identity $\Lambda^0 = \exp(-s^0/w^0)$, the value of the critical clock speed up to order ϑ follows as

$$w = w^0 \left[1 + \vartheta e^{2s^0/w^0} \frac{(\bar{A}^0, \mathbf{L}^1 A^0)}{(\bar{A}^0, (v^* + s^0\bar{v}) A^0)} + O(\vartheta^2) \right].$$

This is the value of the clock speed that enters into the Lyapunov exponent, according to Eq. (3), so

$$\lambda^+ = w^0 \bar{v} \left[\ln \frac{1}{\tilde{n}} + e^{2s^0/w^0} \frac{(\bar{A}^0, \mathbf{L}^1 A^0)}{(\bar{A}^0, (v^* + s^0\bar{v}) A^0)} \right]. \tag{55}$$

Correction terms to this expression are $O(\bar{v}\vartheta)$.

7. EQUILIBRIUM CASE

We will now explicitly evaluate Eq. (55) for the equilibrium case. In that case, i.e., $\gamma = 0$, Eqs. (45) and (46) simplify strongly. One simplification is that the velocity distribution is known to be the Maxwellian, i.e., $f(\mathbf{V}) = \varphi(\mathbf{V})$, so in the integrand, $f_1^{-1} f_1' f_2' = \varphi_2$. Furthermore $\dot{\mathbf{V}} = 0$, which, according to Eq. (22), makes $v^*(\mathbf{V})$ and $v(\mathbf{V})$ equal to the equilibrium collision frequency $v_0(\mathbf{V})$ of a particle with velocity $\mathbf{V}$. The expression in Eq. (43) now gives

$$P_s(\tau \mid \mathbf{V}) = (v_0(\mathbf{V}) + s\bar{v}) \exp\{-[v_0(\mathbf{V}) + s\bar{v}_0]\,\tau\}.$$

The expression for the function b in Eq. (31) simplifies because $\mathbf{S}_t = \mathbb{1}$:

$$b(\mathbf{V}, \tau, \hat{\mathbf{e}}, \hat{\boldsymbol{\sigma}}) = \ln\left(\frac{\tau\tilde{n}\,|\mathbf{RV}\cdot\hat{\mathbf{e}}|}{a\,|\hat{\mathbf{V}}\cdot\hat{\boldsymbol{\sigma}}|}\right).$$

We see that now the integration over τ in Eqs. (45) and (46) can be performed. The result is that Eq. (48) becomes

$$\Lambda_0(v_0 + s\bar{v}_0)\,A_0 = \mathbf{L}_0^0 A_0 - \vartheta\,\frac{\ln \Lambda_0}{\Lambda_0}\,\mathbf{L}_0^1 A_0 \tag{56}$$

where

$$[\mathbf{L}_0^0 A](\mathbf{V}_1) = \int\cdots\int{}' na\,|\hat{\boldsymbol{\sigma}}\cdot\mathbf{V}_{12}|\,[A_1' + A_2']\,\varphi_2\,d\mathbf{V}_2\,d\hat{\boldsymbol{\sigma}},$$

Here $A_k' = A(\mathbf{V}_k')$, and, analogously to Eq. (49),

$$\mathbf{L}_0^1 = \bar{\mathbf{P}}\hat{\mathbf{L}}_0^1 (v_0 + s\bar{v}_0)^{-1}\,\bar{\mathbf{L}}_0^0,$$

where

$$[\bar{\mathbf{L}}_0^0 A](\hat{\mathbf{e}}, \mathbf{V}_1) = \int\cdots\int{}' na\,|\hat{\boldsymbol{\sigma}}\cdot\mathbf{V}_{12}|\sum_{k=1,2}\pi A_k'\,\delta(\hat{\mathbf{e}}\cdot\hat{\mathbf{V}}_{12})\,\varphi_2\,d\mathbf{V}_2\,d\hat{\boldsymbol{\sigma}}$$

$$[\hat{\mathbf{L}}_0^1 \hat{A}](\hat{\mathbf{e}}, \mathbf{V}_1) = \int\cdots\int{}' \frac{1}{2}na\,|\hat{\boldsymbol{\sigma}}\cdot\mathbf{V}_{12}|\sum_{k=1,2}\hat{A}(\hat{\mathbf{e}}^*, \mathbf{V}_k')$$
$$\times \ln\left[\frac{nae^{-C}|\mathbf{V}_{12}|}{v_0(\mathbf{V}_k') + s\bar{v}_0}\frac{|\mathbf{R}\hat{\mathbf{V}}_{12}\cdot\hat{\mathbf{e}}^*|}{|\hat{\mathbf{V}}_{12}\cdot\hat{\boldsymbol{\sigma}}|}\right]\delta(\hat{\mathbf{e}}\cdot\hat{\mathbf{V}}_{12})\,\varphi_2\,d\mathbf{V}_2\,d\hat{\boldsymbol{\sigma}}\,d\hat{\mathbf{e}}^*$$

Here C is Euler's number, $0.577\dots$. In general, subscripts 0 denote the equilibrium values of quantities introduced before.

To zeroth order in ϑ, Eq. (56) reads

$$\Lambda_0^0(v_0 + s\bar{v}_0)\, A_0^0 = \mathbf{L}_0^0 A_0^0.$$

This is the very same eigenvalue problem that was found in a more heuristic derivation of a Boltzmann equation for clock values in ref. 21, with exactly the same operators, except that s was represented as γw and $\mathbf{L}_0^0$ and $v_0 + s\bar{v}_0$ were denoted as $\mathbf{L}$ and $\bar{v}_0 \mathbf{W}_s$, respectively. The largest eigenvalue $\Lambda_0^0(s)$ was determined numerically in that paper, for a range of s, such that the minimum of $\tilde{w}$ could be determined. Briefly, the method used was the following. A basis of functions was constructed that are orthogonal with respect to the inner product defined in Eq. (52), starting with 1, $\mathbf{V}/v_0$, $\frac{1}{2}|\mathbf{V}/v_0|^2 - 1$ and $\frac{1}{8}|\mathbf{V}/v_0|^4 - |\mathbf{V}/v_0|^2 + 1$. Finite matrices were constructed containing the matrix elements of the operators with respect to the four mentioned basis-functions. These finite matrices were used in Eq. (56) instead of the real operators, to get a numerically feasible eigenvalue problem. In ref. 21 it was checked that omitting the basis function containing $|\mathbf{V}|^4$, only changes the result by a few tenth of percents, so that is the accuracy of the numerical results. In this paper we choose to work with just 1, $\mathbf{V}/v_0$, and $\frac{1}{2}|\mathbf{V}/v_0|^2 - 1$, as this simplifies the calculations. On that truncated basis the value and position of the minimum are found to be

$$w_0^0 \approx 4.732, \tag{57}$$

$$s_0^0 \approx 3.506. \tag{58}$$

and the eigenfunction A_0^0 is

$$A_0^0(\mathbf{V}) \approx 0.612 + 0.194 v_0^{-2}\, |\mathbf{V}|^2. \tag{59}$$

The value of w_0^0 gives the leading behavior of the largest Lyapunov exponent: $\lambda_0^+ = -w_0^0 \bar{v}_0 \ln \tilde{n} + O(1)$.

Using these results we can obtain the first correction term. For that, we adapt Eq. (55) to this case:

$$\lambda^+ = w_0^0 \bar{v}_0 \left[\ln \frac{1}{\tilde{n}} + \exp\left(\frac{2s_0^0}{w_0^0}\right) \frac{(A_0^0, \mathbf{L}_0^1 A_0^0)}{(A_0^0, (v_0 + s_0^0 \bar{v}_0)\, A_0^0)} \right].$$

Note that $\mathbf{L}_0^0$ is self adjoint and therefore the left and right eigenvectors are the same. We have calculated the matrix elements $(A_0^0, \mathbf{L}_0^1 A_0^0)$ and

$(A_0^0, (v_0 + s_0^0 \bar{v}_0) A_0^0)$ numerically respectively analytically, using the numbers of Eqs. (58), (59) and (57). The numerical integration uses a sampling from the Maxwellian and subsequent averaging of the rest of the integrand appearing in the matrix elements (including the collision frequency, for which we used a numerical approximation). The results are $(A_0^0, \mathbf{L}_0^1 A_0^0) = -10.85 \, nav_0$ and $(A_0^0, (v_0 + s_0^0 \bar{v}_0) A_0^0) = 19.28 \, nav_0$ Thus we obtain the result that

$$\lambda_0^+ = 4.732 \bar{v}_0 [-\ln \tilde{n} - 2.48 + O(1/\ln \tilde{n})]. \tag{60}$$

8. PERTURBATION IN THE SHEAR RATE

The result in the previous section can be the starting point of a perturbation theory in the shear rate in the case that $\tilde{\gamma}$ is non-zero, but small. From symmetry ($\gamma \to -\gamma$), it follows that the Lyapunov exponent λ^+ is even in γ, so to see the effect of the shear we need a second order perturbation theory at least. We will sketch the solution formally in this section, and leave the explicit calculations for the future.

We start with the eigenvalue equation in Eq. (48) to zeroth order, i.e.,

$$\mathbf{L}^0 A^0 = \Lambda^0 (v^* + s\bar{v}) A^0,$$

and write $\mathbf{L}^0 = \mathbf{L}_0^0 + \tilde{\gamma} \mathbf{L}_1^0 + \tilde{\gamma}^2 \mathbf{L}_2^0 + \mathcal{O}(\tilde{\gamma}^3)$, $v^* = v_0 + \tilde{\gamma} v_1^* + \tilde{\gamma}^2 v_2^* + \mathcal{O}(\tilde{\gamma}^3)$, $A^0 = A_0^0 + \tilde{\gamma} A_1^0 + \tilde{\gamma}^2 A_2^0 + \mathcal{O}(\tilde{\gamma}^3)$ and

$$\Lambda^0(s) = \Lambda_0^0 + \tilde{\gamma}^2 \Lambda_2^0(s) + \mathcal{O}(\tilde{\gamma}^4) \tag{61}$$

where we used that Λ^0 is an even function of $\tilde{\gamma}$. For the same reason we may expand $\bar{v}$ as $\bar{v} = \bar{v}_0 + \tilde{\gamma}^2 \bar{v}_2$ Substituting these expressions into the eigenvalue problem and equating equal powers of $\tilde{\gamma}$ one finds

$$A_1^0 = \mathscr{R}[\Lambda_0^0 v_1^* - \mathbf{L}_1^0] A_0^0,$$

$$A_2^0 = \frac{(A_0^0, [\mathbf{L}_2^0 - \Lambda_0^0(v_2^* + s\bar{v}_2)] A_0^0 + (\mathbf{L}_1^0 - \Lambda_0^0 v_1^*) A_1^0)}{(A_0^0, (v_0 + s\bar{v}_0) A_0^0)},$$

$$A_2^0 = \mathscr{R}(\Lambda_0^0 v_1^* - \mathbf{L}_1^0) A_1^0 + \mathscr{R}[\Lambda_0^0(v_2^* + \bar{v}_2 s) + \Lambda_2^0(v_0 + s\bar{v}_0) - \mathbf{L}_2^0] A_0^0,$$

where $\mathscr{R}$ is the inverse of $\mathbf{L}_0^0 - \Lambda_0^0(v_0 + s\bar{v}_0)$, restricted to the subspace orthogonal to A_0^0 (so A_1^0 and A_2^0 are made unique by requiring orthogonality to A_0^0).

From Eqs. (50) and (61), we obtain $w^0(s) = w_0^0(s) + \tilde{\gamma}^2 w_2^0(s) + \mathcal{O}(\tilde{\gamma}^4)$, where

$$w_0^0(s) = -s/\ln \Lambda_0^0(s)$$
$$w_2^0(s) = s\, \Lambda_2^0/[\Lambda_0^0(s)\ln^2\Lambda_0^0(s)].$$

The location of the minimum of the function $w^0(s)$ is shifted by an amount of order $\tilde{\gamma}^2$, in fact

$$s^0 = s_0^0 - \tilde{\gamma}^2 \frac{\dfrac{dw_2^0}{ds}(s_0^0)}{\dfrac{d^2 w_0^0}{ds^2}(s_0^0)} + \mathcal{O}(\tilde{\gamma}^4) \tag{62}$$

as can be found from $(d/ds)\, w^0(s^0) = 0$ and $(d/ds)\, w_0^0(s_0^0) = 0$. Because we are expanding around a minimum, this shift is not needed for the value of the minimum of the function $w^0(s)$, i.e.,

$$w^0(s^0) = w_0^0(s_0^0) + \tilde{\gamma}^2 w_2^0(s_0^0) + \mathcal{O}(\tilde{\gamma}^4).$$

Thus we can determine the shear corrections to the leading density term in Eq. (55).

To calculate the density correction in Eq. (55) we do need the shift of the minimum as it enters in the matrix elements. This means that one has to insert Eq. (62) and expand all relevant matrix elements in powers of $\tilde{\gamma}$. All of these can be obtained with the help of Eqs. (18), (20)–(22), (23), (25), (26), (31), (46) and (49). In the end the evaluation will have to be done numerically.

9. DISCUSSION

In this paper we developed an analytic method for calculating the largest Lyapunov exponent of a many body system, based on the microscopic equations of motion. To be specific we restricted ourselves to uniform hard disk systems in two dimensions at low densities, but not necessarily in equilibrium. As a particular case we considered the uniformly sheared hard disk gas.

To obtain the largest Lyapunov exponent we derived a generalized Boltzmann equation that describes the time evolution of a distribution function of particle positions and velocities, together with deviation vectors in tangent space. At low densities the position deviations turn out to be

unimportant, to leading orders in the density. The velocity deviation of a particle may be represented conveniently in terms of the logarithms of its norm—the so-called clock value k (Eq. (1))—and an additional unit vector, which in the end plays no essential role.

As in the preceding papers[19–21] the generalized Boltzmann equation may be reinterpreted as describing the propagation of a pulled front on the real line of possible clock values. Therefore, by standard techniques the linearized version of this equation may be used to obtain the asymptotic speed of propagation of the front, which is directly proportional to the largest Lyapunov exponent.

A remarkable property of the generalized Boltzmann equation is that its natural density expansion does not proceed in powers of the dimensionless density $\tilde{n}$, but rather in powers of $\vartheta = 1/|\ln \tilde{n}|$. To lowest order, this reproduces the results of earlier work,[19, 21] which therefore finds a firmer basis here. Here we also give values for the next order in ϑ contribution to the largest Lyapunov exponent, and we give explicit expressions for the first non-vanishing shear rate dependent contribution to this exponent (quadratic in the shear rate) in the uniformly sheared system.

In ref. 21 we made comparisons between our results and the results of numerical simulations of hard disk Lyapunov exponents by Dellago and Posch.[26] Within the numerical accuracy good agreement was found, but it turned out there are two complicating factors. The first one is that the density should be very low to be in the regime where a power series in $1/\ln(\tilde{n})$ can be expected to converge rapidly. The second one is that there are large finite size effects for the front speed w. One cannot (yet) reach the required number of particles in simulations for these effects to become negligible. The finite size effects can be estimated for asymptotically large N using front propagation techniques, and they would scale as $1/\ln^2(N)$. It is not known at which number of particles this asymptotic result suffices, though.

To conclude we mention some possible extensions of this work and some interesting problems that are still open for research. First of all the expressions for the shear rate dependent contribution should be worked out numerically. We plan to do this on short notice. Then one would like to go more general potentials, to general densities and to three-dimensional systems as well as two-dimensional ones. We expect that, as long as one stays at low densities, the generalization to other simple (short ranged and spherically symmetic) potentials should not pose any serious problems; one just has to use the generalized Boltzmann equation that is appropriate for the potential under consideration. Similarly we expect the generalization to three dimensions just will cause some additional technical complications, related to the fact that the directions of the velocity deviations after a

collision will depend on those before, unlike in two dimensions. Generalizations to higher density will be much harder to accomplish. Already the fact that the natural expansion in density proceeds in powers of ϑ rather than $\tilde{n}$ indicates that a systematic expansion up to appreciable density will be forbiddingly hard. On the other hand non-systematic approaches, such as a generalized Enskog equation for hard disks or spheres, may give good approximations, but this has not been explored yet.

One can also try to extend the methods developed here so as to calculate additional Lyapunov exponents. For non-equilibrium systems the most negative Lyapunov exponent is of primary interest, because the sum of this and the largest Lyapunov exponent is directly related to the shear viscosity through the conjugate pairing rule.[23] For the SLLOD equations with a Gaussian or "constant-α" thermostat, there are deviations of this rule,[31–33] but these are of higher order in the shear rate, so that the connection with the *linear* viscosity still stands.

Finally, at low densities, the methods developed here may probably be combined with those of refs. 12 and 22 in order to calculate the sum of all positive Lyapunov exponents, or the KS-entropy, for non-equilibrium cases. However, a theoretical calculation of the full spectrum of Lyapunov exponents, which probably requires similar techniques, remains a very challenging open problem.

ACKNOWLEDGMENTS

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