Lyapunov hydrodynamics in the dilute limit

Michel Mareschal and Sean McNamara

Centre Européen de Calcul Atomique et Molécluaire
46, allée d'Italie
69364 Lyon Cedex 07

Abstract

We study the hydrodynamic Lyapunov exponents of the hard disk fluid in the dilute limit. These exponents appear in discrete groups and their values depend on the system size. In a previous paper [1], we presented a theory for these exponents, explaining them as the growth rate of collective, organized perturbations in phase space. That theory successfully described the basic features of the hydrodynamic exponents, but it had some difficulties. Many of these difficulties can be removed by considering the dilute limit.

Key words: Lyapunov spectrum, kinetic theory, hydrodynamic modes
PACS: 05.45.Jn, 51.10.+y, 05.20.Dd

1 Introduction

There have been many recent studies dealing with the relation between Lyapounov exponents and transport properties. Some general relations have been obtained (Gaspard, Nicolis, Dorfman [2,3]), as well as computations in some model systems linking the largest Lyapounov exponent to a transport coefficient (van Beijeren, et al. [4]). These studies investigated in a quantitative way the intuitive idea which connects the divergence of perturbed trajectories to the collision process, the latter being in turn related to transport coefficients as it is known from kinetic theories (Resibois and DeLeener [5]). The computed values of transport coefficients is known to depend on the particle interaction potential and not on the system size or geometry.

It therefore came as a surprise when Posch et al [6] found a somewhat different behavior. For hard-sphere and hard-disk systems, while increasing the system's size, a few Lyapounov exponents appear, disconnected from the main part of the spectrum, and corresponding to perturbation directions in phase space which involve coherent deviations in positions or velocities of essentially all particles of the system (Posch [6], McNamara and Mareschal [1], hereafter MM1). Those new exponents are smaller when compared to the others, with the corresponding times being proportional to the system size. Recent results both on hard-core potential systems and on systems interacting with smooth potentials (Forster and Posch [7]) confirm the existence of those large-scale collective perturbation directions associated with these exponents.

Theoretical explanations have already been attempted for those exponents. First, Eckman and Gat [8] have considered random matrices, sharing certain features with the linearized dynamics of hard spheres, and they have shown that they display a similar Lyapounov spectrum. In a previous article, McNamara and Mareschal (MM1) have presented a theory, based on a generalized Enskog equation, linking the collective exponents to collisional invariant perturbation directions: because of the link between collisional invariants and the hydrodynamic modes of fluids, we have proposed to name those exponents and the perturbation directions "hydrodynamic Lyapounov modes" because their origin is analogous to that of the usual hydrodynamic modes. This terminology is not meant to suggest that there is a relation between these exponents and the transport coefficients of hydrodynamic theory. In fact, the following theoretical development suggests that there is no such relation. We characterize the hydrodynamic Lyapunov modes further and refer specifically to shear modes and sound modes, relating to the kind of collective perturbation directions displayed. (In a different but related approach, de Wijn and van Beijeren name these modes "Goldstone modes" [9]).

In this paper, we present a more detailed theory than the one developed in MM1, but, given the complexity of the computation, we limit ourselves to the dilute limit: this limitation permits us to avoid the uncontrolled approximations that were done in MM1. We introduce a Boltzmann equation that describes the time evolution of the perturbed trajectories as a kind of internal degree of freedom of the particles. We then introduce spatial fields related to the perturbation directions which do not grow at collision and derive equations describing the space and time variation of those fields. The analysis of those equations is then performed, restricted to equilibrium systems, in a limit where one can use scale separation, both in time and space, in a way similar to the derivation of hydrodynamic equations for the fields of conserved variables. This allows us to predict the largest time scales and to compare them with those computed in molecular dynamics simulations done with hard disks. In the conclusion, we end the paper by discussing the strengths and weaknesses of this approach. In particular, we insist on the fact that the same physics takes place at finite and large density and that the consideration of dilute fluids is not a physical limitation.

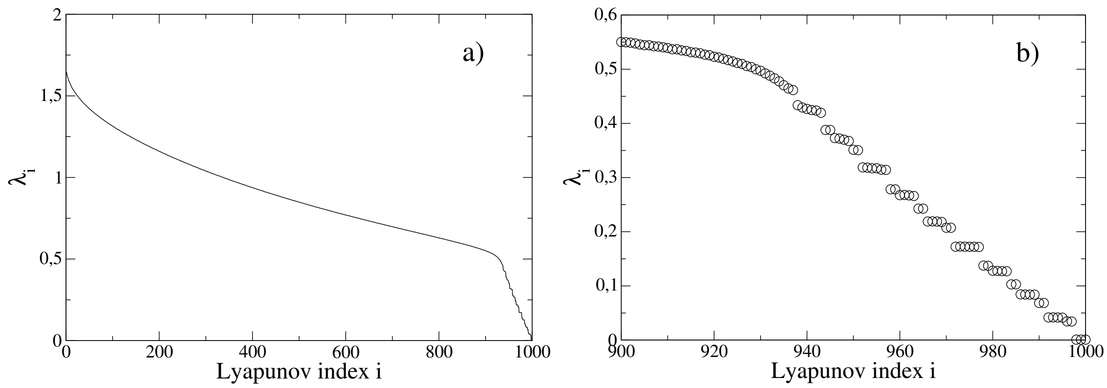

Fig. 1. The Lyapunov spectrum of a hard disk system with $N = 500$ disks in a periodic domain with aspect ratio 25. The disks cover 0.5 of the available space. a) All 1000 positive exponents. b) the spectrum for $900 \leq i \leq 1000$, showing the hydrodynamic exponents.

2 Description of the hydrodynamic Lyapunov modes

In this paper, we study the Lyapunov spectrum of the hard disk fluid with periodic boundary conditions. N disks are confined in a $L_x \times L_y$ periodic domain. We take $L_y > L_x$ because this simplifies the analysis of the hydrodynamic modes. Our algorithm for calculating the Lyapunov spectrum was given by Dellago, Posch, Hoover [10]. All figures show results in simulation units, where the unit of distance is a particle radius, the unit of mass is the particle mass and the unit of time is determined by setting the average kinetic energy per particle equal to 1/2.

The hydrodynamic Lyapunov modes have already been described in MM1 [1] and by Posch et al. [6]. Here we present a very brief review, and add some new findings.

In Fig. 1a, we present the Lyapunov spectrum of a relatively dense (area fraction $\nu = 0.5$) hard sphere fluid at equilibrium in a periodic domain with an aspect ratio of 25. At this resolution, the spectrum can be divided into two parts. There is a smooth curve for $1 \leq i \lesssim 920$, where i is the index of the exponent. Near $i \approx 920$, there is a sharp break as the slope descends with constant slope to zero. In Fig. 1b we show a magnification of this linear region. As one can see, it is made up of numerous, roughly equally spaced groups of exponents. These are the hydrodynamic exponents.

Our analysis of the hydrodynamic Lyapunov exponents is based on the idea that particles possess "Lyapunov coordinates". To explain this idea, we present a loose definition of the Lyapunov spectrum. Let $\mathbf{\Gamma}(t) = (\mathbf{r}_1, \mathbf{r}_2, \ldots \mathbf{r}_N, \mathbf{v}_1 \ldots \mathbf{v}_N)$ be a trajectory in phase space. Note that $\mathbf{\Gamma}$ contains as components the positions and velocities of all the particles. Now, let $\mathbf{\Gamma}'(t)$ be a second trajectory in phases space that is infinitesimally close to $\mathbf{\Gamma}(t)$. The separation between these two trajectories is

$$\delta\mathbf{\Gamma} = \mathbf{\Gamma}' - \mathbf{\Gamma} = (\delta\mathbf{r}_1, \delta\mathbf{r}_2, \ldots \delta\mathbf{r}_N, \delta\mathbf{v}_1 \ldots \delta\mathbf{v}_N). \tag{1}$$

At time $t = 0$, $\mathbf{\Gamma}$ and $\mathbf{\Gamma}'$ are infinitesimally close together. As the systems advance through time, their separation $\delta\mathbf{\Gamma}$ will change. The Lyapunov exponent λ is the average growth rate of $\delta\mathbf{\Gamma}$:

$$\lambda = \lim_{t\to\infty} \frac{1}{t} \ln \frac{|\delta\mathbf{\Gamma}(t)|}{|\delta\mathbf{\Gamma}(0)|}. \tag{2}$$

It is important to realize that each Lyapunov exponent λ_i is associated with a vector $\delta\mathbf{\Gamma}_i$ that gives the perturbation whose growth rate is λ_i. The vector $\delta\mathbf{\Gamma}_i$ allows us to characterize the exponents and to know what physical processes underlie the different exponents. The components of $\delta\mathbf{\Gamma}$ are the Lyapunov coordinates mentioned above; $(\delta\mathbf{r}_i, \delta\mathbf{v}_i)$ are the Lyapunov coordinates of particle i. They give the difference between the coordinates that particle i possesses on trajectory $\mathbf{\Gamma}(t)$ and those it posses on trajectory $\mathbf{\Gamma}'(t)$. If particle i is at $\mathbf{r}_i$ on $\mathbf{\Gamma}(t)$, it is at $\mathbf{r}_i + \delta\mathbf{r}_i$ on $\mathbf{\Gamma}'(t)$. In the theory we develop below, we consider the Lyapunov coordinates to be internal degrees of freedom of the particles.

In Fig. 2, we show the Lyapunov coordinates for several different exponents. For nonhydrodynamic exponents (represented by λ_{10} in Fig. 2), the Lyapunov coordinates are disorganized and uncorrelated to the physical velocities. On the other hand, for the hydrodynamic Lyapunov exponents, they are organized into sinusoidal patterns or strongly coupled to the velocities. When the Lyapunov coordinates are organized into global sinusoidal patterns such as those shown in Fig. 2, $i > 10$, the perturbation $\delta\mathbf{\Gamma}$ is called a "hydrodynamic Lyapunov mode". The hydrodynamic modes come in two different types: shear modes and sound modes. In "shear modes" ($i = 231$ and $i = 237$ in Fig. 2), $\delta\mathbf{r}$ and $\delta\mathbf{v}$ are directed perpendicular to the wave vector, like the particle velocities in a usual hydrodynamic shear wave. In the "sound modes" ($i = 234$ and $i = 235$ in Fig. 2), $\delta\mathbf{r}$ and $\delta\mathbf{v}$ are directed parallel to the wave vector. This is harder to see, because in sound modes, the Lyapunov coordinates are also correlated with the velocities.

In Ref. [1], we postulated that the hydrodynamic exponents obey

$$\lambda = \frac{nc_\lambda}{L_y} + \frac{n^2 d_\lambda}{L_y^2} + \frac{n^3 e_\lambda}{L_y^3} + O(L_y^{-4}), \tag{3}$$

where n is the mode number, i.e. the number of wavelengths that fits into the length of the system L_y. The wavelength of the perturbation is thus L_y/n. In

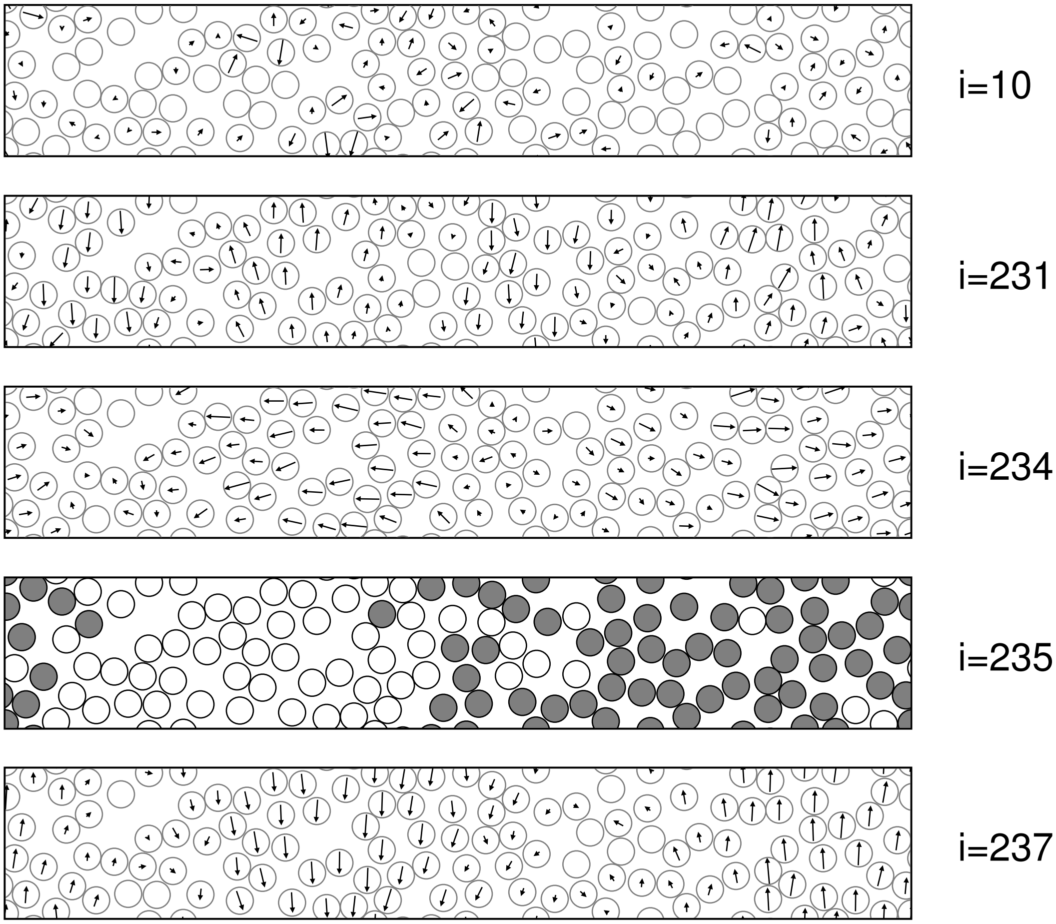

Fig. 2. The Lyapunov coordinates for various exponents. The exponents are taken from an $N = 120$, $\nu = 0.5$ system with periodic boundary conditions and an aspect ratio of 6. The nonhydrodynamic modes are represented by $i = 10$, the shear modes by $i = 231$ (second harmonic, mode number $n = 2$) and $i = 237$. Arrows show the direction and length of $\delta\mathbf{r}$. For $i = 235$, particles with $\mathbf{v} \cdot \delta\mathbf{r} > 0$ are shaded gray; this is a way to show correlations between $\mathbf{v}$ and $\delta\mathbf{r}$.

Fig. 3a, we plot $\lambda L_y/n$ against n/L_y for all the shear modes of the spectrum shown in Fig. 1. Fitting a parabola through the points enables one to extract estimates for c_λ, d_λ, and e_λ. In the remaining panels of Fig. 3, we plot c_λ, d_λ and e_λ as a function of density. On the graph of c_λ we also give the theoretical predictions for the zero density limit given in the next section. There seems to be a transition at the density $\nu \approx 0.25$. For $\nu < 0.25$, $c^{(\text{shear})} > c^{(\text{sound})}$ and both d_λ and e_λ change rapidly with density. For $\nu > 0.25$, $c^{(\text{shear})} < c^{(\text{sound})}$ and d_λ and e_λ change slowly. At $\nu = 0.25$, no points are shown because it is not possible to seperate the sound and shear modes at this density.

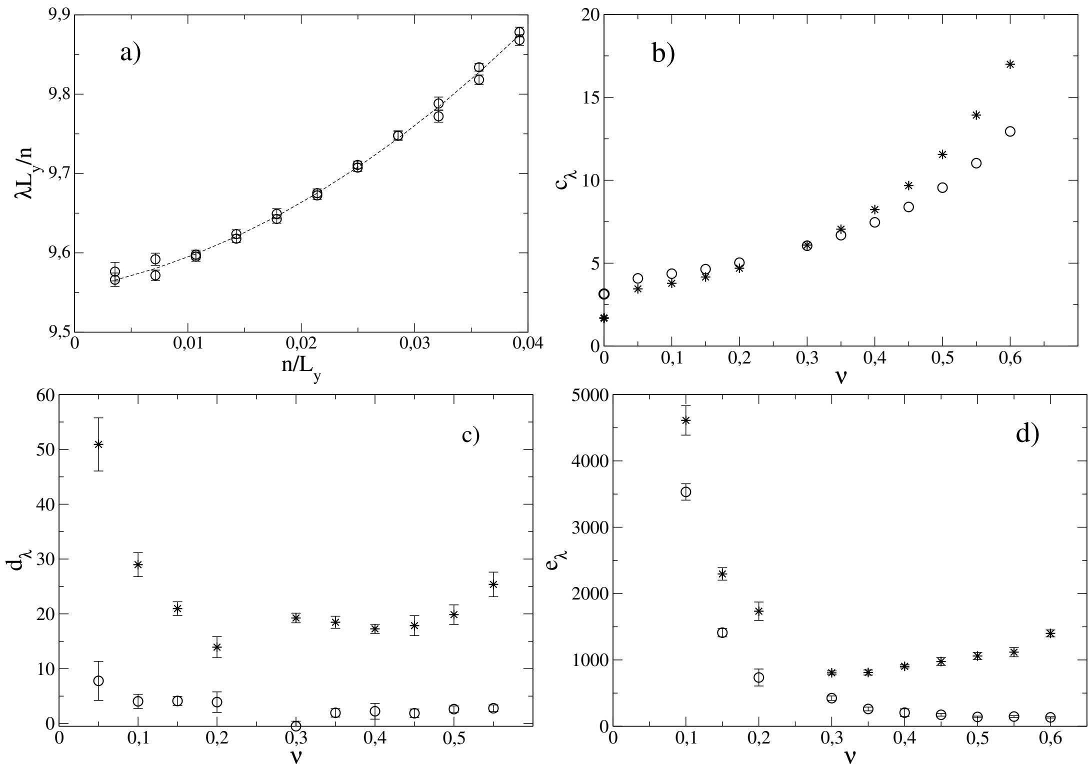

Fig. 3. Figures showing estimates of c_λ, d_λ, and e_λ [defined in Eq. (3)] from the simulations. a) A plot of $\lambda L_y/n$ against n/L_y for the shearing modes of the spectrum shown in Fig. 1. A parabola is fit through the points and c_λ, d_λ, and e_λ appear as the coefficients. The error bars are based on the fluctuations of the exponent during the simulation, which ran for 5×10^6 collisions. All points in the other three panels of this figure were determined from similar simulations. b) observed values of c_λ plotted against area fraction ν. The circles indicate the shearing mode and stars are the sound modes. The dark symbols at $\nu = 0$ are the theoretical predictions given in Eqs. (65) and (87). c) observed values of d_λ. d) observed values of e_λ. The value at $\nu = 0.05$ is not shown; it is $e_\lambda = (1.43 \pm 0.06) \times 10^4$ for the shear mode, and $e_\lambda = (1.77 \pm 0.09) \times 10^4$ for the sound mode.

3 Theory

3.1 General approach

The rationale of our approach is to approximate the exact dynamics in phase space by a statistical treatment, as it is done at the level of the Boltzmann equation, and to neglect all correlations built by collisions among particles. This is not only done for the dynamics itself but also for the evolution of the infinitesimal deviation vectors associated with each trajectory. The physical argument behind this scheme is based on the fact that the evolution of the deviation vectors is driven by the dynamics but they do not in turn influence the latter. The approach formulated here at the level of one-body distributions could therefore be formulated at the level of the Liouville equation.

We therefore begin by defining a generalization of Boltzmann's one-body velocity density function,

$$\phi = \phi(\mathbf{v}, \delta\mathbf{r}, \delta\mathbf{v}; \mathbf{r}, t), \tag{4}$$

that gives the density of particles with velocity $\mathbf{v}$ and Lyapunov coordinates $\delta\mathbf{r}$ and $\delta\mathbf{v}$ at position $\mathbf{r}$ at time t. We can recover the usual velocity density function by integrating out the Lyapunov coordinates:

$$f(\mathbf{v}) = \int\int \phi \, d\delta\mathbf{r} \, d\delta\mathbf{v} = \frac{n}{2\pi T} e^{-v^2/2T}. \tag{5}$$

Since we restrict ourselves to systems in thermal equilibrium, $f(\mathbf{v})$ is always a Gaussian.

We will investigate the behavior of fields defined as moments of ϕ. We use the notation

$$\langle \psi \rangle = \frac{1}{n} \int \psi \, \phi(\mathbf{v}, \delta\mathbf{r}, \delta\mathbf{v}; \mathbf{r}, t) \, d\mathbf{v} \, d\delta\mathbf{r} \, d\delta\mathbf{v}, \tag{6}$$

where n is the number density of the fluid. Since we consider only systems in equilibrium, n is a constant. Not all moments of ϕ are equally important. We will show in Sec. 3.2.2 that four of them are more significant than the rest. Two important fields are

$$\mathbf{X}(\mathbf{r}, t) = \langle \delta\mathbf{r} \rangle, \quad \mathbf{U}(\mathbf{r}, t) = \langle \delta\mathbf{v} \rangle. \tag{7}$$

They resemble the macroscopic velocity $\mathbf{u} = \langle \mathbf{v} \rangle$. On the other hand, the fields

$$D(\mathbf{r}, t) = \frac{1}{2} \langle \mathbf{v} \cdot \delta\mathbf{r} \rangle, \quad E(\mathbf{r}, t) = \frac{1}{2} \langle \mathbf{v} \cdot \delta\mathbf{v} \rangle, \tag{8}$$

resemble the temperature $T = \frac{1}{2}\langle \mathbf{v} \cdot \mathbf{v} \rangle$. Now we will develop evolution equations for these fields and study their stability. The hydrodynamic Lyapunov modes will appear as hydrodynamic instabilities.

We will derive equations for the fields from generalized Boltzmann equation:

$$\frac{\partial \phi}{\partial t} + \mathbf{v} \cdot \nabla_{\mathbf{r}} \phi + \delta\mathbf{v} \cdot \nabla_{\delta\mathbf{r}} \phi = \mathcal{C}. \tag{9}$$

The notation $\nabla_{\mathbf{r}}\phi$ in Eq. (9) indicates the gradient of ϕ with respect to $\mathbf{r}$ and $\nabla_{\delta\mathbf{r}}\phi$ indicates the gradient of ϕ with respect to $\delta\mathbf{r}$. The third term on the left represents the change in $\delta\mathbf{r}$ during the free motion when $\dot{\delta\mathbf{r}} = \delta\mathbf{v}$. The term on the right hand side gives the change in ϕ induced by collisions:

$$\mathcal{C}(\mathbf{q}, \mathbf{r}, t) = \sigma \int \phi_A \phi_B \left[\delta(\mathbf{q}'_A - \mathbf{q}) - \delta(\mathbf{q}_A - \mathbf{q})\right] V \cos\theta \, d\mathbf{q}_A \, d\mathbf{q}_B \, d\theta. \quad (10)$$

To lighten the notation, we have used $\mathbf{q}$ to indicate the coordinates $\mathbf{v}$, $\delta\mathbf{r}$, and $\delta\mathbf{v}$, and the subscript on ϕ to show which particle it represents:

$$\begin{aligned} \mathbf{q}_i &= (\mathbf{v}_i, \delta\mathbf{r}_i, \delta\mathbf{v}_i), \\ d\mathbf{q}_i &= d\mathbf{v}_i \, d\delta\mathbf{r}_i \, d\delta\mathbf{v}_i, \\ \phi_i &= \phi(\mathbf{q}_i, \mathbf{r}, t). \end{aligned} \quad (11)$$

$\mathcal{C}$ is an integral over all possible collisions. The colliding particles and their coordinates are labeled A and B. The δ functions in Eq. (10) select those collisions where a particle with coordinates $\mathbf{q}$ is either created or destroyed.

We will not solve the Eq. (9) for ϕ but rather use it to derive equations for the new hydrodynamic fields. Multiply the Boltzmann equation, Eq. (9), by ψ, integrate over $\mathbf{q}$, and divide by n. The result is

$$\frac{\partial \langle\psi\rangle}{\partial t} + \nabla \cdot \langle \mathbf{v}\psi \rangle + \langle \psi \delta\mathbf{v} \cdot \nabla_{\delta\mathbf{r}} \phi \rangle = \langle \psi \mathcal{C} \rangle. \quad (12)$$

The second term in Eq. (12) gives the streaming transport of ψ. The third term vanishes unless ψ depends on $\delta\mathbf{r}$. This term reflects the amplification of $\delta\mathbf{r}$ by $\delta\mathbf{v}$ during the free motion. The right hand side is the collisional change of ψ. This last term can be simplified to

$$\langle \psi \mathcal{C} \rangle = \frac{\sigma}{2} \int \left[\psi'_A + \psi'_B - \psi_A - \psi_B\right] \phi_A(\mathbf{r}) \phi_B(\mathbf{r}) V \cos\theta \, d\mathbf{q}_A \, d\mathbf{q}_B \, d\theta, \quad (13)$$

where $\psi_i = \psi(\mathbf{q}_i)$, and the definitions of Eq. (11) have been used again. The factor $\Delta\psi = [\psi'_A + \psi'_B - \psi_A - \psi_B]$ in the integrand is the change of ψ during a collision. $\Delta\psi$ must be calculated from the collision rules that give the change of $(\mathbf{v}, \delta\mathbf{r}, \delta\mathbf{v})$ during a collision. These collision rules have two special properties which shape all of Lyapunov hydrodynamics. Let us discuss them now.

3.2 Properties of the collision rules

3.2.1 Nonclassical $\delta\mathbf{v}$ collision rule

The Lyapunov coordinates do not affect the motion of the particles, but they are modified at each collision according to a "collision rule". These collision rules have been derived by Dellago et al [10] and by van Zon [11]. The collision rule for $\delta\mathbf{r}$ is

$$\delta\mathbf{r}'_A = \delta\mathbf{r}_A + \mathbf{f}_r, \quad \delta\mathbf{r}'_B = \delta\mathbf{r}_B - \mathbf{f}_r, \quad \mathbf{f}_r \equiv (\delta\mathbf{r}_B - \delta\mathbf{r}_A)\cdot\hat{\mathbf{n}}\hat{\mathbf{n}}, \tag{14}$$

where A and B label the colliding particles. Primes indicate post-collisional values; unprimed variables are pre-collisional. The unit vector $\hat{\mathbf{n}}$ points along the line of centers.

It is important to realize that $\delta\mathbf{r}$ obeys exactly the same collision rule as the velocities:

$$\mathbf{v}_A{}' = \mathbf{v}_A + \mathbf{f}, \quad \mathbf{v}_B{}' = \mathbf{v}_B - \mathbf{f}, \quad \mathbf{f} \equiv (\mathbf{v}_B - \mathbf{v}_A)\cdot\hat{\mathbf{n}}\hat{\mathbf{n}}. \tag{15}$$

On the other hand, $\delta\mathbf{v}$ does not follow the velocity collision rule. This is the first important fact about the collision rules. $\delta\mathbf{v}$ obeys

$$\begin{aligned}\delta\mathbf{v}'_A &= \delta\mathbf{v}_A + \mathbf{f}_v + \mathbf{f}^*_v, \quad \delta\mathbf{v}'_B = \delta\mathbf{v}_B - \mathbf{f}_v - \mathbf{f}^*_v,\\ \mathbf{f}_v &\equiv (\delta\mathbf{v}_B - \delta\mathbf{v}_A)\cdot\hat{\mathbf{n}}\hat{\mathbf{n}},\\ \mathbf{f}^*_v &\equiv V\sigma^{-1}\sec\theta(\delta\mathbf{r}_B - \delta\mathbf{r}_A)\cdot\hat{\mathbf{u}}\hat{\mathbf{u}}',\end{aligned} \tag{16}$$

where θ is the angle between $\mathbf{v}_B - \mathbf{v}_A$ and $\hat{\mathbf{n}}$. We define $\hat{\mathbf{u}}$ to be a unit vector perpendicular to the pre-collisional relative velocity and $\hat{\mathbf{u}}'$ to be perpendicular to the post-collisional relative velocity, so that $(\mathbf{v}_B - \mathbf{v}_A)\times\hat{\mathbf{u}} = (\mathbf{v}'_B - \mathbf{v}'_A)\times\hat{\mathbf{u}}' = |\mathbf{v}_B - \mathbf{v}_A| = V$. (Here, we define the cross product to be a scalar: $\mathbf{a}\times\mathbf{b} \equiv a_x b_y - a_y b_x$. If our two dimensional space were embedded in three dimensions, $\mathbf{a}\times\mathbf{b}$ gives the magnitude and direction of the usual vector cross product.)

The change of $\delta\mathbf{v}$ during a collision given in Eq. (16) can be divided into two parts. The first part, denoted $\mathbf{f}_v$, has the same form as the velocity collision rule, Eq. (15). The second part, denoted $\mathbf{f}^*_v$ arises because perturbations in particle position can modify the geometry of the collision, and the post-collisional velocities are sensitive to the collision geometry, especially in grazing collisions (i.e. when θ is close to $\pm\pi/2$), which explains the factor of $\sec\theta$ in Eq. (16). $\mathbf{f}^*_v$ is essential for the existence of the hydrodynamic Lyapunov modes. Suppose for a moment that $\mathbf{f}^*_v = 0$. Then all the coordinates would obey the velocity collision rule, and transformation $(\mathbf{v}, \delta\mathbf{r}, \delta\mathbf{v}) \to (\mathbf{v}', \delta\mathbf{r}', \delta\mathbf{v}')$ would share with the transformation $\mathbf{v} \to \mathbf{v}'$ all the special properties that enable one to prove the H-theorem, microscopic balance, and all the properties of dilute gases at equilibrium. The hydrodynamic Lyapunov exponents would not exist, because any perturbations of the $\mathbf{X}$, $\mathbf{U}$ or any other field would decay. The distribution function ϕ would approach a Gaussian. It would even be impossible for $\delta\mathbf{\Gamma}$ to grow exponentially, because $\delta\mathbf{v}^2$ and $\delta\mathbf{r}^2$ would be conserved during collisions. $\delta\mathbf{\Gamma}$ could grow only linearly with time during the free motion of the particles, when $\dot{\delta\mathbf{v}} = 0$ and $\dot{\delta\mathbf{r}} = \delta\mathbf{v}$. This difference between $\mathbf{f}_v^*$ and the other collisional changes is so important that when we evaluate the collisional term in Eq. (12), we will separate it into two pieces:

$$\langle \mathcal{C}\psi \rangle = \mathcal{C}^\circ[\psi] + \mathcal{C}^*[\psi]. \tag{17}$$

$\mathcal{C}^\circ[\psi]$ contains all the parts of $\Delta\psi$ depending only on $\mathbf{f}$, $\mathbf{f}_r$ and $\mathbf{f}_v$. We will call it the "dissipative" part of the collision integral because it drives ϕ toward a Gaussian, just like the collision integral of classical kinetic theory. $\mathcal{C}^*[\psi]$ contains all the changes depending on $\mathbf{f}_v^*$. We call it the "growth" part of the collisional integral, because it contains the terms which cause the Lyapunov modes to grow, and the hydrodynamic Lyapunov exponents to be nonzero.

3.2.2 Conserved quantities

Another important property of the collision rule is that certain quantities are conserved during collisions. It is a consequence of Eqs.(14), (15) and (16) that

$$\begin{aligned}
\delta\mathbf{r}'_A + \delta\mathbf{r}'_B &= \delta\mathbf{r}_A + \delta\mathbf{r}_B, \\
\delta\mathbf{v}'_A + \delta\mathbf{v}'_B &= \delta\mathbf{v}_A + \delta\mathbf{v}_B, \\
\mathbf{v}'_A \cdot \delta\mathbf{r}'_A + \mathbf{v}'_B \cdot \delta\mathbf{r}'_B &= \mathbf{v}_A \cdot \delta\mathbf{r}_A + \mathbf{v}_B \cdot \delta\mathbf{r}_B, \\
\mathbf{v}'_A \cdot \delta\mathbf{v}'_A + \mathbf{v}'_B \cdot \delta\mathbf{v}'_B &= \mathbf{v}_A \cdot \delta\mathbf{v}_A + \mathbf{v}_B \cdot \delta\mathbf{v}_B.
\end{aligned} \tag{18}$$

These conservation rules are important because they indicate the existence of the Lyapunov hydrodynamic modes. Recall that hydrodynamic modes exist in ordinary fluids because particle interactions conserve certain quantities. For example, momentum cannot be created or destroyed by collisions. Thus, a local concentration of momentum decays slowly because the collisions cannot destroy momentum; the momentum must be transported by diffusion. As a consequence, the fluid velocity $\mathbf{u}$ changes on a time scale much longer than the collision frequency and is thus a hydrodynamic field. In the same way, introducing a local concentration of any of the quantities in Eq. (18) will change slowly since none of these quantities can be destroyed by collisions. Each one of these quantities will give rise to a Lyapunov hydrodynamic field. The fields $\mathbf{X}$, $\mathbf{U}$, D and E that we introduced in Eqs. (7) and (8) are the Lyapunov hydrodynamic fields.

We can generate equations for the Lyapunov hydrodynamic fields by setting ψ equal to each quantity in Eq. (18) and using Eq. (12). For these quantities, $\Delta\psi = 0$, so the collision integral on the left hand side of Eq. (12) vanishes. The results are:

$$
\begin{aligned}
\frac{\partial \mathbf{X}}{\partial t} + \nabla \cdot \langle \mathbf{v}\, \delta\mathbf{r} \rangle &= \mathbf{U}, \\
\frac{\partial \mathbf{U}}{\partial t} + \nabla \cdot \langle \mathbf{v}\, \delta\mathbf{v} \rangle &= 0, \\
\frac{\partial D}{\partial t} + \nabla \cdot \langle \mathbf{v}\,(\mathbf{v} \cdot \delta\mathbf{r}) \rangle &= E, \\
\frac{\partial E}{\partial t} + \nabla \cdot \langle \mathbf{v}\,(\mathbf{v} \cdot \delta\mathbf{v}) \rangle &= 0.
\end{aligned} \tag{19}
$$

The quantities in angle brackets are the streaming fluxes. They give the transport of the concerned quantity by the free motion of the particles. To get a set of closed equations, we must make a closure hypothesis, relating the streaming fluxes to the hydrodynamic fields.

3.3 Closure hypothesis for the fluxes

We denote the flux of $\mathbf{X}$ by the tensor $\mathbf{J}$:

$$
\mathbf{J} \equiv \begin{pmatrix} \langle v_x \delta r_x \rangle & \langle v_x \delta r_y \rangle \\ \langle v_y \delta r_x \rangle & \langle v_y \delta r_y \rangle \end{pmatrix} = \langle \mathbf{v} \delta \mathbf{r} \rangle. \tag{20}
$$

Likewise, we denote the flux of $\mathbf{U}$ by the tensor $\mathbf{K}$:

$$
\mathbf{K} \equiv \langle \mathbf{v} \delta \mathbf{v} \rangle. \tag{21}
$$

Note that the diagonal components of these tensors are related to the hydrodynamic fields D and E:

$$
D = \frac{1}{2}\left(J_{xx} + J_{yy}\right), \quad E = \frac{1}{2}\left(K_{xx} + K_{yy}\right). \tag{22}
$$

Using Eq. (12), we can generate equations for the fluxes

$$
\begin{aligned}
\frac{\partial \mathbf{J}}{\partial t} + \nabla \cdot \mathbf{L} &= \mathcal{C}^{\circ}[\mathbf{v}\delta\mathbf{r}] + \mathbf{K}, \\
\frac{\partial \mathbf{K}}{\partial t} + \nabla \cdot \mathbf{M} &= \mathcal{C}^{\circ}[\mathbf{v}\delta\mathbf{v}] + \mathcal{C}^{*}[\mathbf{v}\delta\mathbf{v}].
\end{aligned} \tag{23}
$$

The tensors $\mathbf{L}$ and $\mathbf{M}$ are defined as:

$$
L_{ijk} = \langle v_i v_j \delta r_k \rangle, \quad M_{ijk} = \langle v_i v_j \delta v_k \rangle. \tag{24}
$$

We can get equations for them, too:

$$
\begin{aligned}
\frac{\partial L_{ijk}}{\partial t} + \frac{\partial \langle v_x v_i v_j \delta r_k \rangle}{\partial x} + \frac{\partial \langle v_y v_i v_j \delta r_k \rangle}{\partial y} &= \mathcal{C}^\circ [v_i v_k \delta r_k] + M_{ijk}, \\
\frac{\partial M_{ijk}}{\partial t} + \frac{\partial \langle v_x v_i v_j \delta v_k \rangle}{\partial x} + \frac{\partial \langle v_y v_i v_j \delta v_k \rangle}{\partial y} &= \mathcal{C}^\circ [v_i v_k \delta v_k] + \mathcal{C}^* [v_i v_k \delta v_k]. \qquad (25)
\end{aligned}
$$

In this way, we could define an infinite hierarchy of equations. But we need to truncate the hierarchy somewhere. For the analysis of the shear modes, it suffices to truncate the hierarchy after $\mathbf{J}$ and $\mathbf{K}$. When L_{ijk} or M_{ijk} appear, we replace them with the approximations

$$
L_{ijk} = \langle v_i v_j \delta r_k \rangle \approx \langle v_i v_j \rangle \langle r_k \rangle = T \delta_{ij} X_k. \qquad (26)
$$

Likewise, we have $M_{ijk} = T \delta_{ij} U_k$.

To study the sound modes, it is necessary to keep $\mathbf{L}$ and $\mathbf{M}$. In that case, we need an approximation for their fluxes. We will use

$$
\begin{aligned}
\langle v_i v_j v_k \delta r_l \rangle &= \langle v_i v_j \rangle \langle v_k \delta r_l \rangle + \langle v_i v_k \rangle \langle v_j \delta r_l \rangle + \langle v_j v_k \rangle \langle v_i \delta r_l \rangle, \\
&= (\delta_{ij} J_{kl} + \delta_{ik} J_{jl} + \delta_{jk} J_{ij}) T. \qquad (27)
\end{aligned}
$$

An analogous approximation holds for $\langle v_i v_j v_k \delta v_l \rangle$. This rule seems quite odd, but consider the average $\langle v_i v_j v_k v_l \rangle$, which can be calculated exactly because after integrating over the Lyapunov coordinates, the distribution function is a Gaussian. It can be shown that

$$
\langle v_i v_j v_k v_l \rangle = (\delta_{ij} \delta_{kl} + \delta_{ik} \delta_{jl} + \delta_{jk} \delta_{ij}) T^2, \qquad (28)
$$

which is the same as Eq. (27) after replacing J_{ij} with $T \delta_{ij}$.

3.4 Evaluation of collision integrals

In this section, we describe our method of estimating the collision integrals, $\langle \mathcal{C} \psi \rangle$. These integrals have the form

$$
\begin{aligned}
\langle \mathcal{C} \psi \rangle &= \frac{\sigma}{2n} \int V \cos\theta \, \phi_A \phi_B \, [\psi'_A + \psi'_B - \psi_A - \psi_B)] \;\; d\hat{\mathbf{n}} \, d\mathbf{q}_A \, d\mathbf{q}_B, \\
&= \frac{\sigma n}{2} \left\langle \left\langle V \int_{-\pi/2}^{\pi/2} \cos\theta \, \Delta\psi \right\rangle \right\rangle, \qquad (29)
\end{aligned}
$$

where $V = |\mathbf{v}_A - \mathbf{v}_B|$. The double angle brackets are defined as

$$
\langle\langle \psi \rangle\rangle = n^{-2} \int \psi \, \phi_A \phi_B \, d\mathbf{q}_A \, d\mathbf{q}_B. \qquad (30)
$$

This notation is intended to suggest two interwoven single particle averages. Indeed, according to molecular chaos, $\langle\langle\psi_A \xi_B\rangle\rangle = \langle\psi\rangle\langle\xi\rangle$.

To illustrate this notation, let us calculate the collision frequency ω that will play an important role in our theory. To calculate ω, let ξ count the number of collision suffered by a given particle. Each particle carries a counter ξ with it, and every time it collides with another particle, it adds one to ξ. During a collision, $\Delta\xi = \xi'_A + \xi'_B - \xi_A - \xi_B = 2$ because both particles increment their counters. We can thus write the collision frequency very simply as

$$n\omega = \langle \mathcal{C}\xi \rangle. \tag{31}$$

(Note that ω is the frequency of collisions suffered by a single particle, not the frequency of collisions everywhere in the gas.) Using Eq. (30), this expands to

$$\omega = \sigma n \left\langle\langle V \rangle\right\rangle \int\limits_{-\pi/2}^{\pi/2} \cos\theta \, d\theta. \tag{32}$$

Doing the integral over θ, we have

$$\omega = 2\sigma n \left\langle\langle V \rangle\right\rangle. \tag{33}$$

Now the quantity in the double angle brackets is just an integral over the usual distribution function f. It can be evaluated to give

$$\omega = 2\sigma n \sqrt{\pi T}. \tag{34}$$

Comparing the two expressions for ω, Eqs. (33) and Eq. (34), we find $\langle\langle V \rangle\rangle = \sqrt{\pi T} = \omega/(2n\sigma)$. We will return to this when we approximate the collision integrals.

Another quantity that will be important is the mean free path

$$\ell_{\mathrm{mfp}} = \frac{\langle |v| \rangle}{\omega} = \frac{1}{2\sqrt{2}\sigma n}. \tag{35}$$

3.4.1 Estimation of the dissipation collisional integrals

We will show how we estimate $\mathcal{C}^\circ[v_x \delta r_y]$, and give the results for the remaining integrals. Note that the collision rule for $\delta\mathbf{r}$ does not involve $\mathbf{f}_v^*$, so $\langle v_x \delta r_y \mathcal{C}\rangle = \mathcal{C}^\circ[v_x \delta r_y]$.

From the collision rule, we can show that

$$\Delta(v_x\delta r_y) = -V\left\{\Delta\mathbf{r}\cdot\hat{\mathbf{n}}(\hat{v}_x - \hat{n}_x\cos\theta)n_y + \Delta r_y\hat{n}_x\cos\theta\right\}, \tag{36}$$

where $\Delta\mathbf{r} \equiv \delta\mathbf{r}_A - \delta\mathbf{r}_B$.

Using Eq. (29), we have

$$\langle v_x\delta r_y\mathcal{C}\rangle = \mathcal{C}^\circ[v_x\delta r_y] = \frac{n\sigma}{2}\left\langle\!\!\left\langle V\int_{-\pi/2}^{\pi/2}\cos\theta\,\Delta(v_x\delta r_y)\,d\theta\right\rangle\!\!\right\rangle. \tag{37}$$

Setting $\hat{\mathbf{n}} = \hat{\mathbf{v}}\cos\theta - \hat{\mathbf{u}}\sin\theta$ where $\hat{\mathbf{v}}$ is a unit vector in the direction of $\mathbf{v}_B - \mathbf{v}_A$ allows us to eliminate $\hat{\mathbf{n}}$, and then do the integral over θ. Since $\hat{\mathbf{u}}$ and $\hat{\mathbf{v}}$ are perpendicular, we use $\hat{u}_x = -\hat{v}_y$ and $\hat{u}_y = \hat{v}_x$ to eliminate $\hat{\mathbf{u}}$. The integral becomes

$$\begin{aligned}\mathcal{C}^\circ[v_x\delta r_y] = &+\frac{2n\sigma}{15}\left\langle\!\!\left\langle V^2\Delta\mathbf{r}\cdot\hat{\mathbf{v}}\,\hat{v}_x\hat{v}_y\right\rangle\!\!\right\rangle - \frac{n\sigma}{5}\left\langle\!\!\left\langle V^2\Delta\mathbf{r}\cdot\hat{\mathbf{u}}\,(1+3\hat{v}_y^2)\right\rangle\!\!\right\rangle\\ &-\frac{2n\sigma}{3}\left\langle\!\!\left\langle V^2\Delta r_y\hat{v}_x\right\rangle\!\!\right\rangle.\end{aligned} \tag{38}$$

Let us consider the average in the last term $\langle\langle V^2\Delta r_y\hat{v}_x\rangle\rangle$ which we can rewrite as $\langle\langle V(v_{Ax} - v_{Bx})(\delta r_{Ay} - \delta r_{By})\rangle\rangle$. The factor of $V = \sqrt{(\mathbf{v}_A - \mathbf{v}_B)^2}$ in the integrand is quite awkward, because the coordinates of the two particles are mixed together. If this factor was not there, we would have simply $\langle\langle(v_{Ax} - v_{Bx})(\delta r_{Ay} - \delta r_{By})\rangle\rangle = 2J_{xy}$. This suggests that $\langle\langle V(v_{Ax} - v_{Bx})(\delta r_{Ay} - \delta r_{By})\rangle\rangle \propto \langle\langle V\rangle\rangle\, J_{xy}$. Combining this with Eq. (33), we have

$$\langle\langle V(v_{Ax} - v_{Bx})(\delta r_{Ay} - \delta r_{By})\rangle\rangle = \alpha\frac{\omega}{n\sigma}J_{xy}, \tag{39}$$

where α is an unknown constant. This is the approximation used to evaluate all the dissipation collision integrals. We always assume the same unknown constant α appears. The factor of $n\sigma$ conveniently cancels when we put this expression back into Eq. (38).

There is a slight complication in the other terms, because they include several factors of the components of the unit vectors:

$$\left\langle\!\!\left\langle V^2\Delta\mathbf{r}\cdot\hat{\mathbf{v}}\,\hat{v}_x\hat{v}_y\right\rangle\!\!\right\rangle = \left\langle\!\!\left\langle V^2\Delta r_x\hat{v}_x^2\hat{v}_y\right\rangle\!\!\right\rangle + \left\langle\!\!\left\langle V^2\Delta r_y\hat{v}_x\hat{v}_y^2\right\rangle\!\!\right\rangle. \tag{40}$$

How do we handle these extra components of the unit vectors $\hat{\mathbf{u}}$ and $\hat{\mathbf{v}}$? First, one can show that $\langle\langle V\hat{v}_i\hat{v}_j\rangle\rangle = \delta_{ij}\langle\langle V\rangle\rangle/2$. Then we apply the same factorization as in Eq. (27) and write

$$\left\langle\left\langle V^2\hat{v}_i\hat{v}_j\hat{v}_k\Delta r_l\right\rangle\right\rangle = \frac{\alpha}{4}\frac{\omega}{n\sigma}\left(\delta_{ij}J_{kl} + \delta_{jk}J_{il} + \delta_{ki}J_{jl}\right). \tag{41}$$

The 4 under the α is required to make this equation consistent with with Eq. (39), i.e. we must have $\langle\langle V^2\hat{v}_x\Delta r_y\rangle\rangle = \left\langle\left\langle V^2(\hat{v}_x^2+\hat{v}_y^2)\hat{v}_x\Delta r_y\right\rangle\right\rangle$. Applying these rules we can reduce Eq. (38) to

$$\mathcal{C}^\circ[v_x\delta r_y] = \frac{\alpha\omega}{60}\left(11J_{yx} - 31J_{xy}\right). \tag{42}$$

We can obtain $\mathcal{C}[v_y\delta r_x]$ by simply exchanging x and y.

Following the same method, we find

$$\mathcal{C}^\circ[v_x\delta r_x] = \frac{7\alpha\omega}{20}\left[J_{yy} - J_{xx}\right]. \tag{43}$$

Although these expressions look awkward, certain combinations of them are simpler, and will be useful in later sections:

$$\begin{aligned}
\mathcal{C}^\circ[v_x\delta r_y + v_y\delta r_x] &= -\frac{7\alpha\omega}{10}(J_{xy}+J_{yx}),\\
\mathcal{C}^\circ[v_x\delta r_y - v_y\delta r_x] &= -\frac{\alpha\omega}{3}(J_{xy}-J_{yx}),\\
\mathcal{C}^\circ[\mathbf{v}\cdot\delta\mathbf{r}] &= 0,\\
\mathcal{C}^\circ[v_x\delta r_x - v_y\delta r_y] &= -\frac{7\alpha\omega}{10}(J_{xx}-J_{yy}).
\end{aligned} \tag{44}$$

3.4.2 The growth terms

In the growth terms, the integrand is simply a polynomial of velocities times a Lyapunov coordinate. They can be easily evaluated using Eq. (27). As an example, we will evaluate $\mathcal{C}^*[v_x\delta v_y]$. The part of $\Delta v_x\delta v_y$ that depends on $\mathbf{f}_v^*$ is

$$\Delta v_x\delta v_y = V^2\sigma^{-1}\sec\theta\left(\hat{v}_x - 2\hat{n}_x\cos\theta\right)\left(\delta\mathbf{r}_B - \delta\mathbf{r}_A\right)\cdot\hat{\mathbf{u}}\hat{u}'_y. \tag{45}$$

We use $\hat{\mathbf{u}}' = -\hat{\mathbf{v}}\sin 2\theta - \hat{\mathbf{u}}\cos 2\theta$, integrate over θ and eliminate $\hat{\mathbf{u}}$ as before to obtain

$$\mathcal{C}^*[v_x\delta v_y] = -\pi\left\langle\left\langle V^3(\delta\mathbf{r}_B - \delta\mathbf{r}_A)\cdot\hat{\mathbf{u}}\right\rangle\right\rangle. \tag{46}$$

The quantity inside the angle brackets is just a long polynomial

$$\mathcal{C}^*[v_x\delta v_y] = \pi\left\langle\left\langle(\mathbf{v}_A-\mathbf{v}_B)^2\left[(\delta r_{Ay}-\delta r_{By})(v_{Ax}-v_{Bx})-(\delta r_{Ax}-\delta r_{Bx})(v_{Ay}-v_{By})\right]\right\rangle\right\rangle. \quad (47)$$

With patience, these terms can all be multiplied out to obtain

$$\mathcal{C}^*[v_x\delta v_y] = 8\pi nT(J_{yx}-J_{xy}). \quad (48)$$

In the same way, we have

$$\mathcal{C}^*[v_x\delta v_x] = 0. \quad (49)$$

3.5 Scaling arguments and solution

We now are in a position to present our theory of the hydrodynamic Lyapunov modes. We adopt the situation presented in the simulations. We suppose that $L_x \ll L_y$, so that all gradients in x vanish. We will first analyze the shear modes. We obtain from Eq. (19) the equations for X_x and U_x, the two fields implicated in the shearing modes:

$$\frac{\partial X_x}{\partial t}+\frac{\partial J_-}{\partial y}+\frac{\partial J_+}{\partial y}=U_x, \quad (50)$$

$$\frac{\partial U_x}{\partial t}+\frac{\partial K_-}{\partial y}+\frac{\partial K_+}{\partial y}=0. \quad (51)$$

Instead of J_{yx} and K_{yx}, we have used

$$J_-\equiv\frac{1}{2}(J_{yx}-J_{xy}), \quad J_+\equiv\frac{1}{2}(J_{yx}+J_{xy}), \quad (52)$$

and analogously for K_+ and K_-. This choice renders the equations for the fluxes simpler. The fluxes J_-, J_+, K_-, and K_+ obey

$$\frac{\partial J_-}{\partial t}+\frac{T}{2}\frac{\partial X_x}{\partial y}=-\alpha_-\omega J_-+K_-, \quad (53)$$

$$\frac{\partial J_+}{\partial t}+\frac{T}{2}\frac{\partial X_x}{\partial y}=-\alpha_+\omega J_++K_+, \quad (54)$$

$$\frac{\partial K_-}{\partial t}+\frac{T}{2}\frac{\partial U_x}{\partial y}=-\alpha_-\omega K_-+\beta nTJ_-, \quad (55)$$

$$\frac{\partial K_+}{\partial t}+\frac{T}{2}\frac{\partial U_x}{\partial y}=-\alpha_+\omega K_+, \quad (56)$$

where the constants can be read off from Eq. (44): $\alpha_- = \alpha/3$, $\alpha_+ = 7\alpha/10$, and $\beta = 8\pi$.

Now we assume that the hydrodynamic fields change on a time scale much longer that the collision frequency. This means that the time derivative on the left hand side of Eqs. (53) through (56) is small compared to the first term on the right hand side. In symbols, we would write

$$O\left(\frac{\partial}{\partial t}\right) = \varepsilon\omega, \tag{57}$$

where $\varepsilon \ll 1$ is the ratio between the hydrodynamic time scale and the collision frequency. We therefore neglect all the time derivatives in Eqs. (53) through (56). Physically, we are assuming that the fluxes are slaved to the gradients of the hydrodynamic fields.

Once the time derivatives are removed, we have simply four equations for the four unknowns J_-, J_+, K_-, and K_+. We can solve for these four quantities in terms of the gradients of X_x and U_x. For example,

$$K_- = \frac{T}{2}\frac{\partial X_x}{\partial y} + \frac{\alpha_- \omega T}{2\beta n T - \alpha_-^2\omega^2}\left(\frac{\partial U_x}{\partial y} + \alpha_-\omega\frac{\partial X_x}{\partial y}\right). \tag{58}$$

When we examine this expression more closely, we see that simplifications can be made in the limit of vanishing density. Consider

$$2\beta n T - \alpha_-^2\omega^2 = nT\left(2\beta - \alpha_-^2\frac{\omega^2}{nT}\right). \tag{59}$$

Using our previous expressions for the collision frequency and the mean free path, Eqs. (34) and (35), we see that

$$\frac{\omega^2}{nT} = \frac{\pi}{\sqrt{2}}\frac{\sigma}{\ell_{\mathrm{mfp}}} \ll 1, \tag{60}$$

because in the low density limit, the particle diameter is much smaller than the mean free path.

Eliminating all the terms that vanish in the low density limit, and putting the resulting expressions for the fluxes into Eqs. (50) and (51), we obtain

$$\frac{\partial X_x}{\partial t} - \frac{T}{2\alpha_+\omega}\frac{\partial^2 X}{\partial y^2} + \frac{T}{4\alpha_+^2\omega^2}\frac{\partial^2 U}{\partial y^2} = U_x,$$

$$\frac{\partial U_x}{\partial t} + \frac{T}{2}\frac{\partial^2 X}{\partial y^2} - \frac{T}{2\alpha_+\omega}\frac{\partial^2 U}{\partial y^2} = 0. \tag{61}$$

Now we make two additional scaling assumptions. First, we assume that the hydrodynamic fields vary on a length scale much longer than the mean free path. This means that

$$O\left(\frac{\partial}{\partial y}\right) = \frac{\varepsilon}{\ell_{\mathrm{mfp}}}. \tag{62}$$

The second scaling assumption is that the term U_x on the right hand side of Eq. (50) is the same size as the time derivative $\frac{\partial X_x}{\partial t}$.

$$O\left(\frac{\partial X_x}{\partial t}\right) = O(U_x) \quad \Longrightarrow \quad \varepsilon\omega O(X_x) = O(U_x). \tag{63}$$

This amounts to assuming that the growth of $\delta\mathbf{r}$ during the free movement of the particles is important. With these assumptions, only one of the flux terms survives, and Eqs. (61) become

$$\begin{aligned} \frac{\partial X_x}{\partial t} &= U_x, \\ \frac{\partial U_x}{\partial t} &= -\frac{T}{2}\frac{\partial^2 X_x}{\partial y^2}. \end{aligned} \tag{64}$$

Taking $X_x, U_x \sim e^{st+ikx}$, we obtain the dispersion relation for Eqs. (64):

$$s = \pm q\sqrt{\frac{T}{2}}. \tag{65}$$

This is our prediction for the dilute limit. It is compared with simulations in Fig. 3. This result does not depend on the details of how the collision integrals where approximated, i.e. it does not depend on α, α_-, α_+ or β.

3.6 The sound modes

To get the complete equations for the sound modes, start with the y component of X and U:

$$\frac{\partial X_y}{\partial t} + \frac{\partial D}{\partial y} + \frac{\partial D'}{\partial y} = U_y, \tag{66}$$

$$\frac{\partial U_y}{\partial t} + \frac{\partial E}{\partial y} + \frac{\partial E'}{\partial y} = 0, \tag{67}$$

where D and E are the fields defined in Eq. (8) and E' and D' are given by

$$D' \equiv \frac{1}{2}(J_{xx} - J_{yy}), \quad E' \equiv \frac{1}{2}(K_{xx} - K_{yy}). \tag{68}$$

These fields are governed by

$$\frac{\partial D}{\partial t} + \frac{\partial L}{\partial y} + \frac{T}{2}\frac{\partial X_y}{\partial y} = E, \tag{69}$$
$$\frac{\partial D'}{\partial t} + \frac{\partial L'}{\partial y} + \frac{T}{2}\frac{\partial X_y}{\partial y} = -\alpha'\omega D' + E', \tag{70}$$
$$\frac{\partial E}{\partial t} + \frac{\partial M}{\partial y} + \frac{T}{2}\frac{\partial U_y}{\partial y} = 0, \tag{71}$$
$$\frac{\partial E'}{\partial t} + \frac{\partial M'}{\partial y} + \frac{T}{2}\frac{\partial U_y}{\partial y} = -\alpha'\omega E', \tag{72}$$

where

$$L \equiv \frac{1}{2}(L_{xyx} + L_{yyy} - TX_y), \quad L' \equiv \frac{1}{2}(L_{xyx} - L_{yyy} + TX_y), \tag{73}$$

with analogous definitions for M and M'. We can now show that D' and E' play no role in the dynamics because they are always much smaller than D and E. To see why this is so, compare the equation for E, Eq. (71) to the equation for E', Eq. (72). These equations have almost exactly the same form, except Eq. (72) contains the additional term $-\alpha'\omega E'$. This difference arises because E is an average of a collisional invariant while E' is not. As we argued in Eq. (57), this additional term will dominate the time derivative so that E' will be slaved to the hydrodynamic fields. E, however, is a hydrodynamic field. After neglecting $\frac{\partial E'}{\partial t}$, the two equations can be rewritten

$$\frac{\partial E}{\partial t} = -\frac{\partial M}{\partial y} - \frac{T}{2}\frac{\partial U_y}{\partial y}, \tag{74}$$
$$-\alpha'\omega E' = -\frac{\partial M'}{\partial y} - \frac{T}{2}\frac{\partial U_y}{\partial y}. \tag{75}$$

From this pair of equations, we can see that $\omega O(E') = O(\frac{\partial E}{\partial t})$ so that $O(E') = \varepsilon O(E)$. A similar argument can be applied to show $O(D') = \varepsilon O(D)$.

Now we must calculate L and M in terms of the gradients of E and D. To do this, one must consider the equations for the various components of $\mathbf{L}$ and

M. After applying Eqs. (57), (60), and (63), the equations for the relevant components of **L** and **M** become:

$$\frac{3T}{2}\frac{\partial D}{\partial y} = -\alpha_1 \omega L + M, \tag{76}$$
$$-\frac{T}{2}\frac{\partial D}{\partial y} = \alpha_7 \omega L + M_*, \tag{77}$$
$$0 = -\alpha_1 \omega M + \alpha_2 \omega M_* - \beta_1 L_*, \tag{78}$$
$$0 = -\alpha_6 \omega M_* + \alpha_7 \omega M + \beta_2 L_*, \tag{79}$$

where $L_* = \frac{1}{2}(L'_{xxy} - L'_{xyx})$, and likewise for M_*. The constants $\alpha_1 = \alpha_2 = 31\alpha/60$, $\alpha_6 = 121\alpha/60$ and $\alpha_7 = \alpha/60$, $\beta_1 = \pi$, $\beta_2 = 3\pi$ come from evaluating the collision integrals. Solving these equations for M gives

$$M \approx \left(\frac{\beta_1 \alpha_6}{\beta_2} - \alpha_2\right) \frac{T}{2}\frac{\partial D}{\partial y} = \gamma \frac{\partial D}{\partial y}, \tag{80}$$

where $\gamma = \frac{\beta_1 \alpha_6}{\beta_2} - \alpha_2$. (We have neglected α_7 compared to the other α_i because it is at least 30 times smaller.) When this result is put into Eqs. (66), (67), (69), and (71), the result is

$$\frac{\partial X_y}{\partial t} + \frac{\partial D}{\partial y} = U_y, \tag{81}$$
$$\frac{\partial U_y}{\partial t} + \frac{\partial E}{\partial y} = 0, \tag{82}$$
$$\frac{\partial D}{\partial t} + \gamma \frac{\partial X_y}{\partial y} = E, \tag{83}$$
$$\frac{\partial E}{\partial t} + \gamma \frac{\partial^2 D}{\partial y^2} + \frac{T}{2}\frac{\partial U_y}{\partial y} = 0, \tag{84}$$

which yields the dispersion relation

$$\left(s^2 + \frac{k^2 T}{2}\right)^2 - \left(s^2 - \frac{k^2 T}{2}\right)\gamma k^2 = 0, \tag{85}$$

From the dispersion relation, we have

$$s^2 = \frac{k^2}{2}\left[\gamma - T \pm \sqrt{\gamma^2 - 4\gamma T}\right] = \frac{k^2 T}{2}\left[\frac{5}{6} \pm \sqrt{\frac{2}{3}}\right]. \tag{86}$$

Unlike Eq. (65), this result depends on the precise results of evaluating the integrals, as one can see from the presence of the γ (which in turn depends on the various constants α_i in the integrals). Putting in the values of α_2, α_6, β_1, and β_2, we find $\gamma \approx \frac{T}{6}$. Evaluating s numerically, we find

$$s \approx k\sqrt{T}(0.38 \pm i0.66). \tag{87}$$

Unlike Eq. (65), this result is sensitive to the approximations of the integrals. The difference between Eq. (87) and the observed values suggest that our method of approximating the integrals gives the correct dependence on the fluxes and the collision frequency, but not the correct constant of proportionality.

4 Conclusions

This work supports the hypothesis of the existence of the Lyapunov hydrodynamic modes because it has shown a way to overcome several difficulties with MM1. In MM1, we obtained terms which were not time reversible and hence were not observed in the simulations. In this article, we show that those terms are small. While this is not the same thing as showing that they vanish, it means that they could be suppressed by some small and yet undiscovered effect. What this effect might be is an open question. Another problem with MM1 was that we obtained $\lambda = 0$ for the sound waves. In this article, we have obtained a frequency with the correct form (i.e. with both a real and imaginary part, indicating a growing or decaying oscillating perturbation). However, the predicted value of λ appears to be too small by a factor of about $\frac{1}{2}$. This discrepancy probably arises because our prediction for λ is sensitive to our method of approximating collision integrals. Finally, we believe that the finite density case will not be qualitatively different from the zero density limit considered here, at least for equilibrium states. We have used the zero density limit in two places: first to avoid calculating the collisional fluxes (these fluxes were calculated for some quantities in MM1), and to simplify some of the coefficients appearing in the equations. We conclude that our theory gives an accurate and informative explanation of the smallest positive Lyapunov exponents of the hard disk fluid.

References

[1] S. McNamara and M. Mareschal, *Phys. Rev. E* **64** 051103 (2001).

[2] P. Gaspard and G. Nicolis, *Phys. Rev. Lett.* **65**, 1693 (1990).

[3] J.R. Dorfman, P. Gaspard, *Phys. Rev. E* **51** 28 (1995).

[4] H. van Beijeren, J. R. Dorfman, E. G. D. Cohen, H. A. Posch, and Ch. Dellago *Phys. Rev. Lett.* **77**, 1974 (1996).

[5] P. Resibois and M. DeLeener, *Classical Kinetic Theory of Fluids*, J. Wiley, New York (1977)

[6] H.A. Posch and R. Hirschl, in **Hard-Ball Systems**, D. Szasz (Editor) Springer Verlag, Berlin (2000).

[7] C. Forster and H. A. Posch, these proceedings.

[8] J.P.Eckman and Omri Gat, J.Stat.Phys. **98**, 775, (2000).

[9] A. de Wijn and H. van Beijeren, these proceedings.

[10] Ch. Dellago, H.A. Posch, and W.G. Hoover, Phys. Rev. E, **53** 1485 (1996); Ch. Dellago and H.A. Posch, Physica A **240** 68 (1997).

[11] R. van Zon, **Chaos in dilute hard sphere gases in and out of equilibrium**, (Ph.D. thesis) Shaker Publishing B.V. (2000).