We consider simulations of a two-dimensional gas of hard disks in a rectangular container and study the Lyapunov spectrum near the vanishing Lyapunov exponents. To this spectrum are associated “eigen-directions”, called Lyapunov modes. We carefully analyze these modes and show how they are naturally associated with vector fields over the container. We also show that the Lyapunov exponents, and the coupled dynamics of the modes (where it exists) follow linear laws, whose coefficients only depend on the density of the gas, but not on aspect ratio and very little on the boundary conditions.

KEY WORDS: Nonlinear dynamics; Hamiltonian dynamics; extended systems; Lyapunov spectrum.

1. INTRODUCTION

In this paper, we study the Lyapunov spectra of two-dimensional hard-disk systems and, in particular, the associated “Lyapunov modes”.

Recently, this topic has received considerable attention, and a lot of progress has been made in the understanding of the issues involved. In the present work, we synthesize and expand the results found earlier. In particular, we completely classify these modes and give a simple interpretation of their dynamics, in particular for systems with arbitrary aspect ratio. We furthermore present new simulations in support of this classification.

The Lyapunov exponents describe the rates of exponential growth, or decay, of infinitesimal phase-space perturbations, and are taken to be...
ordered according to $\lambda(1) > \lambda(2) > \cdots > \lambda(\ell)$. Because of the Hamiltonian nature of the problem, they come in conjugate pairs, $\lambda(j) = -\lambda(\ell - j + 1)$.

As is well-known, 0 is always a Lyapunov exponent for such systems and therefore, as a consequence, $\ell$ is odd. At any point $\xi$ in phase space, the tangent space $T_X(\xi)$ decomposes into a sum $T_X(\xi) = \bigoplus E(1)(\xi) \oplus \cdots \oplus E(\ell)(\xi)$, where $E(j)(\xi)$ is the (linear) space of those perturbations of the initial condition $\xi$ whose growth rate is $\lambda(j)$ for the forward dynamics, and $-\lambda(j)$ for the time reversed dynamics. This decomposition is called the Oseledec splitting.

We say that the Lyapunov exponent $\lambda(j)$ is d-fold degenerate if $\dim E(j)(\xi) = d$. It should be noted that, when the Lyapunov exponents are d-fold degenerate, only the subspace corresponding to all d of them is well defined. The main idea of our full classification of Lyapunov exponents and their modes is based on this simple observation.

The Lyapunov modes are defined as follows: at time $t = 0$, we take $n$ orthogonal tangent vectors at $\xi$ and, by applying to them the tangent-space dynamics for a long-enough time $t$, map them onto $n$ vectors which, generally, are not orthogonal but still span an $n$-dimensional subspace $S_n(t)$. If, instead of $n$, we consider only $n - 1$ vectors, they similarly span an $(n - 1)$-dimensional subspace $S_{n-1}(t)$, such that $S_{n-1}(t) \subset S_n(t)$. The Lyapunov mode is a unit vector in $S_n(t)$ which is orthogonal to the space $S_{n-1}(t)$. We will give a precise definition in the next section, explain the algorithmic aspects in Section 3.1 and relate the modes to Oseledec's subspaces in Section 3.2.

The study of Lyapunov modes has revealed interesting spatial structures which we will define later but which come in two types: localized structures associated with the large positive and negative Lyapunov exponents, and smooth delocalized structures of wave-like type for exponents close to zero. The exponents associated with the latter are degenerate and give rise to a step-like appearance of the Lyapunov spectrum as is shown, for example, in Fig. 1.
Lyapunov Modes in Hard-Disk Systems

Fig. 1. Lyapunov spectrum for $N = 780$ hard disks at a density $\rho \equiv N/(L_x L_y) = 0.8i$ in a rectangular periodic box with an aspect ratio $L_y/L_x = 0.867$. The insert provides a magnified view of the mode regime.

The discovery of these structures has led to several studies (3–7) which go some way in explaining their origin and their dynamics. In this paper, we show how they are related to the symmetries of the container in which the particles move (including the boundary conditions). At the same time, we obtain a classification of the degeneracies of the Lyapunov exponents near zero. This classification allows to view the so-called “mode dynamics” from a new geometrical perspective.

The paper starts with a summary of results, passes through a precise definition of the Lyapunov modes, and then describes them as vector fields. In Section 4 these vector fields are classified, and their dynamics is studied in Section 5. The last sections deal with the density dependence and with possible hydrodynamic aspects.

2. NOTATION AND SUMMARY OF RESULTS

We consider a system of $N$ hard disks of diameter $\sigma$ and mass $m$ moving in a two-dimensional rectangular container with sides of lengths $L_x$ and $L_y$. The phase space of such a system is $X = \mathbb{R}_2^N \times ([0, L_x] \times [0, L_y])^N$.

We will consider reflecting and periodic boundary conditions.
and a phase point \( \xi \) in \( X \) is \( \xi = (p, q) = (p_1, \ldots, p_N, q_1, \ldots, q_N) \).

When necessary, we will write \( q_i = (q_{ix}, q_{iy}) \) to distinguish the two position components of particle \( i \), and similarly for the momenta.

The dynamics of the system is that of free flight, interrupted by elastic binary collisions. If \( \xi_0 \) is the state of the system at time 0, then \( \xi_t = \Phi_1(t)(\xi_0) \) is the state at time \( t \), where \( \Phi_1(t) : X \to X \) defines the flow.

Apart from issues of differentiability, which will be addressed when we describe the numerical implementation in Section 3, we call \( D\Phi_1(t) \) the tangent flow. Informally speaking, it is a \( 4N \times 4N \) matrix of partial derivatives and can be thought of as the first-order term (in \( \varepsilon \)) in an expansion of the perturbed flow, \( \Phi_1(t)(\xi_0 + \varepsilon \delta\xi) = \Phi_1(t)(\xi_0) + \varepsilon D\Phi_1(t)\xi_0 \cdot \delta\xi + O(\varepsilon^2) \).

The vector \( \delta\xi \) lies in the tangent space \( TX(\xi_0) \) to the manifold \( X \); in our case \( TX(\xi_0) = \mathbb{R}^{4N} \).

We next invoke the multiplicative ergodic theorem of Oseledec (9, 10). To do so, we need ergodicity of the Liouville measure. Without further knowledge, we assume this for our case.

Theorem. There exist an integer \( \ell \) and numbers \( \lambda(j), j = 1, \ldots, \ell \) such that for almost every \( \xi \in X \) (with respect to the Liouville measure) the tangent space splits into \( TX(\xi) = E(1)(\xi) \oplus E(2)(\xi) \oplus \cdots \oplus E(\ell)(\xi) \), with the property:

\[
\lim_{t \to \pm \infty} \frac{1}{|t|} \log \|D\Phi_1(t)\xi_0 \cdot \delta\xi\| = \pm \lambda(j)
\]

for \( \delta\xi \in E(j)(\xi) \). The spaces \( E(j) \) are covariant: \( D\Phi_1(t)E(j)(\xi) = E(j)(\Phi_1(t)(\xi)) \).

The dimension \( d(j) \) of \( E(j)(\xi) \) is called multiplicity of the exponent \( \lambda(j) \).

We refer the reader to Oseledec (9, 10) for further details.
To denote the Lyapunov exponents repeated with multiplicities, after the index is referred to as the Lyapunov index. This notation is more adequate for describing numerical methods of measurement, in which tangent-space dynamics is probed by a set of vectors. With these notations the relation between the $\lambda^{(j)}$ and the $\lambda^{i}$ is given by

$$\lambda^{(j)} = \lambda f^{(j-1)} + 1 = \cdots = \lambda f^{(j)} ,$$

where $f^{(j)} = d^{(1)} + \cdots + d^{(j)}$. Choosing $j \in \{1, \ldots, \ell\}$ and letting $F^{(j)} = E^{(1)} \oplus \cdots \oplus E^{(j)}$, we define the $d^{(j)}$ Lyapunov modes associated with $\lambda^{(j)}$ as any orthogonal spanning set of the space $M^{(j)} = (F^{(j-1)})^\perp \cap F^{(j)}$.

A finer decomposition of this spanning set will be obtained when we describe the algorithm used, see Section 3.1. The subspaces $M^{(j)}$ are very similar to the subspaces $E^{(j)}$: they have the same dimension and also satisfy $F^{(j)} = M^{(1)} \oplus \cdots \oplus M^{(j)}$. However, they are not identical, because of the orthogonality constraint in (1). This will be explained in Section 3.2.

In this summary, we focus on rectangular boxes with periodic boundary conditions. Narrow systems ($L_y < 2\sigma$) or systems with reflecting boundaries have a very similar Lyapunov spectrum, but some exponents found in the periodic case are either absent, or appear with smaller multiplicities. We shall treat such systems in Section 4.3 but concentrate, until then, on the "general" periodic case. However, it should be noted that systems with reflecting boundaries give important information on the relation between the vanishing and the small Lyapunov exponents (see Ex. 3 below).

The Lyapunov exponents near zero are found to be proportional to the wave numbers of the system,

$$k^{(n_x,n_y)} = \sqrt{(2\pi L_x n_x)^2 + (2\pi L_y n_y)^2} , n_x, n_y = 0, 1, \ldots ,$$

with

$$\theta = \frac{2\pi}{L} .$$

Remark. This result, as well as all results mentioned below, are to be understood in the limit of an infinite number of disks, at fixed density. In particular, we omit higher order terms (in $k$) in most of our statements.
The Lyapunov exponents have the following properties:

**Lyapunov Spectrum:**
For gases of hard disks, the Lyapunov exponents near zero are fully determined by two (positive) constants, $c_L$ and $c_T$. For small enough $n = (n_x, n_y)$, these exponents lie on two straight lines.

1. **Transverse branch (T):**
   \[ \lambda = \pm c_T k_n, \] with multiplicity 4 (2 if either $n_x$ or $n_y$ is zero)

2. **Longitudinal branch (L):**
   \[ \lambda = \pm c_L k_n, \] with multiplicity 8 (4 if either $n_x$ or $n_y$ is zero)

The multiplicities of both branches will be explained by simple geometric observations in Section 4.2. While the linear laws resemble the square roots of the eigenvalues of a Laplacian in the box, we have no explanation beyond those already given in ref. 3. (The square root is related to the symplectic nature of the problem.) Additional degeneracies arise in square systems and may accidentally appear also for specific aspect ratios $L_y/L_x$.

We next explain how to visualize a mode.

Fix $\xi = (p, q) \in X$, and let $\delta \xi$ be a Lyapunov mode of $T_X(\xi)$. The vector $\delta \xi = (\delta p, \delta q)$ has $4N$ components, $2N$ associated with the momenta and $2N$ with the positions. Consider, for example, the $q$ components, $\delta q_1, \ldots, \delta q_N$, where each $\delta q_j$ is in $\mathbb{R}^2$ (corresponding to the infinitesimal $x$ and $y$ displacements of $q_j$, $j = 1, \ldots, N$). By drawing the perturbation vectors $\delta q_j$ at the positions $q_j$ of the particles in the box, one obtains a field of vectors as is shown in Fig. 2. For dense enough fluids we obtain a vector field in every point of the box by interpolating between the particles.

It has been observed that for those Lyapunov exponents close to zero, this vector field is well approximated by trigonometric functions of the spatial coordinates $x$ and $y$. In particular, the number of nodes $(n_x, n_y)$ of the vector field determines a wave number $k_n$. We then say that $\delta \xi$ is a mode of wave number $k_n$. Our second main result is:

**Mode Classification:**
The subspaces $M_j(\xi)$ (defined in (1)) belonging to Lyapunov exponents $\lambda_j$ close to zero fall into two categories:

1. **Transverse branch:** modes associated with a Lyapunov exponent $\pm c_T k_n$ are divergence-free periodic fields of wave number $k_n$.

For both the longitudinal and transverse modes the linear $k$ dependence of $\lambda$ is only the first term of an expansion in powers of $k$,

\[ \lambda = ck_1 + c_2 k_2 + \cdots \] .

For positive $\lambda$, $c_2$ is positive, but small. For a second order calculation in $k$, see ref. 7.
Longitudinal branch: The modes associated with the Lyapunov exponents \( \pm c_L \) are of two types:

(i) Half of them are irrotational periodic vector fields of wave number \( k_n \) (called L-modes);
(ii) The others are scalar modulations with wave number \( k_n \) of the momentum field, (called P or momentum modes).

The L and the P-modes turn out to be paired: the P-mode has components \( p_i A(q_i) \) and the corresponding L-mode has components \( \nabla A(q_i) \), where \( A \) is a scalar function, see Eq. (9). In the following, we refer to an L-mode and its corresponding P-mode as an LP pair. We will give more details on this relation below. Results in this direction have been obtained in refs. 4, 6, 7.

An interesting question, which is related to some hydrodynamic aspects of the fluid, is an apparent propagation of the L and P-modes in physical space. It is a consequence of the motion of the tangent vectors in the subspaces \( M(j) \) (\( \xi_t \)), to which we refer as mode dynamics. It will be described in detail in Section 5. We note that this motion is not only determined by the tangent flow, but also by the re-orthonormalization process part of the algorithm for the simulation. Mode dynamics was observed early on, (2, 11) but attempts to compute the propagation velocities are still scarce and, at present, only work for low densities. (5, 7) Here, we give a more precise definition and provide numerical results.

Mode Dynamics: In an \( M(j) \) space of longitudinal and P-modes, the mode dynamics couples LP pairs.
Eckmann et al.

subspace spanned by a given LP pair, it reduces to a rotation at constant angular velocity \( \omega_n \) which is proportional to the wave number \( k_n \),

\[ \omega_n = v_k n, \]

where \( v \) has the dimension of a velocity.

In the remainder of the paper we state these results more precisely and give details about how they are obtained. They are of two types: First, a theoretical description of the modes, which is based on the symmetries of the system. Second, a detailed account of the numerical algorithms necessary to substantiate our claims (the difficulty being the decomposition of the \( d \) dimensional spaces \( M(j) \)).

3. TANGENT SPACE DYNAMICS

The dynamics of hard disks consists of phases of free flight interrupted by instantaneous elastic collisions. We denote the map for free flights of duration \( \tau \) by \( F_\tau \), and the collision map by \( C \). Then, the evolution of an initial state, \( \xi_0 \), is given by

\[ \xi_t = F_\tau n \circ \cdots \circ C \circ F_\tau 2 \circ C \circ F_\tau 1 \xi_0, \]

where \( \tau_1, \ldots, \tau_n \) are the time intervals between successive collisions. The tangent-space dynamics of an infinitesimal perturbation \( \delta \xi_0 \) of \( \xi_0 \) is given by the tangent map of the flow (3):

\[ \delta \xi_t = D F_\tau n \bigg|_{\xi_k} \cdot \cdots \cdot D C \bigg|_{\xi_{k-1}} \cdot D F_\tau 2 \bigg|_{\xi_{k-1}} \cdot D C \bigg|_{\xi_{k-2}} \cdot D F_\tau 1 \bigg|_{\xi_0} \delta \xi_0, \]

where \( \xi_{k-1} \) denotes the state just before the \( k \)th collision, and \( \xi_k = C(\xi_{k-1}) \) is the state immediately after.

Here, \( D F_\tau \bigg|_{\xi_k} \) and \( D C \bigg|_{\xi_k} \) are \( 4N \times 4N \) symplectic matrices. For the sake of simplicity, the flow is also called \( \Phi_t \) for

\[ \Phi_t(\xi_0) = \xi_t, \]

and we often write

\[ \delta \xi_t = D \Phi_t \bigg|_{\xi_0} \cdot \delta \xi_0. \]

By convention, if \( t \) is a collision time, \( \delta \xi_t \) denotes a tangent vector immediately before that collision.

We disregard problems of differentiability which appear for the (rare) tangent collisions.
3.1. Numerical Procedure and Lyapunov Modes

Extensive numerical simulations are used to establish the classification and dynamics of the modes. Here, we briefly summarize our algorithm described in detail in refs. 2,12 and provide a precise definition of the Lyapunov modes we observe. It is well known that the exponential growth rate of a typical $k$-dimensional volume element is given by

$$\lambda_1 + \cdots + \lambda_k,$$

where

$$\lambda_1 + \cdots + \lambda_k = \lim_{t \to \infty} \frac{1}{t} \log \|\delta \xi_1 t \wedge \cdots \wedge \delta \xi_k t\|.$$

If the tangent vectors $\delta \xi_1, \ldots, \delta \xi_k$ are linearly independent at time zero, they will remain so, because the tangent flow is time reversible. Orthogonality is not preserved by the tangent flow, because, generally, $D/Phi_1 t$ is not an orthogonal matrix. However, (4) still holds if the vectors $\delta \xi_1 t, \ldots, \delta \xi_k t$ are replaced by a (Gram-Schmidt) orthogonalized set of vectors $\delta \eta_1 t, \ldots, \delta \eta_k t$.

It takes thus the simpler form

$$\lambda_1 + \cdots + \lambda_k = \lim_{t \to \infty} \frac{1}{t} \sum_{i=1}^k \log \|\delta \eta_i t\|.$$

Since (5) holds for every $k \leq 4 N$, the exponent $\lambda_k$ turns out to be equal to the growth rate of the $k$th orthogonalized vector $\delta \eta_k t$.

Our study starts with the observation that we consider a system with non-trivial Lyapunov exponents. To guarantee the convergence of the numerical algorithm, additional properties of the dynamical system are needed: Namely, that the system has well-defined local stable and unstable subspaces associated with every Lyapunov exponent (close to zero).

$$\delta \eta_j t = \delta \xi_j t - \sum_{i=1}^{j-1} \frac{(\delta \xi_j t \cdot \delta \xi_i t)}{\|\delta \xi_i t\|^2} \delta \xi_i t.$$
Results in this direction have been obtained for hard-disk systems in refs. 15–17. A stronger property, hyperbolicity, has been recently proved for hard disk systems with randomly chosen masses in refs. 18–20. We assume here that these results hold for our system as well. As already advocated in ref. 10, what matters from a physicist's point of view is that the numerical studies behave as if this were true. Under the above assumptions, the \( k^{\text{th}} \) mode will align with the corresponding unstable subspace. In other words, measured modes will be orthogonal spanning sets of the \( M_{(j)} \) subspaces defined in Eq. (1).

The algorithm we use in our numerical work is based on the principles just outlined. We restrict our considerations to hard-disk systems without external interaction. Since there is no potential energy, the dynamics is the same at any (total) energy, up to a rescaling of time. The natural unit of time of the system is \( \left( \frac{m\sigma^2 N}{K} \right)^{1/2} \). Throughout, reduced units are used, for which the particle mass \( m \), the disk diameter \( \sigma \), and the kinetic energy per particle, \( K/N \), are unity. The density, defined by \( \rho = \frac{N}{V} \) and the aspect ratio, defined by \( A = \frac{L_y}{L_x} \), are the only relevant macroscopic parameters. Here, \( V = L_x L_y \) is the area of the (rectangular) simulation box whose sides are \( L_x \) and \( L_y \) in the \( x \) and \( y \) directions, respectively. All our numerical examples are for densities \( \rho \leq 0.8 \) characteristic of dense or dilute (if \( \rho \leq 0.1 \)) hard disk gases. The results are insensitive to the time between successive Gram-Schmidt re-orthonormalization steps.

3.2. Modes and Oseledec Subspaces

We have remarked in Section 2 that the spaces \( E_{(j)} \) of Oseledec' theorem are in general not identical to the spaces of the modes \( M_{(j)} \) defined in Eq. (1). Here, we explain this difference. The covariant subspaces \( E_{(1)}, \ldots, E_{(\ell)} \) of the Oseledec splitting are obtained as follows (10): the multiplicative ergodic theorem (for reversible systems) states that the matrices \( a f_{(\frac{\pi}{2})} \equiv \lim_{t \to \pm \infty} \left( \frac{D}{\Phi_1} \pm t \right)^{1/2} \) exist with probability one. The eigenvalues of \( a f_{(\frac{\pi}{2})}^{+} \) are \( \exp(\lambda(1)) > \cdots > \exp(\lambda(\ell)) \) and the eigenvalues of \( a f_{(\frac{\pi}{2})}^{-} \) are \( \exp(-\lambda(1)) > \cdots > \exp(-\lambda(\ell)) \). Since \( a f_{(\frac{\pi}{2})}^{+} \) and \( a f_{(\frac{\pi}{2})}^{-} \) are symmetric, their eigenspaces define two orthogonal decompositions of the tangent space \( TX = U_{(1)}^{\pm} \oplus \cdots \oplus U_{(\ell)}^{\pm} \).
where $U(j)\pm$ is the eigenspace of $\frac{\partial f_i}{\partial x_j}$ associated to $\exp(\pm \lambda(j))$. Note that the $U(j)$ subspaces are pairwise orthogonal but in general not covariant. However, for $j \in \{1, \ldots, \ell\}$, the subspaces $U(j)\oplus \cdots \oplus U(\ell)$ and $U(1)\oplus \cdots \oplus U(j)$ are covariant. They are, respectively, the subspace of the $\ell-j+1$ most stable directions of $f$ and the subspace of the $j$ most unstable directions of $f$. For every $\xi$, the invariant subspaces $E(j)$ are given by

$$E(j) = (U(1)\oplus \cdots \oplus U(j)) \cap (U(j)\oplus \cdots \oplus U(\ell)).$$

The $E(j)$ spaces are covariant but in general not orthogonal. One can show that

$$U(1)\oplus \cdots \oplus U(j) = E(1)\oplus \cdots \oplus E(j) \equiv F(j),$$

where $F(j)$ was introduced in Section 2. Using the definition (1), one easily verifies that $M(j) = U(j)$.\[\]

Remark 1. In our numerical method, the modes are obtained at the phase points $\Phi_t(\xi_0)$ for large $t$, i.e., at the end of integrated trajectories. It is therefore consistent that they should contain information about the past and not the future, that is about $U(\ell)$ and not $U(1)$.\[\]

In general, $U(1)$ and $U(\ell)$ are different. The projection theorem $U(1)\oplus U(\ell) = X$ follows from Theorem B.1.2. The set $U(1)$ and $U(\ell)$ are minimally different. It is clear that these subspaces are minimal.\[\]

Remark 2. In our numerical method, the modes are obtained at the phase points $\Phi_t(\xi_0)$ for large $t$, i.e., at the end of integrated trajectories. It is therefore consistent that they should contain information about the past and not the future, that is about $U(\ell)$ and not $U(1)$.
Two additional properties greatly simplify the classification of the modes:

1. Symplecticity of the tangent flow:
   \[ \frac{D}{\Phi_1} |_\xi J \frac{D}{\Phi_1} |_\xi = J, \]  
   where the $4N \times 4N$ matrix $J$ is defined as
   \[ J = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} \delta p \\ \delta q \end{pmatrix} = \begin{pmatrix} -\delta q \\ \delta p \end{pmatrix}. \]

2. Lyapunov exponents of Hamiltonian systems come in pairs $\lambda(j), \lambda(\ell - j + 1)$ of equal multiplicity. The matrix $J$ relates the $U(j) \pm$ subspaces by
   \[ U(j) \pm (\xi) = J U(\ell - j + 1) \pm (\xi). \]

Therefore, it is sufficient to measure the Lyapunov exponents and the modes for the positive part of the spectrum. Note that $J$ is not the (derivative of the) velocity reversal $\delta p, \delta q \mapsto -\delta p, \delta q$ and does not change the sign of time.

The simulations of our system exhibit an additional structure which considerably simplifies the analysis of Lyapunov modes near zero. Unstable perturbations ($\lambda > 0$) have the (approximate) form
   \[ \delta p = C(\xi, \lambda) \delta q, \quad C > 0, \]
   while the stable ($\lambda < 0$) perturbations are of the form
   \[ -C'(\xi, \lambda) \delta p = \delta q, \quad C' > 0. \]

Here, $C$ and $C'$ are numbers. In Figure 3 we demonstrate that the perturbations $\delta p$ and $\delta q$ associated with each Lyapunov mode are nearly parallel or anti-parallel for large $N$. Equation (7) also suggests $C = C'$, which is well verified by the simulations.

With the reduced units defined above, positions and velocities are dimensionless.
Fig. 3. Value of $\cos(\Theta_1) = (\delta q \cdot \delta p)/(|\delta q| \cdot |\delta p|)$, as a function of the Lyapunov index $l$ for an instantaneous configuration of the system characterized in Fig. 1. Here, $\Theta_1$ is the angle between the $2N$-dimensional vectors of the perturbation components of all particle positions and velocities for a Lyapunov vector $\xi_l$. For the small positive exponents, for which $l < 2N - 2 = 1558$, this angle vanishes, for the small negative exponents, for which $l > 2N + 3 = 1563$, it is equal to $\pi$. For the six zero modes, $1558 \leq l \leq 1563$, the angle lies between these limiting values.

We can therefore center our attention on the log part of the reality coordinates, or perhaps equivalently, we are essentially omitting the term of one particular direction. For the small positive exponents, this is just a particular coordinate system for the small negative exponents.

### 3.4. Tangent Vectors as Vector Fields

The components of a tangent vector $\delta \xi = (\delta p, \delta q)$ are the perturbation components of the positions and velocities of all particles. As a graphical representation of such a vector, we show in the left panel of Fig. 4 the instantaneous positional perturbations of all particles at their positions in physical space, where the arrows indicate the directions and strengths. It belongs to a Lyapunov exponent $\lambda_{1546}$ indicated by the enlarged circle in Fig. 5. A qualitatively identical figure is obtained, if the positional displacements of all particles are replaced by their momentum displacements, as explained in Section 3.3. Thus, this figure is a complete representation.
Fig. 4. The transverse mode $T(1,1)$ for $\lambda = 1546$ of Fig. 5. Left: Interpretation as a vector field; Right: Alternative representation as periodic spatial patterns of the position perturbations $\delta x_i$ and $\delta y_i$ of the particles, which emphasizes the wave vector parallel to a diagonal of the simulation box.

Fig. 5. Lyapunov spectrum and "dispersion relations" for the 780-disk system characterized in Fig. 1, and the density $\rho = 0.8$. Left: Lyapunov exponents are ordered by size and repeated with multiplicities. The specially marked point corresponds to the transverse mode shown in Fig. 4. Right: Lyapunov exponents as a function of their wave number. The respective labels $L$ and $T$ refer to the longitudinal and transverse branches.

The transverse modes for $\lambda = 1549$ on the left panel of Fig. 2, and for $\lambda = 1548$ at the bottom left panel of Fig. 6, are other examples of transverse modes belonging to the same degenerate exponent.

We interpret the left panel of Fig. 4 as a two-dimensional vector field $\phi$ which – up to a constant phase – is well described by:

$$
\left( \begin{array}{c}
\phi_x(x,y) \\
\phi_y(x,y)
\end{array} \right) = \left( \begin{array}{c}
\alpha_1 \cos(k_x x) \sin(k_y y) \\
-\alpha_2 \sin(k_x x) \cos(k_y y)
\end{array} \right),
$$
Fig. 6. Snapshots of Lyapunov modes for the periodic 780-disk system of Section 4. Left, from top to bottom: Transverse modes T(1,0), T(0,1), and T(1,1) belonging to $\lambda_{1557}$, $\lambda_{1555}$, and $\lambda_{1548}$, respectively, of Fig. 5. Right, from top to bottom: Vector fields for longitudinal modes, which belong to the LP pairs LP(1,0), LP(0,1), and LP(1,1), and which are associated with the respective exponents $\lambda_{1553}$, $\lambda_{1545}$, and $\lambda_{1535}$, of Fig. 5.
where \( k_x = 2\pi L_x \) and \( k_y = 2\pi L_y \), and \( \alpha_1, \alpha_2 \) are two constants. For this reason, we assign the node numbers \((n_x, n_y) = (1, 1)\) to this mode.

To be more precise, let \( r = (x, y) \in [0, L_x) \times [0, L_y) \). We say that a two-dimensional smooth vector field \( \phi = (\phi_x, \phi_y) \) over the position space, is sampled by the infinitesimal displacements \( \delta q \) of the \( N \) disks at their reference positions \( q \), when \( \phi(q_j) = \delta q_j \), for all \( j = 1, \ldots, N \).

Thinking of a tangent vector in terms of an associated vector field is meaningful if there are “sufficiently” many particles to sample the field on a typical length scale of its variation. Once this condition breaks down for larger exponents, as it will for large-enough \( k \), the modes disappear, and so do the steps in the Lyapunov spectrum. In the following we use a notation which does not distinguish between tangent vectors and their two-dimensional vector fields.

4. OBSERVATION AND DESCRIPTION OF THE MODES

In this section, we describe the Lyapunov spectrum near 0 and the corresponding modes, as they are measured in numerical experiments. In the two following subsections, we will explain how these modes can be understood on the basis of symmetry breaking of “zero modes”. We illustrate our assertions with the system already introduced in Fig. 1, which contains \( N = 780 \) particles in a rectangular periodic box with an aspect ratio \( L_y / L_x = 0.867 \). It corresponds to a hard-disk gas with a density \( \rho = 0.8 \), slightly below the fluid-to-solid phase transition density.

The left panel of Fig. 5 provides a magnified view of the smallest positive Lyapunov exponents for this system. The exponents, ordered by size and repeated with their multiplicities, are plotted as a function of their index. Degenerate exponents with a multiplicity \( d \geq 2 \) appear therefore as “steps”.

To account for the wave-like appearance of the modes, we associate with each Lyapunov vector a wave number \( k(n_x, n_y) \), as in (2), where the non-negative integers \( n = (n_x, n_y) \) count the nodes in the respective directions. When the small Lyapunov exponents are plotted as a function of their corresponding wave number, they all lie on two curves, sometimes referred to as “bands”.

For the sampled vector field is ill-defined.

The conjugate negative exponents are not shown, see refs. 2, 8.

In many cases, the number of nodes is easy to determine, as in Fig. 4. To facilitate an objective identification of the wave vectors modes associated with larger exponents, which are noisier, Fourier-transforms are used.
Table I. Central Subspace for the Vanishing Lyapunov Exponents. Notation: \(1 = (1, 1, \ldots, 1), \) and \(0 = (0, 0, \ldots, 0).\) All vectors have 4 \(N\) components.

Transformation Generator

\[(p, q) \mapsto (p^x + \varepsilon_1, p_y, q^x, q_y)\delta \xi_1 = (1, 0, 0, 0)\]

\[(p, q) \mapsto (p^x, p_y + \varepsilon_1, q^x, q_y)\delta \xi_2 = (0, 1, 0, 0)\]

\[(p, q) \mapsto (p^x, p_y, q^x + \varepsilon_1, q_y)\delta \xi_3 = (0, 0, 1, 0)\]

\[(p, q) \mapsto (p^x + \varepsilon p^x, p_y + \varepsilon p_y, q^x, q_y)\delta \xi_4 = (0, 0, 0, 1)\]

\[(p, q) \mapsto (p^x, p_y, q^x, q_y + \varepsilon p_y)\delta \xi_5 = (p^x, p_y, 0, 0)\]

\[(p, q) \mapsto (p^x, p_y, q^x, q_y + \varepsilon p_y)\delta \xi_6 = (0, 0, p^x, p_y)\]

Note that in the table, \(\delta \xi_i\) represents a vector transformation that is induced by the symmetries of the system. The zero modes play a fundamental role in understanding the nature of the modes associated with Lyapunov exponents close to zero.

Remark 2. The space \(N(\xi)\) can be further decomposed into three covariant subspaces:

\[N_x = \text{Span}\{\delta \xi_1, \delta \xi_3\}, \]

\[N_y = \text{Span}\{\delta \xi_2, \delta \xi_4\}, \]

\[N_p = \text{Span}\{\delta \xi_5, \delta \xi_6\}.\]
Span \{\delta \xi_5, \delta \xi_6\}, each of which independently satisfies the properties listed for \(N(\xi)\). In systems with reflecting boundaries, only \(N_p\) is present, while \(N_x\) and \(N_y\) are absent, because they are related to translation invariance.

If only the \(x\) direction is periodic, (6) the space of zero modes is reduced to \(N_x \oplus N_p\).

### 4.2. Longitudinal, Transverse and P-Modes

Following our argument of Section 3.3, we need only describe the \(\delta q\) part of the modes. Therefore, we consider the three transformations (see Table I):

- \(\delta \xi_3: (q_x,j, q_y,j) \mapsto (q_x,j + \varepsilon, q_y,j)\)
- \(\delta \xi_4: (q_x,j, q_y,j) \mapsto (q_x,j, q_y,j + \varepsilon)\)
- \(\delta \xi_6: (q_x,j, q_y,j) \mapsto (q_x,j + \varepsilon p_x,j, q_y,j + \varepsilon p_y,j)\),

associated to zero modes, and claim the following:

**Modes Classification I:** Modes of wave number \(k_n\) are scalar modulations of (8) with wave number \(k_n\). More precisely, they are obtained by replacing \(\varepsilon\) with \(\varepsilon A(q_x,j, q_y,j)\) in (8), where the real scalar function \(A\) is of the form

\[
A(x,y) = \sum_{|\ell| = n_x, |m| = n_y} c_{\ell,m} e^{i(\ell k_x x + m k_y y)}.
\]

The space of such modulations has dimension 4 in general and dimension 2 if either \(n_x\) or \(n_y\) vanishes.

**Example 1.** We consider \(n = (1,0), (0,1),\) and \((1,1)\). We use the notation \(c_x = \cos (k_x x), \sin (k_x x), c_y = \cos (k_y y), \sin (k_y y)\). A basis of the space of functions with wave number \(k_n\) is shown in Table II.

| Function | dim |
|----------|-----|
| \(c_x\), \(s_x\) | 2 |
| \(c_y\), \(s_y\) | 2 |
| \(c_x c_y, s_x s_y\) | 4 |

Of course, this choice fixes a constant phase for the sine and cosine functions.
If the Lyapunov exponent were a function of \( k_n \) only, we would expect 12-fold degeneracy in Fig. 5, (resp. 6-fold if either \( n_x \) or \( n_y = 0 \)), since each of the three perturbations of (8) can be modulated by the four (resp. two) functions of Table II. However, this degeneracy is broken into an 8 + 4 (resp. 4 + 2) structure:

**Mode Classification II:**

The Lyapunov vectors of wave number \( k_n \) have two possible Lyapunov exponents:

\[ |\lambda| = c_T |k_n| \text{ or } |\lambda| = c_L |k_n| \]

corresponding to the Transverse or Longitudinal branch of Fig. 5. The modes for these two branches are obtained as follows:

(1) **Transverse branch:** transverse modes are obtained by combining the modulations of \( \delta_3 \) and \( \delta_4 \) in a divergence-free vector field. We denote by \( T(n) \) the space of such vector fields.

(2) **Longitudinal branch:**
   (i) Longitudinal modes are irrotational vector fields one obtains by combining the modulations of \( \delta_6 \) and \( \delta_7 \). We denote the corresponding space by \( L(n) \).
   (ii) **P-modes** are modulations of \( \delta_8 \), and we denote the corresponding subspace by \( P(n) \).

The three subspaces \( T(n), L(n), \) and \( P(n) \) have dimension 4 (or dimension 2 if either \( n_x \) or \( n_y \) vanishes). We denote by \( LP(n) \equiv L(n) \oplus P(n) \) the subspace corresponding to the Longitudinal branch. It has dimension 8 (4 if either \( n_x \) or \( n_y \) vanishes).

**Remark 3.** The divergence and curl of a vector field \( \mathbf{v} = (v_x, v_y) \) are, of course,

\[ \nabla \cdot \mathbf{v} = \frac{\partial v_x}{\partial x} + \frac{\partial v_y}{\partial y}, \quad \nabla \times \mathbf{v} = \frac{\partial v_y}{\partial x} - \frac{\partial v_x}{\partial y}. \]

Since every two-dimensional vector field uniquely decomposes into a sum of a divergence-free and an irrotational vector field, the spaces \( L(n) \) and \( T(n) \) span all possible two-dimensional vector fields of wave number \( k_n \).

There is a simple way to build \( P(n), L(n), \) and \( T(n) \) from the scalar modulations of Table II. If \( A \) is a modulation of wave number \( k_n \), we have

\[ pA \in P(n), \quad \nabla A \in L(n), \quad \nabla \times A \in T(n), \quad (9) \]
\[ \nabla A = \left( \frac{\partial x}{\partial x} A \frac{\partial y}{\partial y} A \right), \]
\[ \nabla \wedge A = \left( \frac{\partial y}{\partial x} A - \frac{\partial x}{\partial y} A \right). \]

This construction is also useful because it naturally defines what we shall call LP pairs, by which we denote a field of \( L(n) \) and a field of \( P(n) \) originating from the same scalar modulation, as in (9). We show below that LP pairs play an important role. Indeed, when only some of the modes are present because of the boundary conditions, LP pairs are never broken: both fields are present, or both are missing (see Section 4.3). We shall also see in Section 5 that the dynamics of the modes mostly takes place between LP pairs.

Example 2. For the three modes of lowest wave number, Table III lists a basis of \( T(n), L(n) \) and \( P(n) \). Fields are given in a non-normalized form to keep notation short. Corresponding \( L(n) \) fields and \( P(n) \) fields are LP pairs. Figure 6 provides examples for T- and L-modes.

Modes of \( L(n) \) and \( T(n) \) are wavelike perturbations of the position space, and, therefore, are similar to the modes that appear in hydrodynamics (see Section 7). In particular, when either \( n_x \) or \( n_y \) vanish, the fields of \( L(n) \) and \( T(n) \) are, respectively, longitudinal and transverse to the wave vector. This observation is the reason for the names of the two branches in Fig. 5. To stay in line with this now-accepted terminology, we keep it also for the case \( n_x \cdot n_y \neq 0 \). P-modes are more complex than the other modes, because they depend not only on the positions of the perturbed particles but also on their velocities.

| Basis of \( T(n) \) | Basis of \( L(n) \) | Basis of \( P(n) \) |
|-----------------|-----------------|-----------------|
| \((1,0)\)       | \((0,0)c_x, (0,0)s_x\) | \((0,0)c_x, (0,0)s_x\) |
| \((0,1)\)       | \((0,0)c_y, (0,0)s_y\) | \((0,0)c_y, (0,0)s_y\) |
| \((1,1)\)       | \((1,0)k_x c_x s_y - (0,0)k_y s_x c_y\) | \((1,0)k_x c_x s_y - (0,0)k_y s_x c_y\) |

Table III. Decomposition of \( n \)-Modes for Rectangular Systems with Periodic Boundaries
At this point we are able to characterize the spectrum and its multiplicities with only two constants, \(c_L\) and \(c_T\), which have the physical dimension of velocities. We shall see in Section 6 that these velocities depend on the density of the system, but are insensitive to the system size, the boundary type, and the aspect ratio. Therefore, it is tempting to think of \(c_L\) and \(c_T\) as thermodynamic velocities. However, as discussed in Section 6, no obvious interpretation could be found so far.

4.3. Other Aspect Ratios and Boundary Conditions

In this section, we summarize some observations which concern different boundary conditions and degeneracies.

(i) The Lyapunov spectrum is more degenerate for square systems, for which \(k(n_x, n_y) = k(n_y, n_x)\). In this case the multiplicities are doubled with respect to the general case, for which \(n_x \neq n_y\). Other "accidental" degeneracies may occur: for instance, parameters can be found for which \(c_T|_{k(1,1)} = c_L|_{k(1,0)}\).

(ii) Systems with reflecting boundaries develop only a subset of the modes encountered so far, which can be found by the following simple, and obvious, rules:

• The fundamental wave vectors are \(k_x = \pi L_x\) and \(k_y = \pi L_y\) (not \(2\pi L_x\)). Here, \(L_x\) and \(L_y\) are the effective box sizes, obtained from the actual side lengths by subtracting one particle diameter \(\sigma\).

• The fields of \(T(n)\) and \(L(n)\) have to satisfy Dirichlet conditions, namely to be tangent to the boundary:

\[
\phi_x(0,y) = \phi_x(L_x,y) = 0 \quad \text{and} \quad \phi_y(x,0) = \phi_y(x,L_y) = 0
\]

If expressed in terms of sines and cosines, this means that \(\phi_x\) may contain \(\sin(k_x x)\) but not \(\cos(k_x x)\), and so on.

• As for periodic boundary conditions, when an L-mode is present, its paired P-mode is always present.

(iii) Hybrid systems with reflecting boundaries in one direction and periodic boundaries along the other behave as expected:

(6) the fundamental wave vectors are chosen according to the boundary type, and the Dirichlet conditions are only applied to one component of the field.
### Table IV. Mode Decomposition for Rectangular Systems with Reflecting Boundaries

| n  | Mode Description                  | L(nx,0) | T(nx,0) |
|----|-----------------------------------|---------|---------|
| (1,0) | none                              |         |         |
| (0,1) | none                              |         |         |
| (1,1) | \(s_x c_y - c_x s_y\)\((s_x c_y c_x s_y)\) |         |         |

#### Remarks
- Only develop modes with \(n_y = 0\).

**Example 3.** Table IV shows which modes of Table III satisfy the Dirichlet condition and are thus present in a system with reflecting boundaries.

- We stress that such a system has only two vanishing Lyapunov exponents which are associated with \(\delta \xi_5\) and \(\delta \xi_6\) of Table I. Therefore, modes appear which are not modulations of zero modes of the system.

**Systems with reflecting boundaries and narrow systems.** Systems with reflecting boundaries and narrow systems are easier to study numerically, because the multiplicities of the L, P and T spaces are smaller than in the periodic rectangular case. In particular, the LP(1,1) space has only dimension 2 when the boundaries are reflecting. For that reason, we illustrate some of the issues below also with the "reflecting-wall version" of the 780-disk system introduced in Fig. 8.
4.4. How to Measure P-Modes

Contrary to $L(n)$ and $T(n)$, the tangent subspace $P(n)$ depends on the state that it perturbs. Moreover, modes of $P(n)$ are not really vector fields, because the velocities of the particles in a typical configuration do not depend smoothly on position. In order to "see" a P-mode, we face two problems:

(i) A typical measured vector of an LP($n$) space is a superposition of vectors of $L(n)$ and $P(n)$.

(ii) Even when a mode of $P(n)$ is isolated, it is not smooth and does not "look like" a vector field over the box.

We explain our solution to the first problem with the simplest possible example: the LP($1$,$0$) space for a rectangular system with reflecting boundaries (see Section 4.3). This space has dimension two and is defined by the two normalized spanning vectors

$$\phi_L = (\phi_L^x, \phi_L^y) = (1, 0),$$
$$\phi_P = (\phi_P^x, \phi_P^y) = (\pi L^x, 0),$$

where $z_1$ and $z_2$ are normalization constants. At any time $t$, we have two measured modes, $\psi_1$ and $\psi_2$ (vectors with $2N$ components, since only the $\delta q$ part is observed), whose span is (numerically very close to) LP($1$,$0$).

Therefore, there are constants $a$, $b$, $c$, $d$ with

$$\phi_L = \psi_1 a + \psi_2 b,$$
$$\phi_P = \psi_1 c + \psi_2 d.$$  

Since all these vectors are normalized, one should also have $a^2 + b^2 = c^2 + d^2 = 1$. However, Eq. (11) is over-determined: four constants have to satisfy $4N$ equations. Numerically, we use a least-square method to find the best values for $a$, $b$, $c$, $d$, which we denote by $\alpha$, $\beta$, $\gamma$, $\delta$.

Thus, the measured modes, $\psi_1$ and $\psi_2$, are decomposed according to

$$\tilde{\phi}_L = \psi_1 \alpha + \psi_2 \beta,$$
$$\tilde{\phi}_P = \psi_1 \gamma + \psi_2 \delta.$$
where the vectors $\tilde{\phi}_L$ and $\tilde{\phi}_P$ are the best-possible LP-pair, $\phi_L$ and $\phi_P$, reconstructed from experimental data.

Now we can deal with our second problem: whereas the vector $\tilde{\phi}_L$ is easily recognized as a vector field, the vector $\tilde{\phi}_P$ is not. However, from (10) we deduce that

\[
(\phi_P x/p x \phi_P y/p y) = (c x c_x),
\]

or, more precisely,

\[
(\phi_P x,j/p x,j \phi_P y,j/p y,j) = (\cos(k x q_{x,j}) \cos(k x q_{x,j})), j = 1, \ldots, N.
\]

Therefore, both $\phi_P x/p_x$ and $\phi_P y/p_y$ are smooth functions and can be easily visualized.

Remark.

(i) This procedure readily extends to higher-dimensional LP spaces, for instance to the four-dimensional LP $n_1 = 1$ space of a periodic system. We take this case as an example to illustrate in Fig. 7 our method of mode reconstruction: from the four measured modes the analogue to Eq. (11) generates four spanning vectors, namely two L-modes (one of which is shown at the top-right position of Fig. 4) and two P-modes. The $x$ and $y$ components of one of the P-modes, namely $\tilde{\phi}_P x, y \approx p_{x,y}$, are shown in the top row of Fig. 7. No smooth functions are recognized. However, after dividing by the momentum components, $p_x,j$ and $p_y,j$, as required by (12), the figures for the fields $\tilde{\phi}_P x/p_x$ and $\tilde{\phi}_P y/p_y$ in the bottom row of Fig. 7 clearly display the expected $s_x$-dependence.

(ii) Division by $p_x,j$ or $p_y,j$ in (12) is numerically unstable when particle $j$ has a very small momentum along a coordinate axis. We avoid this by multiplying instead by $p_x,j/(p_x^2 + \epsilon)$, where $\epsilon \ll 1$. One could also ignore particle $j$ in this case and only sample the field at those points where both $p_x,j$ and $p_y,j$ are not too small.

5. DYNAMICS OF THE MODES

Remark.

The interested reader can look up animated pictures on the web at the address http://theory.physics.unige.ch/modes/.

In this section we turn to the "dynamics of the modes" and study what has been called the velocity of the longitudinal modes. This might clarify hydrodynamic theories, which are mostly based on a partial classification of the modes. In numerical simulations, the transverse...
Fig. 7. Example for the P-mode reconstruction for the four-dimensional LP(1,0) space of a system with periodic boundaries. Only half of the components are shown, namely those corresponding to $s_x$. The $c_x$ components are similar. Top row: the fields $\tilde{\phi}_P / p_x$ and $\tilde{\phi}_P / p_y$ are wavelike again. Note that in the top row one can recognize the sinusoidal envelope.

modes are stationary in space and time: although the particles move, the vector field of the mode does not. In other words, the vector field of an S-mode does not move: it is a fixed point in Eulerian space.

For longitudinal modes, however, one seems to observe a propagation in the direction of the wave vector.

Using the geometrical picture developed above, we can interpret this motion and explain why no propagation is observed for the LP dynamics in systems with reflecting boundaries as demonstrated in Fig. 8 below. Since multiplicities are not so essential here, we illustrate the interpretation for the (simpler) LP($1,1$) space of a rectangular system with reflecting boundaries (dimension 2). In Section 4.4 we pointed out that any

When either $n_x$ or $n_y$ vanish, for instance in the L($1,0$) or L($0,1$) space.
Fig. 8. LP(1,1) dynamics for a system of 780 disks in a box with an aspect ratio 0.867, a density 0.8, and with reflecting boundaries. Left: coordinates of the measured fields in the "standard basis" of LP(1,1). The (unit) circle is nearly reached, showing that indeed $\psi_1$ and $\psi_2$ span the same subspace as $\phi_L$ and $\phi_P$. Center and right: the measured fields $\psi_1(t)$ and $\psi_2(t)$. The rows from top to bottom are consecutive snapshots separated by time steps of $t = 3 \times 20$, which corresponds to a phase shift of $\pi/2$ in the LP(1,1) rotation. (A color figure is available online.)
Lyapunov Modes in Hard-Disk Systems

Given time \( t \), the state is \( \xi_t \), where the measured modes \( \psi_1(t) \) and \( \psi_2(t) \) are combinations of the two spanning vectors \( \phi_L(\xi_t) \) and \( \phi_P(\xi_t) \).

We write Eq. (11) in matrix form, but now with explicit time dependence:

\[
(\phi_L(\xi_t), \phi_P(\xi_t)) = (\psi_1(t), \psi_2(t)) \cdot Q(t),
\]

where \( Q(t) = \begin{pmatrix} a(t) & b(t) \\ c(t) & d(t) \end{pmatrix} \).

Therefore, the dynamics of the modes reduces to that of the \( 2 \times 2 \) matrix \( Q(t) \). In our simulations we keep the spanning vectors orthonormal. Since (in the experiment) the two fields \( \phi_L \) and \( \phi_P \) are also (nearly) orthogonal, the matrix \( Q(t) \) is close to a rotation matrix (that is \( c \approx -b \), \( d \approx a \), and \( a^2 + b^2 \approx 1 \)). Therefore, the dynamics in the two-dimensional subspace is well described by a phase \( \phi(t) = \arctan(b(t)/a(t)) \).

LP-dynamics in 2 dimensions: The matrix \( Q(t) \) is a rotation with constant angular velocity \( \omega_n \). This velocity is proportional to the wave number \( k_n \), namely \( \phi(t) = \omega_n t = \nu k_n t \).

Here, \( \nu \) is the product of a frequency and a wavelength and describes a velocity. According to the simulations, \( \nu \) depends only on the density of the system.

Example 4. In Fig. 8 we demonstrate this rotation in the LP(1,1) space of a system with reflecting boundaries. Snapshots of the two measured fields at consecutive times show the rotation of the two vectors between the L and the P direction.

A similar rotation has been found in narrow systems in ref. 6 and explained in refs. 5, 7 in the low density limit using a Boltzmann-equation approach.

Remark 4. The velocity \( \nu = \omega_n / |k_n| \) has been interpreted earlier as the phase velocity of a traveling wave in physical space. In Appendix A we demonstrate how the two interpretations can be reconciled. The definitions given above allow us to apply the same concepts also to the LP-dynamics of systems with reflecting boundaries, although they do not show traveling but standing waves.

The scalar product \( \phi_L \cdot \phi_P = \mathcal{O}(1) \) a priori does not vanish. However, as the simulations show, it is of the same order as \( \mathcal{O}(1) \), which is also small and non-vanishing due to the uneven spacing of the particles.
Next, we consider the dynamics for the general case of a 2\textsuperscript{d}-fold degenerate LP space. As explained in Section 4, an LP space is defined by a spanning set of \(d\) longitudinal modes, \(\phi_{L1}, \ldots, \phi_{Ld}\), and \(d\) P-modes, \(\phi_{P1}, \ldots, \phi_{Pd}\), where each pair \((\phi_{Lk}, \phi_{Pk})\) is an LP pair. The following description is valid for any type of boundary conditions.

**Dynamics in LP\((n)\).** The dynamics in LP\((n)\), when restricted to a two-dimensional subspace spanned by an LP pair \(\text{Span}\{\phi_{Lk}, \phi_{Pk}\}\), is a two-dimensional rotation at a constant angular velocity \(\pm \omega_n\), where \(\omega_n = \frac{v_k}{\lambda_n}\), with \(v\) independent of \(n\).

**Example 5.** The LP dynamics for higher-dimensional spaces is illustrated in Fig. 9. In the following we concentrate on LP\((1,1)\). This space has dimension 8, that is four LP pairs. Generically, a measured mode has a non-vanishing projection onto all four LP pairs, and four different phases can be defined. The four time series of phases for LP\((1,1)\) in Fig. 9 belong to different projections of the same mode.

## 6. INFLUENCE OF GEOMETRY AND SYSTEM SIZE

In this section, we study how changes in the density, aspect ratio, and boundary conditions affect \(c_T\), \(c_L\), and \(v\). The influence of the density is examined in Section 5, and the aspect ratio in Section 6. The boundary conditions are described in Section 3.
Fig. 10. Slopes of the transverse and longitudinal branches $c_L$ and $c_T$ of Fig. 5, and of phase velocity $v$. The simulations are for a system containing $N = 780$ particles in a rectangular periodic box with a fixed aspect ratio $L_y/L_x = 0.867$.

Left: $c_L$ and $c_T$ as a function of the particle density $\rho$. The smooth lines are polynomial fits added to guide the eyes. Although the fits have no theoretical basis, we provide the fit parameters for convenience:

$$c_L = 0.790 + 0.970 \rho + 0.785 \rho^2 + 6.24 \rho^4$$

$$c_T = 0.902 + 1.050 \rho - 0.053 \rho^2 + 3.85 \rho^4$$

Right: Almost linear relations between all three quantities. There are two observations which are of interest: First, as seen in the left panel, $c_T$ and $c_L$ cross for lower densities. Thus, the intuitively natural conjecture, $c_L \geq c_T$, is not supported by the numerical evidence. Second, the three "velocities" $c_L$, $c_T$, and $v$ are almost linearly related. In particular, the phase velocity $v$ agrees rather well with $c_L$ for fluid densities $\rho < 0.6$ (see the full line in the right panel of Fig. 10), thus lending support to referring to the curves $\lambda(k)$ as "dispersion relations".

On the left panel of Fig. 11 we plot the longitudinal and transverse dispersion relations for a moderately-dense gas with a density $\rho = 0.4$. The full and open points are for systems with periodic and reflecting boundaries, respectively. In all cases, $\lambda$ was determined from the lowest step of the Lyapunov spectrum for the system, for which the aspect ratio varied between 0.5 and 1, and the particle number between 400 and 800. The figure demonstrates that periodic and reflecting boundary conditions give the same $\lambda(k)$. We have experimentally verified (but not shown here) that the same is true also for larger and lower densities.

The situation becomes a little more complicated when we consider the dependence of the slopes, $c_L$ and $c_T$, on the aspect ratio $A$. This is addressed in Fig. 12, which shows that the slopes, $c_L$, $c_T$, and $v$, vary smoothly with $A$.

However, the slopes do not vary smoothly with $A$ when we consider the dependence of the slopes, $c_L$, $c_T$, and $v$, on the aspect ratio $A$. This is addressed in Fig. 12, which shows that the slopes, $c_L$, $c_T$, and $v$, vary smoothly with $A$. The slopes are determined from the lowest step of the Lyapunov spectrum for the system, for which the aspect ratio varied between 0.5 and 1, and the particle number between 400 and 800. The figure demonstrates that periodic and reflecting boundary conditions give the same $\lambda(k)$. We have experimentally verified (but not shown here) that the same is true also for larger and lower densities.

As we mentioned earlier, the slopes do not vary smoothly with $A$. This is addressed in Fig. 12, which shows that the slopes, $c_L$, $c_T$, and $v$, vary smoothly with $A$. The slopes are determined from the lowest step of the Lyapunov spectrum for the system, for which the aspect ratio varied between 0.5 and 1, and the particle number between 400 and 800. The figure demonstrates that periodic and reflecting boundary conditions give the same $\lambda(k)$. We have experimentally verified (but not shown here) that the same is true also for larger and lower densities.

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Fig. 11. Simulation results for a hard-disk gas with a density $\rho = 0.4$. The full and open points refer to periodic and reflecting boundary conditions, respectively. Left: The smallest positive Lyapunov exponent for $T$- and $L$-modes, respectively, as a function of the wave-number $k$. The curves for periodic and reflecting boundary conditions agree. To the second order in $k$, a fit to the data gives $c_L = 1.422 k + 0.55 k^2$ and $c_T = 1.412 k + 0.086 k^2$. Right: The slopes, $c_L$ and $c_T$, are plotted as a function of the aspect ratio $A$ of the simulation box. For a given $A$ we compare points with the same $k$ to eliminate the influence of the nonlinearity of the dispersion relations. This means that for periodic boundaries the linear extensions of the simulation box, $L_x$ and $L_y$, are twice those of the respective reflecting box. The data for periodic and reflecting boundaries agree to within numerical accuracy. The right panel of Fig. 11. The dispersion curves are not strictly linear in $k$ and non-gradual for small $A$, as we have pointed out already in a footnote in Section 2. A fit to the points in the left panel of Fig. 11 reveals that the term proportional to $k^2$ is much larger for $L$ than for $T$. To eliminate this nonlinearity in a comparison of the slopes for reflecting and periodic systems with a given $A$, modes with the same values for $k^2$ are used in the right panel of Fig. 11. With this precaution the figure demonstrates that the slopes of the dispersion relations do not depend on the boundary conditions in any significant way, as long as the box does not degenerate to a narrow channel.

7. HYDRODYNAMIC EQUIVALENT OF THE MODES

There is a general expectation that the Lyapunov modes should be related to the hydrodynamic behavior of the system, and several papers have attempted to establish this connection. However, the dispersion curves are not strictly linear in $k$, and non-gradual for small $A$, as we have pointed out already in a footnote in Section 2. A fit to the points in the left panel of Fig. 11 reveals that the term proportional to $k^2$ is much larger for $L$ than for $T$. To eliminate this nonlinearity in a comparison of the slopes for reflecting and periodic systems with a given $A$, modes with the same values for $k^2$ are used in the right panel of Fig. 11. With this precaution the figure demonstrates that the slopes of the dispersion relations do not depend on the boundary conditions in any significant way, as long as the box does not degenerate to a narrow channel.
Table V. Modulations of the Hydrodynamic Fields (Multiplicative Constants are Omitted)

| mode | \( \delta \xi \) | \( \delta \rho \) | \( \delta u \) | \( \delta E \) |
|------|-----------------|----------------|-------------|-------------|
|      | \( \nabla \wedge \mathbf{A} \) | \( \nabla \wedge \mathbf{A} \) | \( \nabla \wedge \mathbf{A} \) | \( \nabla \wedge \mathbf{A} \) |

point in this direction. \((3–6)\)

It should be noted, however, that none of these studies has reached a totally convincing interpretation, and, furthermore, it is obvious from this body of work that the LP-modes are more difficult to explain than the \( T \)-modes. Here, we add to this a simple calculation which might be helpful in the future: we determine how the modes perturb the hydrodynamic fields or, in other words, what would be the hydrodynamic equivalent of the modes we measure. The results, given in Table V, have quite a simple form, but do not reproduce the usual modes of hydrodynamics.

Consider a general transformation \( T \) of the one-particle phase space \( \mu \equiv [0, L_x) \times [0, L_y) \times \mathbb{R}^2 \) given by

\[
T: \begin{array}{c}
\mathbf{r} \mapsto \mathbf{r}' = \mathbf{r} + \epsilon \delta \xi \nabla \mathbf{r} \\
\mathbf{v} \mapsto \mathbf{v}' = \mathbf{v} + \epsilon \delta \eta \mathbf{v}
\end{array}
\]

and \( \epsilon \) is probability density, see \( \mathbb{B} \). If \( \mathbf{f} \) is Boltzmann, then the new probability density is

\[
\mathbf{f}' = \mathbf{f} + \epsilon \delta \mathbf{f} = \mathbf{f} - \int \delta \mathbf{f} g(\mathbf{r}, \mathbf{v})
\]

where \( g(\mathbf{r}, \mathbf{v}) = \nabla \mathbf{r} \cdot \delta \xi + \mathbf{v} \cdot \delta \eta \).

We define the variations of the three hydrodynamic fields (density \( \rho \), momentum \( u \), and energy \( E \)) by

\[
\begin{align*}
\delta \rho &= \int \delta \mathbf{f} d^3 \mathbf{v} \\
\delta u &= \int \delta \mathbf{f} \mathbf{v} d^3 \mathbf{v} \\
\delta E &= \int \delta \mathbf{f} |\mathbf{v}|^2 d^3 \mathbf{v}
\end{align*}
\]

*With \( k_B T = 1 \) as in the simulations.*
For each of the three types of modes, one can compute these quantities as a function of the scalar modulation $A$ introduced in (9). The results are given in Table V. Since $\delta \rho = -k^2 n A$, we note that the scalar fields $\delta \rho$ and $\delta E$ are proportional to the initial scalar modulation $A$. Note also that the energy field is only affected by the L and P-modes but not by the T-mode.

8. CONCLUSIONS

The picture developed in this paper is for two-dimensional hard disks, but the method is sufficiently geometric and general to allow easy extensions to other systems: For example, the generalization to three-dimensional hard disks is straightforward. The existence of L- and T-modes for this case has been confirmed by computer simulation. (25) Recently, Lyapunov modes were also found for two-dimensional soft-particle systems interacting either with a Weeks-Chandler-Anderson potential (26) or a Lennard–Jones potential. (27, 28) It would also be interesting to extend the work to, say, circular geometries. Another extension concerns linear molecules such as hard dumbbells in a periodic box. (1, 11) In this case two qualitatively different degrees of freedom play a role, translation and rotation. The existence of modes has already been demonstrated in this case.

We have ended our wanderings through the rich landscape of Lyapunov modes. To summarize, we have carefully identified and analyzed the modes, giving a beginning of a theoretical classification. Furthermore, we have seen that the Lyapunov exponents and the phase velocity of the LP-modes seem to be functions of the density alone. In particular, they are practically independent of the aspect ratio of the box (and, where applicable, also insensitive to the boundary conditions).

APPENDIX A: TRAVELING WAVES OF LP DYNAMICS

We consider the LP, a type of traveling wave with periodic boundary conditions, defined if the free boundary value

$$\psi(x) < \psi(0), \quad -\psi'(x) < -\psi'(0).$$

We take as initial tangent vector $a$.
After a time \( \tau = \frac{2\pi}{4\omega n} \), the vector is transformed to
\[
\delta \xi_{\tau} = a\phi P \cos + b\phi L \sin.
\]
(A.2)

Assume that \( a \) and \( b \) are more or less equal. Then (A.1) will resemble a sinus, with much "noise" due to the \( P \) component, while (A.2) will look more like a cosine. In the dynamics leading from (A.1) to (A.2) a kind of "traveling wave" is therefore visible, which seems to cover a distance \( 2\pi |k_n| - 1 \) in a time \( 2\pi\omega - 1 \), thus "moving" at velocity \( v = \omega n / |k_n| \). In actual simulations, we cannot expect typical vectors to have a phase difference of \( \pi/2 \) between their \( \phi L \sin \) and \( \phi L \cos \) components, as in our example. Therefore, the observed wave displacement as seen in refs. 24, 25 has the shape of "steps" in a space–time diagram, with an average slope equal to \( v \).

**APPENDIX B: TRANSFORMATION OF THE ONE-PARTICLE DISTRIBUTION**

Let \( f \) be a given distribution. For \( \frac{1}{\Gamma(x)} \subset \mu \), we have
\[
F(\frac{1}{\Gamma(x)}) \equiv \text{Prob}(\text{one particle} \in \frac{1}{\Gamma(x)}) = \int_{\frac{1}{\Gamma(x)}} dr dv f(r, v).
\]
The transported probability \( F' \) is defined by
\[
F'(\frac{1}{\Gamma(x)'})) = F(\frac{1}{\Gamma(x)}),
\]
where \( \frac{1}{\Gamma(x)'} = T(\frac{1}{\Gamma(x)}) \). We shall compute its density \( f' \). In the integral
\[
F(\frac{1}{\Gamma(x)}) = \int_{T^{-1}(\frac{1}{\Gamma(x)'})} dr dv f(r, v),
\]
we change the variables to \((r', v') = T(r, v)\). To first order in \( \varepsilon \), we have
\[
T^{-1}: \begin{cases} r' \mapsto r = r' - \varepsilon \delta \xi(r', v') \\ v' \mapsto v = v' - \varepsilon \delta \eta(r', v') \end{cases}
\]
so (B.1) becomes
\[
F(\frac{1}{\Gamma(x)}) = \int_{\frac{1}{\Gamma(x)'}} dr' dv' \det \begin{bmatrix} D T^{-1} & |r', v' \end{bmatrix} f(r' - \varepsilon \delta \xi(r', v'), v' - \varepsilon \delta \eta(r', v')).
\]
(B.2)

The determinant is
\[
\det \begin{bmatrix} D T^{-1} & |r', v' \end{bmatrix} = \det \left( \begin{bmatrix} \text{Id} - \varepsilon D r \delta \xi - \varepsilon D v \delta \xi - \varepsilon D r \delta \eta \text{Id} - \varepsilon D v \delta \eta \end{bmatrix} \right).$$
To first order in $\epsilon$, we obtain with (B.2) and (B.3)

$$F(\Gamma_1) = F(\Gamma_1') - \epsilon \int_{\Gamma_1'} \frac{d\mathbf{r}'}{\mathbf{v}'} f(\mathbf{r}', \mathbf{v}') \left[ \mathbf{\nabla}_r \cdot \delta \xi + \mathbf{\nabla}_v \cdot \delta \eta \right] \mathbf{r}'', \mathbf{v}''. \quad (B.3)$$

which is equivalent to (13).

ACKNOWLEDGMENTS

Financial support from the Austrian Science Foundation (FWF), project P15348, and the Fonds National Suisse is gratefully acknowledged.

REFERENCES

1. Lj. Milanović, H. A. Posch, and Wm. G. Hoover, What is 'Liquid'? Understanding the states of matter, Mol. Phys. 95:281–287 (1998).
2. H. A. Posch and R. Hirschl, Simulation of Billiards and of Hard-Body Fluids, in Hard Ball Systems and the Lorenz Gas, D. Szasz, ed. Encyclopedia of the mathematical sciences Vol. 101, (Springer Verlag, Berlin, 2000).
3. J.-P. Eckmann and O. Gat, Hydrodynamic Lyapunov modes in translation-invariant systems, J. Stat. Phys. 98:775 (2000).
4. S. McNamara and M. Mareschal, The Lyapunov spectrum of granular gases, Phys. Rev. E 63:061306 (2001).
5. S. McNamara and M. Mareschal, On the origin of the hydrodynamic Lyapunov modes, Phys. Rev. E 64:051103 (2001).
6. T. Taniguchi and G. P. Morriss, Boundary effects in the stepwise structure of the Lyapunov spectra for quasi-one-dimensional systems, Phys. Rev. E 68:026218 (2003).
7. A. de Wijn and H. van Beijeren, Goldstone modes in Lyapunov spectra of hard sphere systems, Phys. Rev. E 70:016207 (2004).
8. Ch. Forster, R. Hirschl, H. A. Posch, and Wm. G. Hoover, Perturbed phase-space dynamics of hard-disk fluids, Physica D 187:294 (2004).
9. V. I. Oseledec, A multiplicative ergodic theorem. Lyapunov characteristic numbers for dynamical Systems, Trudy Mosk. Mat. Obsc. 19:179 [Moscow Math. Soc. 19:197 (1968)].
10. J.-P. Eckmann and D. Ruelle, Ergodic theory of chaos and strange attractors, Rev. Mod. Phys. 57:617 (1985).
11. Lj. Milanović and H. A. Posch, Localized and delocalized modes in the tangent-space dynamics of planar hard dumbbell fluids, J. Mol. Liquids 96–97:221 (2002).
12. Ch. Dellago, H. A. Posch, and Wm. G. Hoover, Lyapunov instability of hard disks in equilibrium and nonequilibrium steady states, Phys. Rev. E 53:1485 (1996).
13. G. Benettin, L. Galgani, and A. Giorgilli, J.-M. Strelcyn, Meccanica 15:21 (1980).
14. I. Shimada and T. Nagashima, A numerical approach to ergodic problem of dissipative dynamical system, Prog. Theor. Phys. 61:1605 (1979).
15. N. Chernov, Construction of transverse fiberings in multi-dimensional semidispersed billiards, Funct. Anal. Appl. 16:270–280 (1983).
16. M. Wojtkowski, Systems of classical interacting particles with non-vanishing Lyapunov
exponents in Lyapunov exponents (Oberwolfach, 1990), Lecture Notes in Math. Vol. 1486
(Springer, 1991).
17. L. Bunimovich, C. Liverani, A. Pellegrinotti, and Y. Suhov, Ergodic systems of
balls in a billiard table, Commun. Math. Phys. 146:357 (1992).
18. N. Simányi and D. Szasz, Hard ball systems are completely hyperbolic, Ann. Math.
149:35–96 (1999).
19. N. Simányi, The complete hyperbolicity of cylindric billiard, Erg. Th. Dyn. Syst.
22:281–302.
20. N. Simányi, Proof of the ergodic hypothesis for typical hard ball systems, Ann. Henri Po-
icaré 5:203–233 (2004).
21. M. Wojtkowski, "Measure theoretic entropy of the system of hard spheres", Ergod. Th.
&Dynam. 8:133 (1988).
22. Ch. Dellago and H. A. Posch, Kolmogorov–Sinai entropy and Lyapunov spectra of a
hard sphere gas, Physica D 240:68 (1997).
23. Ch. Forster, D. Mukamel, and H. A. Posch, Hard disk in narrow channels, Phys. Rev. E
69:066124 (2004).
24. Ch. Forster, R. Hirschl, and H. A. Posch, Analysis of Lyapunov modes for hard-disk
systems, Proceedings of ICMP 2003.
25. R. Hirschl, Computer simulation of hard-disk systems: "Lyapunov modes" and stochas-
tic color conductivity, diploma thesis, University of Vienna (1999).
26. Ch. Forster and H. A. Posch, Lyapunov modes for soft-disk fluids, New J. Phys. 7,
article 32 (2005).
27. G. Radons and H. Yang, Static and dynamic correlations in many-particle Lyapunov
vectors, submitted to Phys. Rev. Lett. (2004).
28. H. Yang and G. Radons, Lyapunov instabilities of Lennard-Jones fluids, Phys. Rev. E,
submitted (2004).