From Lyapunov modes to their exponents for hard disk systems

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We demonstrate the preservation of the Lyapunov modes in a system of hard disks by the underlying tangent space dynamics. This result is exact for the Zero modes and correct to order ϵ for the Transverse and Longitudinal-Momentum modes, where ϵ is linear in the mode number. For sufficiently large mode numbers, the ϵ terms become significant and the dynamics no longer preserves the mode structure. We propose a modified Gram-Schmidt procedure based on orthogonality with respect to the center zero space that produces the *exact* numerical mode. This Gram-Schmidt procedure can also exploit the orthogonality between conjugate modes and their symplectic structure in order to find a simple relation that determines the Lyapunov exponent from the Lyapunov mode. This involves a reclassification of the modes into either *direction preserving* or *form preserving*. These analytic methods assume a knowledge of the ordering of the modes within the Lyapunov spectrum, but gives both predictive power for the values of the exponents from the modes and describes the modes in greater detail than was previously achievable. Thus the modes and the exponents contain the same information.

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I. INTRODUCTION

In a chaotic system, the difference between two nearby phase space trajectories, called the Lyapunov vector, diverges exponentially in time. If one or more of the rates of divergence are positive, then the dynamics of a single initial condition is unpredictable and global behavior becomes important. The statistical mechanics of chaotic many particle systems is an illustrative example of a probabilistic treatment of the global behavior of deterministic microscopic dynamics. It is believed that using the probabilistic axioms of statistical mechanics in what is otherwise a deterministic system can be justified by the chaotic nature of the dynamics. Much effort has been devoted to finding links between macroscopic fluid quantities, such as transport coefficients, and chaotic properties of microscopic systems such as the Lyapunov exponents [1–3]. There have been some successes in bridging this divide, such as the conjugate pairing rule for the Lyapunov spectrum in some thermostated systems [4–6] and the fluctuation theorem [7,8].

The existence of a step structure in the smallest nonzero values in the Lyapunov spectrum (the full set of Lyapunov exponents) is another chaotic property which has been studied extensively [9–20]. Each step in the exponent spectrum is associated with delocalized wavelike structure in the corresponding Lyapunov vector; distinguished now as a Lyapunov mode [21]. These modes connect to macroscopic fluid properties as the delocalized modes relate to the slowest global dynamics of the fluid. In order to understand how this phenomenon manifests itself many analytical approaches—such as random matrix theory [22,23], kinetic theory [12,24] and periodic orbit theory [25]—have been attempted.

A clue to understanding the nature of the ordered collation of the step structure in the Lyapunov spectrum and the global Lyapunov modes is in the behavior of the Lyapunov vectors associated with the zero Lyapunov exponents of the system [15]. It is now understood that these Zero modes are Noether transformations [26] generated either by the conserved quantities in the system, or by time translations along the phase space trajectory that are invariant. It is thought then that the Lyapunov modes associated with the steps in the spectrum are k-vector analogs of the Zero modes and have the same basis in the fundamental symmetries of the system [13–15].

The standard numerical scheme for calculating the Lyapunov exponents and modes is the Benettin algorithm [27–29]. This uses a combination of tangent space dynamics and the standard Gram-Schmidt (GS) procedure to obtain orthogonal Lyapunov vectors. Recently, new methods have become available to calculate covariant Lyapunov vectors [30–34]. It has been observed that the numerical time evolution of the Lyapunov modes in the Benettin algorithm is especially simple; the modes develop into approximately invariant directions or approximately invariant subspaces of the tangent space [9–11]. Here we exploit the simplicity of the mode dynamics to develop a more complete understanding of their properties.

The paper is organized as follows. Section II introduces the quasi-one-dimensional (QOD) model used in the numerical calculations, and Sec. III introduces Lyapunov exponents, vectors and modes with a brief description of the numerically observed Lyapunov spectrum and modes. In Sec. IV the tangent space dynamics for hard particle systems is introduced and a form appropriate for the QOD system is derived. Section V applies the tangent space dynamics to each of the numerically observed modes in order to understand how the modes become either direction preserving or form preserving. In Part D we develop the connection between the modes obtained from the Benettin scheme which are perfectly orthogonal and the assumed functional forms for the modes [35] that are not perfectly orthogonal. Section VI introduces a conjugate Gram-Schmidt procedure to obtain the values on the Lyapunov exponents from knowledge of the functional form of the modes and compares these with the numerical values of the exponents.

Although the approach we have taken is applicable to the QOD system, it can easily be extended to two-dimension systems of hard disks with only minor modifications. A step

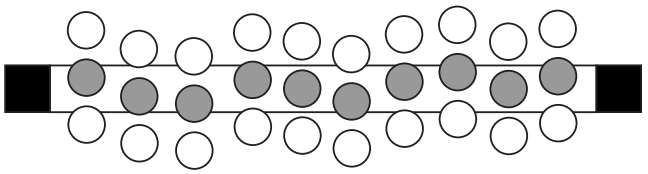

FIG. 1. A schematic of the quasi-one-dimensional system with hard wall boundaries in the x direction and periodic boundaries in the y direction. That is, (H,P) boundary conditions. The shaded disks are within the QOD system and the unshaded disks are the first periodic images above and below each particle.

structure in the Lyapunov spectrum has been observed in many different systems, such as coupled map lattices [34], partial differential equation [36] and appears to be a general feature of dynamical systems with conserved quantities. The results obtained here suggest that it may not be too difficult to understand the origin of these steps and the associated Lyapunov modes in other dynamical systems.

II. QUASI-ONE-DIMENSIONAL SYSTEM

The model used was a particular hard disk system referred to as quasi-one-dimensional [10]. The system contains N hard disks (typically $N=150$ or 200) in a two-dimensional rectangular space $L_x \times L_y$. When $L_y < 2\sigma$, where σ is the diameter of the disks (set so $\sigma=1$), the space becomes QOD and the hard disks cannot interchange positions, remaining ordered in the x direction. For our system we use $L_y = 1.15\sigma$ to ensure the QOD condition, as can be seen in Fig. 1. It is possible to use particles with smooth interaction potentials but it has proved much more difficult using these to get clear numerical evidence for the steps in the Lyapunov spectrum and to obtain delocalized modes [20,37].

The boundaries of the QOD system can either be hardwalls (H) or be periodic (P); much of the variations in the Lyapunov exponent step structure of the system stem from the choice of these boundaries. For our system we use Hardwall boundary conditions in the x-direction and Periodic boundary conditions in the y-direction (labeled succinctly as (H,P) boundary conditions).

The significant advantage of using the QOD system for study is that both the Lyapunov exponents and the Lyapunov modes of the system can be obtained to high accuracy by the standard numerical schemes with fast convergence rates [27–29,31–34]. Although more difficult to obtain, the same structure must exist in all other particle systems [20,37], as their dynamics are subject to the same invariances and conservation properties as the QOD system.

III. LYAPUNOV EXPONENTS, VECTORS AND MODES

The complete description of the state of the QOD system at any time is contained in the single $4N$-dimensional phase vector $(q,p)^T$ which contains all the positions $q \equiv \mathbf{q}_1, \ldots, \mathbf{q}_N$ and momenta $p \equiv \mathbf{p}_1, \ldots, \mathbf{p}_N$ of each particle in the system (the superscript T here indicates transpose). Note that $\mathbf{q}_i$ and $\mathbf{p}_i$ contain both the x and y components of particle i, thus $\mathbf{q}_i = (q_{xi}, q_{yi})^T$.

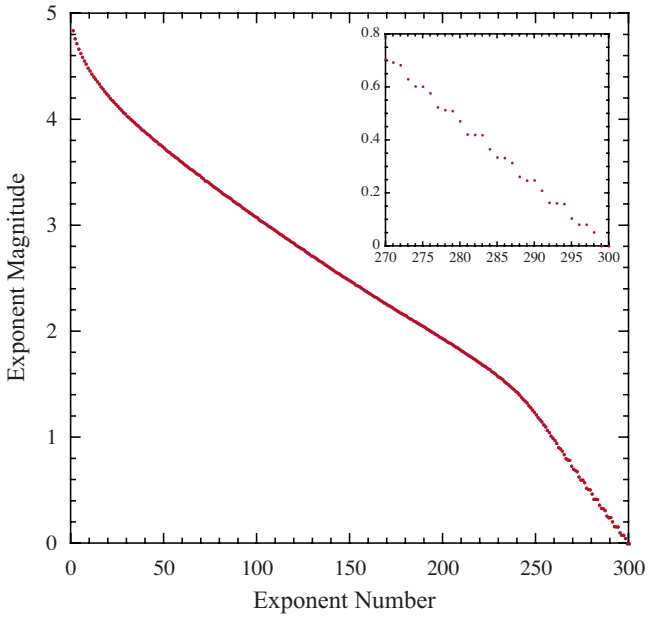

FIG. 2. (Color online) The Lyapunov spectrum for a QOD system of 150 hard disks at a density of 0.8 and temperature of 1. The inset is an enlargement of the step region of the spectrum from exponent number 270 to 300.

The tangent vectors of the system describe displacements away from the phase vector represented by the $4N$-dimensional vector $\delta\Gamma = (\delta q, \delta p)^T$. Here δq and δp are N-dimensional vectors containing the two-dimensional entries for each particle position separation $\delta\mathbf{q}_i$ or momentum separation $\delta\mathbf{p}_i$. These separations are between the original phase vector $(q,p)^T$ and a similar infinitesimally perturbed phase vector. For further explanation see Chapter 1 of [1], for example.

The important distinction is that although there is a single phase vector, there are $4N$ different tangent vectors, as the infinitesimal perturbations span the $4N$-dimensional phase space. The numerical scheme begins with $4N$ orthogonal unit perturbations; the Lyapunov vectors form from the accumulated results of the tangent space dynamics acting on these.

These $4N$ separations all diverge from the phase vector at some rate—the different rates being characterized by the Lyapunov exponents, λ_j

$$\delta\Gamma_j(t) = e^{\lambda_j t}\delta\Gamma_j(0) \tag{1}$$

The form of each divergent vector differs—the Lyapunov vectors are all unique, or at least, in the case of multiple vectors with degenerate eigenvalues, orthogonal. These vectors are the corresponding eigenvectors to the Lyapunov exponent eigenvalues.

The Lyapunov spectrum contains all $4N$ Lyapunov exponents of the system (the j^{th} exponent labeled λ_j) arranged specifically from largest to smallest. The positive half of the Lyapunov spectrum is shown in Fig. 2. As the system studied evolves under symplectic hamiltonian dynamics [38] the spectrum of exponents exhibits the conjugate pairing property of the Lyapunov exponents $\lambda_j = -\lambda_{4N+1-j}$ [35]. This sym-

plectic structure also relates the Lyapunov vectors associated with conjugate exponents [39]. If the Lyapunov vector for the positive exponent is given by

$$\delta\Gamma_j = \begin{pmatrix} \delta q \\ \delta p \end{pmatrix} \tag{2}$$

then the Lyapunov vector for the corresponding conjugate negative exponent is given by

$$\delta\Gamma_{4N+1-j} = \begin{pmatrix} -\delta p \\ \delta q \end{pmatrix}. \tag{3}$$

There are three distinct regions to the Lyapunov exponent spectrum and accordingly the Lyapunov vectors in each of these regions show distinct characteristics. The first region, from exponent number 1 to approximately 250, shown in Fig. 2, is called the "continuous region." Here the exponents vary smoothly, with no apparent fine structure. The highest value exponents describe the fastest processes in the system and are known to have highly localized vectors [18].

The second region of the spectrum is the step region, where the exponents form discrete steps, dependent upon the boundary conditions [10], starting approximately after exponent number 250, as seen in Fig. 2 inset. The associated Lyapunov vectors are important because they contain delocalized structure; as opposed to localized components or random fluctuations typical of the tangent vectors in the continuum region. Here we refer to Lyapunov vectors with delocalized structure as Lyapunov modes. There are three types of Lyapunov modes, Transverse (T), Longitudinal (L) and momentum dependent (P) modes [35]. The Transverse modes are associated with one point steps in the Lyapunov spectrum and contain nonzero components only in the y direction, "Transverse" to the dominant direction of the system (see Fig. 1). The Longitudinal and Momentum modes occur together in orthogonal pairings known as LP modes and are associated with two point degenerate steps in the Lyapunov spectrum. The L modes contain nonzero components only in the x direction, while the P modes have components dependent on the instantaneous momenta of each particle.

The third region in Fig. 2 contains the zero exponents of the system, exponent numbers 299 and 300. These exponents and their modes are vital to the system and are related to the conservation properties and symmetries of the system [15,26].

It is well known that the numerical modes that form in the step region can be approximated by simple functional forms. These assumed forms for the modes are an approximation to the numerical vectors, rather than an exact representation. Later, we will investigate this point in more detail for the Transverse modes.

IV. TANGENT SPACE DYNAMICS

The time evolution of a system of hard disks proceeds via repeated mappings of collisions and free flights of all particles between collisions. The phase vector (q,p) moves to a new phase vector (q',p') with a free flight of length τ followed by a collision between two particles (or perhaps with a boundary). The fundamental iteration of free flight followed by a collision is given by the matrix equation

$$\begin{pmatrix} q' \\ p' \end{pmatrix} = \begin{pmatrix} \mathcal{I} & \tau\mathcal{I} \\ \mathcal{O} & \mathcal{N} \end{pmatrix} \begin{pmatrix} q \\ p \end{pmatrix} = \begin{pmatrix} q + \tau p \\ \mathcal{N}p \end{pmatrix}. \tag{4}$$

The positions are translated by an amount τp and two momenta have been changed due to the collision. Each scripted matrix is an $N\times N$ matrix containing 2×2 submatrices, giving a $4N\times 4N$ evolution matrix. $\mathcal{I}$ is the identity and $\mathcal{O}$ is the zero matrix.

The matrix $\mathcal{N}$ acts only on the momenta of the two colliding disks; changing their momenta via the collision rules of the system. It is represented as

$$\mathcal{N} = \begin{pmatrix} I & . & 0 & 0 & . & 0 \\ . & . & . & . & . & . \\ 0 & . & I - N_{ij} & N_{ij} & . & 0 \\ 0 & . & N_{ij} & I - N_{ij} & . & 0 \\ . & . & . & . & . & . \\ 0 & . & 0 & 0 & . & I \end{pmatrix}. \tag{5}$$

Again, each element in this matrix is itself a 2×2 submatrix with I the 2×2 identity and 0 the 2×2 zero matrix. The N_{ij} matrix is a 2×2 matrix composed of the dyadic product $\mathbf{n}_{ij}\mathbf{n}_{ij}^T$ where the $\mathbf{n}_{ij}^T=(x_{ij},y_{ij})$ term is a row vector containing the x and y components of the separation between particles i and j at collision $\mathbf{n}_{ij}=\mathbf{q}_j-\mathbf{q}_j$ (the length of this term is equal to the diameter of the disks σ). Note that for a QOD system $j=i+1$, but otherwise the result is general.

The time evolution equations for the Lyapunov tangent vectors consist of many repeats of a free flight, then a collision and then a Gram-Schmidt procedure. Much like the phase vector the first two of these steps—the application of a free flight matrix then a collision matrix—evolve each of the tangent vectors in time from t to $t+\tau$ and can be written as

$$\begin{pmatrix} \delta q(\tau) \\ \delta p(\tau) \end{pmatrix} = \begin{pmatrix} \mathcal{N} & \tau\mathcal{N} \\ \mathcal{Q} & \tau\mathcal{Q}+\mathcal{N} \end{pmatrix} \begin{pmatrix} \delta q \\ \delta p \end{pmatrix}. \tag{6}$$

Here we are treating the time evolution of an arbitrary tangent vector. It is straightforward to show that the time evolution matrix in Eq. (6) satisfies the symplectic condition $M^TJM=J$, where J is the usual symplectic matrix [40]. The matrix $\mathcal{Q}$ changes the dynamics of the momenta exchange due to the change in collision point because of the infinitesimal perturbation. It is represented as

$$\mathcal{Q} = \begin{pmatrix} 0 & . & 0 & 0 & . & 0 \\ . & . & . & . & . & . \\ 0 & . & -Q_{ij} & Q_{ij} & . & 0 \\ 0 & . & Q_{ij} & -Q_{ij} & . & 0 \\ . & . & . & . & . & . \\ 0 & . & 0 & 0 & . & 0 \end{pmatrix}. \tag{7}$$

Each component of this matrix is a 2×2 submatrix where the only nontrivial components are those associated with the two particles that collide, i and j, through the four Q_{ij} elements. The Q_{ij} submatrix is given by

$$Q_{ij} = (\mathbf{n}_{ij} \cdot \mathbf{p}_{ij}) \left[I + \frac{\mathbf{n}_{ij}\mathbf{p}_{ij}^T}{\mathbf{n}_{ij} \cdot \mathbf{p}_{ij}} \right] \cdot \left[I - \frac{\mathbf{p}_{ij}\mathbf{n}_{ij}^T}{\mathbf{n}_{ij} \cdot \mathbf{p}_{ij}} \right]. \quad (8)$$

where $\mathbf{p}_{ij}^T = (p_{xij}, p_{yij})$ is a row vector containing the x and y components of the relative momenta at collision ($\mathbf{p}_{ij} = \mathbf{p}_j - \mathbf{p}_i$). The principle property of this term that we wish to exploit in what follows is that $Q_{ij} \cdot \mathbf{p}_{ij}^T = 0$. To understand the result of the dynamics on each of the tangent vectors we consider the action of the matrix $\mathcal{N}$ on either δq or δp. This gives

$$\mathcal{N}\delta q = \delta q + N_{ij} \cdot (\delta \mathbf{q}_j - \delta \mathbf{q}_i) X, \quad (9)$$

$$\mathcal{N}\delta p = \delta p + N_{ij} \cdot (\delta \mathbf{p}_j - \delta \mathbf{p}_i) X, \quad (10)$$

where X is the N-dimensional column vector which selects the nonzero elements of $\mathcal{N}\delta q$. All elements of X are equal to zero except for $X_i = 1$ and $X_j = -1$.

Similarly, the action of the matrix $\mathcal{Q}$ gives

$$\mathcal{Q}\delta q = Q_{ij} \cdot (\delta \mathbf{q}_j - \delta \mathbf{q}_i) X, \quad (11)$$

$$\mathcal{Q}\delta p = Q_{ij} \cdot (\delta \mathbf{p}_j - \delta \mathbf{p}_i) X. \quad (12)$$

All of these results follow simply from the definitions of the matrices in Eqs. (5) and (7). Any interesting structure in the mode dynamics is a consequence of the form of the mode itself and in particular the form of the $\delta \mathbf{q}_j$ and the $\delta \mathbf{p}_j$.

V. LYAPUNOV MODE DYNAMICS

To understand the dynamics in a more fundamental way we begin by looking in depth at the action of the tangent space dynamics on particular modes. The question that we seek to answer is what part of the dynamics leads to the invariant directions or invariant subspaces that are characteristic of the modes. It has even been suggested that the dynamics of the mode space could be separate from the dynamics of the rest of the system [26]. The functional forms for the Lyapunov modes are now well established [14,15] and we probe the time evolution of each mode individually. This could provide some clues as to the nature of the Lyapunov modes; it is indeed hard to understand why a GS procedure working down through many hundreds of dimensions should suddenly give rise to steps in the exponents and delocalized modes.

A. Gram-Schmidt procedure

The Gram-Schmidt procedure is a key component of both the Benettin algorithm and also in the analysis following. The Gram-Schmidt procedure is an algebraic method that takes a set of linearly independent vectors $\{\mathbf{v}_1, \mathbf{v}_2, \ldots, \mathbf{v}_n\} \in \mathbb{R}^n$ and transforms them into a spanning set of orthogonal vectors $\{\mathbf{u}_1, \mathbf{u}_2, \ldots, \mathbf{u}_n\} \in \mathbb{R}^n$. The procedure works sequentially on each vector beginning at $k=2$ and ending at n using

$$\mathbf{u}_k = \mathbf{v}_k - \sum_{j=1}^{k-1} \frac{(\mathbf{u}_j \cdot \mathbf{v}_k)}{(\mathbf{u}_j \cdot \mathbf{u}_j)} \mathbf{u}_j. \quad (13)$$

Where the centered dot $(\mathbf{u}_j \cdot \mathbf{v}_k)$ indicates an inner product. This removes the components of $\mathbf{v}_k$ that are in the direction of $\mathbf{v}_1, \ldots, \mathbf{v}_{k-1}$, to form the new vector $\mathbf{u}_k$. This set can then be normalized trivially. In the numerical simulation the largest Lyapunov exponent comes from $\delta\Gamma_1$ (taking the place of $\mathbf{u}_1$), followed by the second largest exponent from $\delta\Gamma_2$, which is $\mathbf{u}_2$, and so on. Further detail about the application of the Benettin algorithm to systems of hard particles can be found in [41,42].

B. Zero modes

In Fig. 2 there are two zero exponents, giving a total of four for the full spectrum; these are exponent numbers 299, 300, 301, and 302. These four exponents gives rise to a four-dimensional subspace spanned by 4 basis vectors. The first two of these basis vectors are

$$\delta\Gamma_y = \frac{1}{\sqrt{N}} \begin{pmatrix} c_0 \\ 0 \end{pmatrix} \quad \delta\Gamma_{p_y} = \frac{1}{\sqrt{N}} \begin{pmatrix} 0 \\ c_0 \end{pmatrix}. \quad (14)$$

Following the notation convention of Eq. (2), the jth element of the N-dimensional vector c_n is $(0, \cos k_n x_j)^T$ where $k_n = n\pi/L_x$ and x_j is the x position of the jth particle. Clearly, when $n=0$, $\cos k_n x_j = 1$. These arise from the symmetry present in the y-direction, due to the periodic boundary condition. There are *not* corresponding vectors for the x direction because of the hard wall boundary conditions in that direction. The second two basis vectors are

$$\delta\Gamma_t = \frac{1}{\sqrt{2K}} \begin{pmatrix} p \\ 0 \end{pmatrix} \quad \delta\Gamma_e = \frac{1}{\sqrt{2K}} \begin{pmatrix} 0 \\ p \end{pmatrix}, \quad (15)$$

which are related to the time translational invariance and conservation of energy respectively. Here it is apparent that each entry is N dimensional and that the jth component of p is $(p_{xj}, p_{yj})^T$. The K term is simply the total kinetic energy of the system, which is conserved.

It is readily apparent that Eqs. (14) and (15) show the conjugate structure observed in Eqs. (2) and (3). It is important to remember that these basis vectors are *not* the modes themselves, only that the Zero modes are made of linear combinations of this basis. The Zero modes are perfectly described by linear combinations of these four basis vectors [11,35].

The four Zero modes $\delta\Gamma_y$, $\delta\Gamma_{p_y}$, $\delta\Gamma_t$, and $\delta\Gamma_e$ are also unique among the Lyapunov modes because of their simple structure. As can be seen in Eq. (14) the $\delta\Gamma_y$ mode contains no intricate structure to the δq terms, simply constants $\delta \mathbf{q}_j = (0,1)^T$, while the δp terms are zero. This means that $\delta \mathbf{q}_i - \delta \mathbf{q}_j = 0$ and $\delta \mathbf{p}_i - \delta \mathbf{p}_j = 0$. Applying Eq. (6) we see that $\delta\Gamma_y$ is preserved exactly by the dynamics as

$$\delta\Gamma_y(\tau) = \frac{1}{\sqrt{N}} \begin{pmatrix} \mathcal{N}c_0 \\ \mathcal{Q}c_0 \end{pmatrix} = \frac{1}{\sqrt{N}} \begin{pmatrix} c_0 \\ 0 \end{pmatrix} = \delta\Gamma_y. \quad (16)$$

The conjugate mode $\delta\Gamma_{p_y}$ will have $\delta \mathbf{p}_j = (0,1)^T$ and $\delta q = 0$, thus undergoing the same evolution will mean that the mode will grow linearly in time [26] as

$$\delta\Gamma_{p_y}(\tau) = \frac{1}{\sqrt{N}}\begin{pmatrix} \mathcal{N}\tau c_0 \\ \mathcal{Q}\tau c_0 + \mathcal{N} c_0 \end{pmatrix} = \delta\Gamma_{p_y} + \tau\delta\Gamma_y. \quad (17)$$

What we see is that the conjugate mode will grow toward the direction of the "positive exponent" mode $\delta\Gamma_y$ over time. So although $\delta\Gamma_y$ is preserved by the dynamics alone, the Gram-Schmidt procedure is needed to keep $\delta\Gamma_{p_y}$ orthogonal to $\delta\Gamma_y$.

The application of the dynamics on the momentum dependent Zero modes $\delta\Gamma_t$ and $\delta\Gamma_e$ results in a change similar to the constant modes. For $\delta\Gamma_t$ we have that $\mathcal{N}p = p'$ and $\mathcal{Q}\cdot p = 0$ so essentially we get

$$\delta\Gamma_t(\tau) = \frac{1}{\sqrt{2K}}\begin{pmatrix} \mathcal{N}p \\ \mathcal{Q}p \end{pmatrix} = \frac{1}{\sqrt{2K}}\begin{pmatrix} p' \\ 0 \end{pmatrix}. \quad (18)$$

Which has exactly the same *functional form* as the original vector $\delta\Gamma_t$, however, this vector now has two precollision momenta replaced by their postcollision values, so the direction of $\delta\Gamma_t$ has changed. Similarly, the time evolution of $\delta\Gamma_e$ gives $\delta\Gamma_e(\tau) = \delta\Gamma_e + \tau\delta\Gamma_t$.

Left to evolve under just the numerical dynamics alone only two of the Zero modes will remain preserved, the other two will quickly evolve toward their conjugates. Importantly the mode that does evolve moves only within the subspace defined by the mode and its conjugate. At no stage does it move outside that subspace. This observation is critical to the conjugate GS scheme that we will introduce later.

The Zero modes reveal a very important aspect of the Lyapunov modes. We see that some of the modes preserve their direction; the dynamics is irrelevant to the structure of these modes, they are fixed within the $4N$-dimensional space, such as $\delta\Gamma_y$ and $\delta\Gamma_{p_y}$. We also see that some of the modes preserve their functional form; the dynamics may change their direction, but leaves their functional form intact, like $\delta\Gamma_t$ and $\delta\Gamma_e$. This compels the idea of separating the Lyapunov modes into two sub groups, one group "direction preserving" and one group "form preserving." This allows us to separate the basis vectors that describe the mode into two types, which will be beneficial in the coming analysis.

C. Transverse modes

The first step of the Lyapunov Spectrum is a one point step and is therefore associated with the first Transverse (T) mode [35]. The nth Transverse mode can be written as

$$\delta T^n = \begin{pmatrix} \gamma_n c_n \\ \gamma_n' c_n \end{pmatrix}. \quad (19)$$

Following from the definition of c_n previously, it is apparent that the Transverse mode only contains nonzero y components. It is important to note that the coordinate and momentum parts are *not* the same, only their functional forms are the same; the difference between them comes from the magnitude of the constants γ_n and γ_n'. This is an application of the known relation that, for long time averaging, the Lyapunov modes obey $\delta p = C\delta q$ [9].

The dynamics of the Transverse modes are more problematic than the Zero modes; from Eq. (19) we can see that the term $(\delta\mathbf{q}_j - \delta\mathbf{q}_i)$ is not removed from the dynamics like the Zero modes. After the evolution from Eqs. (9) and (11) the separation components would become

$$(c_{nj} - c_{ni}) \to (\delta y_j - \delta y_i) = -\epsilon\gamma_n \sin(k_n x_i), \quad (20)$$

where $\epsilon = k_n x_{ij} = n\pi x_{ij}/L_x$. x_{ij} is the x component of the distance between particles i and j at collision $|(x_j - x_i)| \le 1$ and L_x is the length of the system in the x direction, which is $O(N)$. Therefore $\epsilon \sim n\pi/L_x$ is a small parameter for the first few modes (as $n = 1, 2, 3, \ldots$ is the mode number). Due to the structure of the T modes, this separation is also true for the momentum components $(\delta\mathbf{p}_j - \delta\mathbf{p}_i)$.

Therefore evolution of the T modes under the tangent space dynamics is analogous to the Zero modes, but will involve order ϵ terms. Following Eq. (6) the full time evolution of a T modes is given by

$$\begin{pmatrix} \delta q(\tau) \\ \delta p(\tau) \end{pmatrix} = \begin{pmatrix} \delta q + \tau\delta p \\ \delta p \end{pmatrix} + O(\epsilon). \quad (21)$$

We will initially neglect the ϵ dependent terms. Clearly the small parameter ϵ is linear in the mode number n so for sufficiently large ϵ the dynamics without the order ϵ term will become incorrect and a new approach will have to be taken.

We assume that below a threshold value, we can ignore the order ϵ terms in the dynamics in Eq. (21). Much like the Zero modes, the dynamics of both positive and negative Transverse modes consists of a leading term that is invariant and a time dependent term that rotates the vector. The dynamics of the conjugate pair of modes is coupled and this is the dominant term in the dynamics. Although there is some other motion of the pair, it is much smaller [26].

D. First transverse mode reorthogonalization

We have seen that the Zero modes can be obtained exactly from the system dynamics and are also preserved exactly by the dynamics. With the addition of the GS procedure for the conjugate Zero modes they define a stable center space where all Lyapunov exponents are zero (completing the Benettin algorithm). This stable orthonormal center space can be used as a reference point for all other Lyapunov modes. All the numerical Lyapunov modes generated by the combination of tangent space dynamics and Gram-Schmidt are orthogonal, although the assumed functional forms for the Lyapunov modes [for example, in Eq. (19)] are not *exactly* orthogonal.

We know the first Lyapunov mode after the Zero modes is a Transverse mode. Figure 3 shows the first Transverse mode across all $4N$ components (the circles). It is apparent that the assumed functional form for the T modes, Eq. (19), when $n = 1$ is a very good approximation to the numerically observed mode but it is not an exact representation. The *noise* apparent in the mode means that the numerical mode for δy is not a smooth cosine function as we may have expected.

We hypothesized that this noise was not due to errors in the system description or imprecision in the calculations, but due to the assumed functional form for the T mode not being *exactly* orthogonal to the center space. If the numerically observed mode is thought to be made up of the known as-

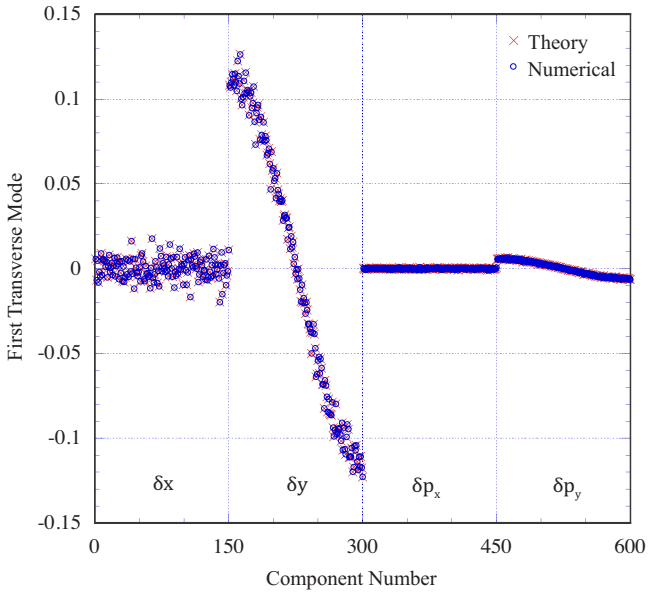

FIG. 3. (Color online) The circles are the *numerical* values of the first Transverse mode calculated from the Benettin algorithm for a QOD system of 150 disks. The crosses are the tangent space vector obtained from the assumed functional form for the Transverse mode (with coefficients γ and γ' determined numerically) explicitly orthogonalized to the zero space using the Gram-Schmidt procedure in Eq. (22). This essentially gives the exact numerical Transverse mode.

sumed functional form plus small contributions in the direction of the zero space then making the smooth cosine explicitly orthogonal to the center space via a GS procedure may give a more accurate representation of the mode. To do this we write the corrected mode as

$$\delta T^n = \begin{pmatrix} \gamma c_n \\ \gamma' c_n \end{pmatrix} - \frac{c_0 \cdot c_n}{N} \begin{pmatrix} \gamma c_0 \\ \gamma' c_0 \end{pmatrix} - \frac{p \cdot c_n}{2K} \begin{pmatrix} \gamma p \\ \gamma' p \end{pmatrix}. \quad (22)$$

The four Zero mode basis vectors are combined into the two last terms. The first orthogonalization is with respect to the two vectors $\delta\Gamma_y$ and $\delta\Gamma_{p_y}$, while the second orthogonalization is with respect to $\delta\Gamma_t$ and $\delta\Gamma_e$. The result of this Zero mode reorthogonalization on the first mode is shown in Fig. 3 (the crosses). Not only does this process improve the representation obtained from the assumed functional form, but the corrected mode is essentially the *exact* numerically observed mode, as it gives point-wise agreement across all $4N$ components.

This accuracy can be seen by noting that as the Zero modes are perfectly described by the theoretical functional forms, it is an instance where the numerical mode and the theoretical mode that is thought to describe it are the same. Importantly, when we form the inner product of the Zero modes functional form to the first T modes *new* functional form, we get *exactly* zero, not approximately zero, which is what was found for the simple description of the first T mode. What we had previously described as noise in the δx and δy components can now be seen to be thermal velocity contributions from the Gram-Schmidt procedure with respect to the Zero modes $\delta\Gamma_t$ and $\delta\Gamma_e$.

The two correction terms have coefficients with an extensive term in the denominator, while the numerator is at best $O(N^{1/2})$, so both of the correction terms approach zero as $N \to \infty$. As the number of particles in the system gets larger, the assumed form for the Lyapunov modes becomes more accurate and more orthogonal to the center space. This result suggests that applying this new kind of GS procedure with respect to the center space gives more accurate Lyapunov modes for a finite system. A crucial observation is that the form (or direction) of the first positive and negative T modes are preserved and they remain orthogonal once the dynamics has evolved them and the full GS procedure has been performed.

E. *LP* modes

The LP modes are associated with the two-point steps in the Lyapunov Spectrum [35] and are an amalgamation of two separately orthogonal modes; one mode containing momentum proportional components (the P mode), the other mode containing only nonzero x components (the L mode). The LP modes, due to the degeneracy of their exponents, come in pairs. The pair of LP modes are given by

$$\delta LP_1^n = s_{nt} \begin{pmatrix} \beta_n p c_n \\ \beta_n' p c_n \end{pmatrix} + c_{nt} \begin{pmatrix} \alpha_n s_n \\ \alpha_n' s_n \end{pmatrix}, \quad (23)$$

and

$$\delta LP_2^n = c_{nt} \begin{pmatrix} \beta_n p c_n \\ \beta_n' p c_n \end{pmatrix} + s_{nt} \begin{pmatrix} \alpha_n s_n \\ \alpha_n' s_n \end{pmatrix}, \quad (24)$$

where we have followed the same conventions as for the Transverse mode. Each component of the mode is an N dimensional vector made up of two-dimensional vector elements, totaling $4N$ components. The first vector is the momentum dependent mode, where each element of pc_n contains

$$pc_{nj} = \begin{pmatrix} p_{xj} \cos k_n x_j \\ p_{yj} \cos k_n x_j \end{pmatrix}. \quad (25)$$

The second vector is the Longitudinal mode which contains only nonzero x components. Analogous to the T modes, we define an N-dimensional vector s_n with two-dimensional elements s_{nj} as

$$s_{nj} = \begin{pmatrix} \sin k_n x_j \\ 0 \end{pmatrix}. \quad (26)$$

Clearly all the y components are zero. Both δLP_1^n and δLP_2^n are time dependent as well, represented through

$$s_{nt} = \sin \omega_n t \quad c_{nt} = \cos \omega_n t, \quad (27)$$

which ensure the modes remain orthogonal (or almost orthogonal). The constants α_n, α_n', β_n, and β_n' again reflect the observed relation $\delta p = C \delta q$.

As a result of the L and P components of the LP mode being almost orthogonal, their evolution under the tangent space dynamics can be treated separately.

The dynamics of the L modes is comparable to the T modes, due to the similarities in their structures. Because of this the L mode evolution is described by Eq. (21), just like the T mode.

The P mode is slightly more complicated, due to the mode being linear in the momentum; $\delta\mathbf{q}_i = \beta_n \mathbf{p}_i \cos k_n x_i$. This complication means that

$$\delta\mathbf{q}_i - \delta\mathbf{q}_j = \beta_n(\mathbf{p}_{ij} \cos k_n x_i - \epsilon \mathbf{p}_j \sin k_n x_i) \tag{28}$$

where ϵ is the same small parameter defined previously after Eq. (20). This seemingly complex result is simplified through $Q_{ij} \cdot \mathbf{p}_{ij}^T = 0$. Using this, the first term in Eq. (28) is zero and the final result is again order ϵ, like the other modes.

There are two different approaches that could be taken with the LP modes (as well as the T modes), we can follow the time evolution of the two modes δLP_1^n and δLP_2^n, with their individual time dependences, or we can follow the time evolution of two stationary basis vectors that span the space in which δLP_1^n and δLP_2^n rotate. Here we choose the second approach and consider basis vectors δL_1^n and δP_1^n, where δP_1^n is the first vector component in Eq. (23) without the time dependent pre-factor s_{nt} and δL_1^n is the second term without the prefactor c_{nt}. The tangent space evolution of the basis vector δP_1^n is given by

$$\delta P_1^n(\tau) = \begin{pmatrix} (\beta_n + \tau\beta_n')p' c_n \\ \beta_n' p' c_n \end{pmatrix} + O(\epsilon). \tag{29}$$

After removal of the ϵ term, the action of the tangent space dynamics alone modifies δP_1^n. However, the basis vector must preserve its functional form so this modification, the combined tangent space dynamics and GS procedure, must lead to

$$\delta P_1^n(\tau) = \begin{pmatrix} \beta_n p' c_n \\ \beta_n' p' c_n \end{pmatrix}. \tag{30}$$

VI. CONJUGATE GRAM-SCHMIDT PROCEDURE

The step structure component of the Lyapunov Spectrum, which encompasses the Lyapunov modes, defines a subspace of the phase space that is spanned by the basis vectors described in the previous section. These basis vectors have now been classed into two distinct types, from their similarities to the Zero modes. Analogous to the Zero modes $\delta\Gamma_y$ and $\delta\Gamma_{p_y}$, the numerical dynamics gives Transverse modes δT^n and Longitudinal modes δL^n which have fixed directions in the phase space. The numerically observed T and L modes are invariants of the dynamics (omitting the $O(\epsilon)$ term) once the GS procedure has been performed. Similarly, the P modes are analogous to the Zero modes $\delta\Gamma_t$ and $\delta\Gamma_e$; under the dynamics their directions in phase space are *not* preserved, but the *form* of the mode is preserved; it is described by the same functional form after the dynamics and the GS procedure. The combined action of the dynamics and GS procedure therefore simply results in each Lyapunov mode being preserved either in direction or form.

We now introduce a *conjugate* Gram-Schmidt procedure that has the same effect as the combination of dynamics and standard Gram-Schmidt for the Lyapunov modes. To do this we make two assumptions: (1) that the functional forms for the T, L and P modes are known; (2) that the numerical values for the amplitude coefficients are known. The simplified *conjugate* GS procedure also makes the assumption that the complete Lyapunov mode subspace of the dynamics can be treated as separate pairs of conjugate modes and that these pairs of modes are *already* orthogonal to the center space (by construction). We have already seen that the assumed functional forms for the Lyapunov modes are not exactly orthogonal to the center space, only approximately orthogonal.

After one iteration step in the program the tangent vectors have been modified by the dynamics; using the conjugate GS procedure, the phase space direction of the Lyapunov mode is kept constant (or its form constant) and the mode is allowed to grow slightly, by a factor of ζ (this is true because all the nonzero exponent modes are characterized by different growth rates). Next one, and only one, element from the summation in Eq. (13) is taken, where the j in Eq. (13) is the Lyapunov exponent *number* of the Lyapunov mode in question and $4N+1-j$ is the corresponding conjugate Lyapunov mode. This is the main step in the conjugate GS procedure and is given by

$$\delta\Gamma_j' = \delta\Gamma_j - \frac{(\delta\Gamma_j \cdot \delta\Gamma_{4N+1-j})}{(\delta\Gamma_{4N+1-j} \cdot \delta\Gamma_{4N+1-j})} \delta\Gamma_{4N+1-j}. \tag{31}$$

This equation does not take into account the evolution of the mode due to the dynamics; this aspect will be incorporated below. The simplified process then ensures orthogonality with respect to the conjugate mode *only*. Interestingly, given these two assumptions the simplified GS procedure can calculate the values of the Lyapunov exponents in the step region.

Following the dynamics and the new conjugate GS procedure, the original Lyapunov mode will evolve to a new mode as

$$\zeta\begin{pmatrix} \delta q \\ \delta p \end{pmatrix} = \begin{pmatrix} \mathcal{N}(\delta q + \tau\delta p) \\ \mathcal{Q}(\delta q + \tau\delta p) + \mathcal{N}\delta p \end{pmatrix} - \begin{pmatrix} \mathcal{N}(\delta q + \tau\delta p) \\ \mathcal{Q}(\delta q + \tau\delta p) + \mathcal{N}\delta p \end{pmatrix} \cdot \begin{pmatrix} -\delta p \\ \delta q \end{pmatrix} \begin{pmatrix} -\delta p \\ \delta q \end{pmatrix}.$$

The first term is the time evolution under the tangent space dynamics, while the second term is the Gram-Schmidt procedure which ensures that the new vector is orthogonal to the direction of the original conjugate vector.

We can separate this vector equation into one for δq and one for δp. These two vector equations can be transformed into two scalar equations; the first by multiplying the transpose of δp into the δq equation and the second by the transpose of δq into the δp equation. This results in two scalar equations for ζ, which both give the same result

$$\zeta = \frac{\delta q \mathcal{N} \delta p + \tau \delta p \mathcal{N} \delta p (\delta q \cdot \delta q) + \delta q \mathcal{Q} (\delta q + \tau \delta p)(\delta p \cdot \delta p)}{\delta q \cdot \delta p}. \tag{32}$$

This equation is completely general, as it does not pertain to any specific Lyapunov mode. Using the matrix forms for $\mathcal{N}$ and $\mathcal{Q}$ given in Eqs. (5) and (7) we can simplify this as

$$\delta p \mathcal{N} \delta p = \delta p \cdot \delta p - \delta \mathbf{p}_{ij}^T N_{ij} \delta \mathbf{p}_{ij} \tag{33}$$

and

$$\delta q \mathcal{Q} (\delta q + \tau \delta p) = - \delta \mathbf{q}_{ij}^T Q_{ij} (\delta \mathbf{q}_{ij} + \tau \delta \mathbf{p}_{ij}) \tag{34}$$

where $\delta \mathbf{q}_{ij} = \delta \mathbf{q}_i - \delta \mathbf{q}_j$ and the dot products have been suppressed.

If $\delta \mathbf{q}$ and $\delta \mathbf{p}$ vary smoothly with the particle index—as they do for a Lyapunov mode—then both $\delta \mathbf{q}_{ij}$ and $\delta \mathbf{p}_{ij}$ are small—of order ϵ—and ζ is given by

$$\zeta = 1 + \tau \frac{(\delta p \cdot \delta p)(\delta q \cdot \delta q)}{\delta q \cdot \delta p} + O(\epsilon^2). \tag{35}$$

The full evolution of the system involves many repeats of this three step process: free flight, collision, Gram-Schmidt. Therefore the Lyapunov exponent will result from the accumulation of all the ζ's from each cycle. In the infinite time limit the scaling factor ζ yields the Lyapunov exponent.

The idea that a Lyapunov mode will preferentially evolve toward a specific mode, forgoing other directions, has been shown to occur in the Zero modes. We saw previously that the Lyapunov modes will evolve toward their conjugate modes at the fastest rate [26], so this is a good approximation.

A. Application to the *T* modes

As a solid example of the information garnered from the conjugate GS procedure, consider a T or L mode under a free flight and collision iteration. Using Eq. (21) the mode modifies, but then the GS procedure returns it to its initial direction with some scaling factor ζ, as

$$\begin{pmatrix} \delta q \\ \delta p \end{pmatrix} \overset{\tau,coll}{\rightarrow} \begin{pmatrix} \delta q + \tau \delta p \\ \delta p \end{pmatrix} \overset{GS}{\rightarrow} \zeta \begin{pmatrix} \delta q \\ \delta p \end{pmatrix}. \tag{36}$$

The first right arrow represents the action of the tangent space dynamics (free flight and collision) while the second represents the result of the GS procedure (note that $O(\epsilon)$ terms are neglected).

The same dynamics applies to the conjugate mode so its evolution will be

$$\begin{pmatrix} -\delta p \\ \delta q \end{pmatrix} \overset{\tau,coll}{\rightarrow} \begin{pmatrix} -\delta p + \tau \delta q \\ \delta q \end{pmatrix} \overset{GS}{\rightarrow} \zeta^* \begin{pmatrix} -\delta p \\ \delta q \end{pmatrix}, \tag{37}$$

where ζ^* is the expansion (or contraction) factor for the conjugate mode.

As the mode is normalized it is straight forward to see that $\delta q \cdot \delta q + \delta p \cdot \delta p = 1$, so using the results of Eq. (35) the scalar solution for the mode is again

$$\zeta = 1 + \tau \frac{(\delta p \cdot \delta p)(\delta q \cdot \delta q)}{\delta q \cdot \delta p}. \tag{38}$$

Applying the same procedure to the conjugate mode gives

$$\zeta^* = 1 - \tau \frac{(\delta p \cdot \delta p)(\delta q \cdot \delta q)}{\delta q \cdot \delta p}. \tag{39}$$

As the dynamics is the serial accumulation of these processes, the Lyapunov exponent is given by the product of the ζ factors

$$\lambda = \lim_{m \to \infty} \frac{1}{T} \ln \prod_{i=1}^{m} \zeta_i \tag{40}$$

and $\lambda^* = -\lambda$ which is consistent with the conjugate pairing Lyapunov exponents. For the mode δT^n, $\delta y_j = \gamma_n c_{nj}$ and $\delta p_{yj} = \gamma_n' c_{nj}$ so using $\Sigma_j^N c_{nj}^2 = N/2$

$$\lambda_n = \frac{N}{2} \gamma_n' \gamma_n. \tag{41}$$

Similarly, we find that the accumulation of the ζ^* terms for the conjugate mode δT^{-n} results in $\lambda_{-n} = \frac{N}{2} \gamma_{-n}' \gamma_{-n} = -\lambda_n$, which is expected.

B. LP modes

The functional form of the *LP* modes is given in Eqs. (23) and (24) and it is evident that the two numerical modes δLP_1 and δLP_2 rotate in a two-dimensional subspace with basis vectors

$$\delta P^n = \begin{pmatrix} \beta_n p c_n \\ \beta_n' p c_n \end{pmatrix} \quad \delta L^n = \begin{pmatrix} \alpha_n s_n \\ \alpha_n' s_n \end{pmatrix}. \tag{42}$$

Where we have moved the time rotation into the constants over one iteration of the dynamics. As the vector δL^n behaves in the same way as the Transverse mode, maintaining a constant direction in phase space, the simplified GS result is already known. The momentum dependent basis vector δP^n behaves differently. Instead of having a fixed phase space direction, we have claimed that the functional form of the mode is preserved, thus in each step of the dynamics the vector δP^n is of the same form but with the *instantaneous* values of position and momentum changed. Both of these basis vectors have conjugate vectors defined through Eq. (3).

For the Longitudinal mode component δL^n, the result is similar to the Transverse mode,

$$\lambda_n = \frac{N}{2} \alpha_n' \alpha_n. \tag{43}$$

To a good approximation we can express the momentum dependent part of the basis δP^n mode immediately after a collision as

$$\begin{pmatrix} \delta q' \\ \delta p' \end{pmatrix} = \begin{pmatrix} \beta_n p' c_n \\ \beta_n' p' c_n \end{pmatrix} = \begin{pmatrix} \mathcal{N} & 0 \\ 0 & \mathcal{N} \end{pmatrix} \begin{pmatrix} \beta_n p c_n \\ \beta_n' p c_n \end{pmatrix}. \tag{44}$$

The conjugate Gram-Schmidt procedure in the case of form preservation is different to the one used for direction preser-

TABLE I. A comparison of predicted [Eqs. (41), (43), and (45)] and numerically observed Lyapunov exponents for a 200 particle QOD system with (H,P) boundary conditions at density $\rho=0.8$ and total kinetic energy $K=N$. We use units where the mass and disk radius R are 1, the total energy is N and the system size is $L_y=1.15R$ and $L_x=N/\rho L_y$ where ρ is the density. There are small differences between the x and y projections of β so we include both results.

	T mode		P_x mode	P_y mode	L mode	
n	$\frac{N}{2}\gamma\gamma'$	λ_T	$K\beta_x\beta_x'$	$K\beta_y\beta_y'$	$\frac{N}{2}\alpha\alpha'$	λ_{LP}
1	0.0388	0.0393	0.0599	0.0559	0.0502	0.0605
2	0.0749	0.0784	0.1169	0.1044	0.0965	0.1229
3	0.1099	0.1177	0.1507	0.1348	0.1344	0.1848
4	0.1431	0.1571	0.1753	0.1472	0.1591	0.2484
5	0.1748	0.1961	0.1693	0.1391	0.1595	0.3140
6	0.2007	0.2352	0.1855	0.1409	0.1823	0.3791

vation. Here rather than doing a Gram-Schmidt with respect to the initial conjugate mode, we Gram-Schmidt with respect to the form preserved mode at the new time. Thus we have

$$\zeta\begin{pmatrix}\delta q'\\ \delta p'\end{pmatrix}=\begin{pmatrix}\mathcal{N}(\delta q+\tau\delta p)\\ \mathcal{Q}(\delta q+\tau\delta p)+\mathcal{N}\delta p\end{pmatrix}-\begin{pmatrix}\mathcal{N}(\delta q+\tau\delta p)\\ \mathcal{Q}(\delta q+\tau\delta p)+\mathcal{N}\delta p\end{pmatrix}\cdot\begin{pmatrix}-\delta p'\\ \delta q'\end{pmatrix}\begin{pmatrix}-\delta p'\\ \delta q'\end{pmatrix}.$$

Similar to before, the first term is the time evolution under the tangent space dynamics and the second term ensures that this vector is orthogonal to the form evolved conjugate vector. This leads to two equations for the variable ζ. Using Eq. (44) and the result that $\mathcal{N}$ is its own inverse, it can be shown that operating on $\delta q'$ on the left with $\delta p\mathcal{N}$ gives the same result (to order ϵ) as operating on $\delta p'$ on the left with $\delta q\mathcal{N}$. Again the normalization condition $\delta q\cdot\delta q+\delta p\cdot\delta p=1$ is used and the order ϵ terms in the $\mathcal{Q}(\delta q+\tau\delta p)$ are neglected, so that Eq. (35) is obtained for ζ.

The same argument as the T and L modes then leads to the result for the Lyapunov exponent for the P modes

$$\lambda_n=K\beta_n'\beta_n, \tag{45}$$

where the total kinetic energy is given by $2K=\Sigma_j\mathbf{p}_j^2$. Again the negative exponent is simply $\lambda_{-n}=-\lambda_n$ for the P basis vector of the mode.

C. Comparisons with experiment

In Table I we compare the predicted values and numerical results for the Lyapunov exponents of the first six modes of each type, for a system where $N=200$. The first few T and P modes are quite accurate but the first L mode differs by 20% from the numerical result. Generally the results become less accurate with increasing mode number.

There are a number of possible sources of error. The accuracy of the dynamics is limited by the size of the neglected term ϵ and this increases with mode number n. Probably the most important limitation in the simplified conjugate GS procedure is that it assumes the functional forms for the modes are already orthogonal to the center space of Zero modes. At any finite N this is not correct and any more exact conjugate GS procedure would need to work systematically to ensure orthogonality with all previous modes. Thus, for example, to Gram-Schmidt the third T mode it should be explicitly made orthogonal to the center space, the first and second T modes and any LP modes with lower exponent values. This is because we are purposefully choosing to disregard the standard GS procedure—which works from the highest exponent down—and *after the fact* working outwards from the stable center zero space. This would be accomplished using only the knowledge of the placement of the Lyapunov modes within the spectrum and the known theoretical functional forms for the modes. Although we have performed this after the dynamics, there is no reason why this procedure could not easily be accomplished while the dynamics are performed. This suggests that a more sophisticated GS procedure may produce better results but this would be at the expense of the simplicity of the current scheme.

It has been shown previously [35] that the assumed functional form of the modes become less accurate as the mode number increases. The magnitude of the assumed functional form is initially very close to unity, but as the mode number increases, the magnitude decreases. This effect was more prevalent for LP modes, as the accuracy of the functional form for the $n=6$ LP mode was only 45% [35]. As this happens the fitted coefficients of the mode are smaller than they should be and thus the exponents calculated from them are also smaller. To correct the exponent values we divide them by the calculated magnitude of the functional form. Table II shows how the accuracy of the conjugate GS procedure changes if this known inaccuracy of the modes is taken into account. As expected, the increase in the accuracy is more noticeable for the LP modes than for the T modes. Table II shows that the corrected conjugate GS procedure produces exponents that are greater than 90% accurate, dropping to only 80% accurate for the least accurate.

We have now outlined the various forms of GS procedures: one for the first Transverse against all the modes "below" it (the zero space) and one where we use the conjugate mode only, showing that this gives us interesting insights. We propose that in order to gain a complete description of the system, including accurate modes and exponent values, a

TABLE II. A comparison of the corrected exponent predictions λ_{pred}^{corr} and the numerically observed Lyapunov exponents for a 200 particle QOD system with (H,P) boundary conditions at density $\rho=0.8$ and total kinetic energy $K=N$.

	T mode		P mode		L mode	
n	λ_{pred}^{corr}	λ_T	λ_{pred}^{corr}	λ_{LP}	λ_{pred}^{corr}	λ_{LP}
1	0.0388	0.0393	0.0603	0.0605	0.0515	0.0605
2	0.0757	0.0784	0.1215	0.1229	0.1033	0.1229
3	0.1121	0.1177	0.1718	0.1848	0.1552	0.1848
4	0.1471	0.1571	0.2170	0.2484	0.2046	0.2484
5	0.1838	0.1961	0.2460	0.3140	0.2384	0.3140
6	0.2156	0.2352	0.3709	0.3791	0.3944	0.3791

conjugate GS procedure should be introduced that systematically describes each mode as the original fitting function as well as a reorthogonalization with every mode "below" it from the center zero space out to the mode in question, ending in the conjugate orthogonalization we have shown.

VII. CONCLUSION

In conclusion, we have shown that the Lyapunov exponents for all Lyapunov modes can be calculated using a conjugate Gram-Schmidt procedure and a complete knowledge of the functional form of the modes. The same information that is obtained from the exponents is also encoded in the modes.

The simplified Gram-Schmidt procedure has only high accuracy for the first T and P mode components but the systematic approach suggested above may improve the accuracy, at the cost of the simplicity of the result. This result derives from the fact that some Lyapunov modes are "direction preserving" like the Zero modes $\delta\Gamma_y$ and $\delta\Gamma_{p_y}$, while others are "form preserving" like the Zero modes $\delta\Gamma_t$ and $\delta\Gamma_e$.

We have seen that the Lyapunov exponents—invariant eigenvalues of the system, quantities not dependent on the structure, basis or description of the phase space—can be found via the Lyapunov modes—eigenvectors of the system which depend greatly on the description of the phase space. There is always a relationship between an eigenvalue and its eigenvector, but usually not such a direct and explicit relation.

It has been shown that an *exact* theoretical description of the numerical mode can be found if the assumed form of the mode is made orthogonal to the center zero space; implying that any mode would be found with the same procedure extended to include any modes that are "between" the mode and the zero space.

In all numerical calculations of Lyapunov modes there are a set of modes which are stable below some maximum mode number $n_{\max}$. Here we require that ϵ in the dynamics of Eq. (21) is less than some threshold $\epsilon_{\max}$ which we can estimate from the numerics used to generate Table I. For a system of $N=200$ disks we find that $n_{\max}\sim 24$, and for the QOD system x_{ij} is positive and bounded by $\sqrt{1-L_y^2/4}<x_{ij}<1$. Therefore $\epsilon_{\max}\sim 0.35x_{ij}$ which corresponds to about eight particles per half wavelength. If the initial Lyapunov vector is modelike for a particular n then the dynamics will preserve its modelike character for $n<n_{\max}$ and it will be unstable for $n>n_{\max}$. The question of the stability or otherwise of a particular mode near $n_{\max}$ is a different level of stability for this system which we do not consider here.

A referee has commented that for a Lyapunov mode the long time average of the time derivative of δq is equal to $\lambda\delta q=\delta p$. This comes from the fact that δq changes continuously but δp only changes at collisions. This implies, for example, that the Lyapunov exponent for the first Transverse mode can be written as

$$\lambda_1=\frac{\gamma_1'}{\gamma_1}=\frac{N}{2}\frac{\gamma_1'\gamma_1}{1-\frac{N}{2}\gamma_1'^2}. \tag{46}$$

This is equal to our Eq. (41) when $\frac{N}{2}\gamma_1'^2$ is small and can be neglected. This implies that the conjugate Gram-Schmidt procedure is sufficient, by not necessary, to obtain the result we have presented. We thank the referee for this observation.

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