From Lyapunov modes to the exponents for hard disk systems

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(Dated: April 8, 2009)

We demonstrate the preservation of the Lyapunov modes by the underlying tangent space dynamics of hard disks. This result is exact for the zero modes and correct to order $\epsilon$ for the transverse and LP modes where $\epsilon$ is linear in the mode number. For sufficiently large mode numbers the dynamics no longer preserves the mode structure. We propose a Gram-Schmidt procedure based on orthogonality with respect to the centre space that determines the values of the Lyapunov exponents for the modes. This assumes a detailed knowledge of the modes, but from that predicts the values of the exponents from the modes. Thus the modes and the exponents contain the same information.

PACS numbers: 05.45.Jn, 05.45.Pq, 02.70.Ns, 05.20.Jj

In a chaotic system, the difference between two nearby phase space trajectories, the so called 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 example of a probabilistic treatment of the global behavior of deterministic microscopic dynamics. It is believed that the probabilistic axioms of statistical mechanics can be justified by the chaotic nature of the underlying dynamics, so much effort has been devoted to finding links between macroscopic quantities, such as transport coefficients, and chaotic properties such as the Lyapunov exponents. There have been some successes such as the conjugate pairing rule for the Lyapunov spectrum (the full set of Lyapunov exponents) and the fluctuation theorem. The stepwise structure of the Lyapunov spectrum consists of one-point steps and two-point steps. The one-point steps correspond to transverse modes while the two-points steps correspond to longitudinal and momentum proportional modes. The significant advantage of the QOD system is that both the exponents and the modes can be obtained to high accuracy by standard numerical schemes. For systems with smooth interaction potentials it has proved much more difficult to get clear numerical evidence for the steps in the Lyapunov spectrum and to find modes. However, the same structure must exist as the dynamics is subject to the same invariances and conservation properties.

The QOD system with (H,P) boundary conditions we studied contained $N$ hard disk particles. The complete description of the system at any time is contained in the $4N$-dimensional phase vector $(q,p)$ where $q = \{q_1, ..., q_N\}$ and $p = \{p_1, ..., p_N\}$ where $q_i$ and $p_i$ contain the $x$ and $y$ coordinates and momentum of particle $i$. The time evolution of the phase vector through a free flight, and then collision, is given by the matrix equation

$$\begin{pmatrix} q' \\ p' \end{pmatrix} = \begin{pmatrix} I & \tau I \\ O & N \end{pmatrix} \begin{pmatrix} q \\ p \end{pmatrix} \quad (1)$$

where each scripted matrix is an $N \times N$ matrix containing $2 \times 2$ sub matrices, $I$ is the identity and $O$ is the zero matrix. The matrix $N$ that changes the moments at collisions is given by

$$N = \begin{pmatrix} I & 0 & 0 & 0 \\ 0 & I - n_{ij}^T n_{ij} & n_{ij}^T & 0 \\ 0 & n_{ij} & I - n_{ij} n_{ij}^T & 0 \\ 0 & 0 & 0 & I \end{pmatrix} \quad (2)$$

where $n_{ij}$ are the $2 \times 2$ sub matrices of the vectors $q_i$ and $p_i$. The dynamics is then determined by the matrix $N$. The elements of $N$ are determined by the effective invariants and conservation properties.
Again, each element is itself a $2 \times 2$ sub-matrix. The term $n_{ij}^T = (x_{ij}, y_{ij})$ is a row vector containing the $x$ and $y$ components of the separation between particles $i$ and $j$ at collision, so that the dyadic product $n_{ij}n_{ij}^T$ is a $2 \times 2$ matrix.

We write the Lyapunov vectors as $(\delta q, \delta p)^T$ where $\delta q$ and $\delta p$ are $N$-dimensional vectors containing the 2-dimensional entries for each particle position separation $\delta q_j$ or momentum separation $\delta p_j$. For this QOD system there are four zero-Lyapunov exponents and hence four associated Zero (Z) Lyapunov modes. The numerically observed Z modes can be written as linear combinations of elements of the basis set [21] $\delta \Gamma_y = (\delta q, 0)$, $\delta \Gamma_{yy} = (0, \delta p)$, $\delta \Gamma_{ix} = (p, 0)/||p||$ and $\delta \Gamma_{e} = (0, p)/||p||$ where the $j^{th}$ element of $\delta q$ and $\delta p$ in $\delta \Gamma_y$ and $\delta \Gamma_{yy}$ is given by $\delta q_j \sim \delta p_j \sim \frac{1}{\sqrt{2}}$ (1), while $p$ is an $N$-dimensional vector whose $j^{th}$ component is $p_j$ (the momentum of particle $j$) and $||p||$ is the magnitude of the total momentum.

The time evolution equations for tangent space dynamics consist of many repeats of a free-flight followed by a collision and the Gram-Schmidt procedure. The first two of these steps, the application of a free-flight matrix then a collision matrix, evolve the tangent vector in time from 0 to $\tau$ and can be written as

$$
\begin{pmatrix}
\delta q(\tau)
\\
\delta p(\tau)
\end{pmatrix}
= 
\begin{pmatrix}
\mathcal{N} & 0 \\
\mathcal{Q} & \mathcal{N}
\end{pmatrix}
\begin{pmatrix}
I & \tau I
\\
0 & I
\end{pmatrix}
\begin{pmatrix}
\delta q
\\
\delta p
\end{pmatrix}
$$

(3)

where

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

(4)

Each component of the matrix $\mathcal{Q}$ is a $2 \times 2$ sub-matrix where the only non-trivial components are those associated with the two particles that collide, $i$ and $j$ through $Q_{ij}$. Then $Q_{ij}$ is given by

$$
Q_{ij} = (n_{ij} \cdot p_{ij}) \left[ I + \frac{n_{ij}n_{ij}^T}{n_{ij} \cdot p_{ij}} \right] \cdot \left[ I - \frac{p_{ij}n_{ij}^T}{n_{ij} \cdot p_{ij}} \right].
$$

(5)

where $p_{ij}^T = (p_{xij}, p_{yij})$ is a row vector containing the $x$ and $y$ components of the relative momenta at collision $(p_{ij} = p_j - p_i)$. The principle property that we will exploit now is that $Q_{ij} \cdot p_{ij} = 0$.

To understand the tangent vector dynamics we consider the action of the matrix $\mathcal{N}$ on either $\delta q$ or $\delta p$ which gives

$$
\mathcal{N} \delta q = \delta q + n_{ij}n_{ij}^T \cdot (\delta q_j - \delta q_i)X.
$$

(6)

where $X$ is the $N$-dimensional column vector with all elements equal to zero except for $X_i = 1$ and $X_j = -1$.

Note that for a QOD system $j = i + 1$, but otherwise the result is general.

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

$$
\mathcal{Q} \delta q = Q_{ij} \cdot (\delta q_j - \delta q_i)X.
$$

(7)

Any Lyapunov mode for which $\delta q_j - \delta q_i = 0$ or $\delta p_j - \delta p_i = 0$ exactly - such as the zero mode $\delta \Gamma_y$ - is preserved by the dynamics, while the conjugate zero mode grows linearly with time, so for example $\delta \Gamma_{yy}(\tau) = \delta \Gamma_{yy} + \tau \delta \Gamma_y$ [22].

The application of the dynamics on the momentum dependent $Z$ modes gives for $\delta \Gamma_i$ that $\mathcal{N}p = p$ and $\mathcal{Q}p = 0$ so that $(p, 0)/||p|| \to (p, 0)/||p||$ which is $\delta \Gamma_i$ at the new time. Therefore the functional form of $\delta \Gamma_i$ is preserved exactly. The conjugate mode is linear in time $\delta \Gamma_x(\tau) = \delta \Gamma_x + \tau \delta \Gamma_x$.

The numerically observed Lyapunov modes are of four types, $Z$ modes, transverse ($T$) modes, longitudinal ($L$) modes and momentum proportional ($P$) modes. The $L$ and $P$ are usually observed together as a combined $LP$ mode. The $T$ modes are given by

$$
\delta T^n = \begin{pmatrix}
\delta q \\
\delta p
\end{pmatrix}
= \begin{pmatrix}
\gamma_n \delta q_T \\
\gamma_n \delta p_T
\end{pmatrix}
$$

(8)

where $\gamma$ and $\gamma'$ are constants [23]. The components of both $\delta q_T$ and $\delta p_T$ are of the form $\delta q_j = \begin{pmatrix} 0 \end{pmatrix}$ where $c_{nj} = \cos k_n x_j$.

In a transverse mode the term $(\delta q_j - \delta q_i)$ in equations (8) and (9), becomes $(\delta y_j - \delta y_i) = -\epsilon \gamma n \sin(k_n x_i)$ where $\epsilon = k_n x_j = n \pi x_{ij}/L$. Here $x_{ij}$ is the $x$-component of the distance between particles $i$ and $j$ at collision and $L$ is the length of the system in the $x$-direction. The small parameter $\epsilon$ is linear in the mode number $n$. Thus the time evolution of a $T$ modes is given by

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

(9)

and henceforth we neglect the $\epsilon$ dependent terms. Clearly for sufficiently large $\epsilon$ the dynamics without the order $\epsilon$ term will become incorrect. We assume that below a threshold value of $\epsilon$ the dynamics in equation (9) is correct.

Further, for the $LP$ mode, the $P$ component is linear in the momentum, so that for example $\delta q_j = \beta_p p_j \cos k_n x_i$ then $\delta p_j - \delta q_j = \beta_p p_j \cos k_n x_i - c_{nj} \sin k_n x_i$. As $Q_{ij} \cdot p_{ij} = 0$ the first term is zero and the result is order $\epsilon$. The $LP$ modes are of the form

$$
\delta LP_1^n = \begin{pmatrix}
\delta q \\
\delta p
\end{pmatrix}
= s_{nt} \begin{pmatrix}
\beta_n p c \\
\beta_n p c
\end{pmatrix}
+ c_{nt} \begin{pmatrix}
\alpha_n \delta q_L \\
\alpha_n \delta p_L
\end{pmatrix}
$$

(10)

where $\beta_n$, $\beta_n'$, $\alpha_n$ and $\alpha_n'$ are constants [23]. The $N$-dimensional vector $pc$ has components $p_{ij}c_{nj}$, $s_{nt} = \sin \omega_n t$ and $c_{nt} = \cos \omega_n t$ (with frequency $\omega_n$). In the
case of (H,P) boundary conditions the LP exponents are doubly degenerate so there is a second LP mode $\delta LP^2_n$ with $s_n$ and $c_n$ interchanged which is orthogonal in time to $\delta LP^1_n$. This result means that the LP modes also have a time evolution governed by equation (11) with a different order $\epsilon$ term and again we assume that this dynamics is correct below some threshold $\epsilon$.

The numerically observed $T$ modes are invariants of the dynamics and the pair of LP modes define a two-dimensional sub-space. The action of the dynamics and Gram-Schmidt procedure therefore simply results in the $T$ mode remaining orthogonal to the centre space defined by the zero modes. This suggests that we can define an inside-out Gram-Schmidt procedure to obtain the same effect. 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 coefficients are known.

Given these assumptions we can calculate the values of the Lyapunov exponents in the step region. If we consider a $T$ or $L$ mode then under a free flight and collision using equation (9) the mode changes, but then the Gram-Schmidt procedure returns it to its initial direction with some scaling factor $\zeta$, as

$$
\left( \begin{array}{c} \delta q \\ \delta p \end{array} \right) \stackrel{\tau, \text{coll}}{\rightarrow} \zeta \left( \begin{array}{c} \delta q + \tau \delta p \\ \delta p \end{array} \right).
$$

The first right arrow is the action of the free flight and collision while the second right arrow is the result of the Gram-Schmidt procedure. Here we use a simplified inside-out Gram-Schmidt procedure in which we assume that the mode is already orthogonal to the centre space and then ensure orthogonality with respect to the conjugate mode.

Using the symplectic property of the system [28] the mode conjugate to $\delta T^{(n)}$ is

$$
\delta T^{(-n)} = \left( \begin{array}{c} -\delta p \\ \delta q \end{array} \right).
$$

Applying the inside-out Gram-Schmidt procedure to equations (11) gives

$$
\zeta \left( \begin{array}{c} \delta q \\ \delta p \end{array} \right) = \left( \begin{array}{c} \delta q + \tau \delta p \\ \delta p \end{array} \right) + \tau (\delta p \cdot \delta p) \left( \begin{array}{c} -\delta q \\ \delta q \end{array} \right)
$$

or two equations to solve for the scale factor $\zeta$. It is straightforward to see that as the mode is normalised $\delta q \cdot \delta q + \delta p \cdot \delta p = 1$ so both components of equation (13) give the same solution

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

The full time evolution is infinitely many repeats of this process: free-flight, collision and Gram-Schmidt, so the Lyapunov exponent is given by

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

For the mode $\delta T^n$, $\delta y_j = \gamma_n c_{nj}$ and $\delta p_{yj} = \gamma'_n c_{nj}$ so assuming that $\sum_j c_{nj}^2 = N/2$, we have

$$
\lambda_n = \frac{N}{2} \gamma'_n \gamma_n.
$$

Similarly, we can consider the evolution of the negative mode $\delta T^{-n}$ and by ensuring orthogonality with respect to its conjugate mode $\delta T^n$, the result will be $\lambda_{-n} = \frac{N}{2} \gamma_n \gamma'_n = -\lambda_n$.

Next treat the longitudinal part of the $LP$ mode without its explicit time dependence. Clearly this is just the same as the transverse mode and the result is

$$
\lambda_n = \frac{N}{2} \alpha'_n \alpha_n.
$$

We treat the momentum dependent part of the $LP$ mode without its explicit time dependence and ensure orthogonality with respect to the conjugate $P$ component. A similar argument leads to the result

$$
\lambda_n = N \beta'_n \beta_n T.
$$

where the temperature is given by $2NT = \sum_j p_j^2$. Again the negative exponent is simply $\lambda_{-n} = -\lambda_n$ for both $L$ and $P$ components of the mode.

In table I we compare the predicted and numerical results for the Lyapunov exponents of the first six modes of each type. The first $T$ mode and $P$ mode are quite accurate but the first $L$ mode is 20\% less than the numerical result. Generally the results become worse for higher order modes.

| $n$ | $\frac{1}{\rho} \delta n$ | $\lambda_n$ | $N \beta_n \gamma_n / T$ | $N \beta'_n \beta_n T$ | $N \alpha'_n \alpha_n$ | $N \lambda_n / T$ |
|-----|-----------------|-----------|--------------------------|--------------------------|--------------------------|----------------|
| 1   | 0.0388 0.0393  | 0.0599 0.0559 | 0.0602 0.0605 | 0.0602 0.0605 | 0.0602 0.0605 | 0.0602 0.0605 |
| 2   | 0.0749 0.0784  | 0.1169 0.1044 | 0.0965 0.1229 | 0.0965 0.1229 | 0.0965 0.1229 | 0.0965 0.1229 |
| 3   | 0.1099 0.1177  | 0.1507 0.1348 | 0.1344 0.1848 | 0.1344 0.1848 | 0.1344 0.1848 | 0.1344 0.1848 |
| 4   | 0.1431 0.1571  | 0.1753 0.1472 | 0.1591 0.2484 | 0.1591 0.2484 | 0.1591 0.2484 | 0.1591 0.2484 |
| 5   | 0.1748 0.1961  | 0.1693 0.1391 | 0.1595 0.3140 | 0.1595 0.3140 | 0.1595 0.3140 | 0.1595 0.3140 |
| 6   | 0.2007 0.2352  | 0.1855 0.1409 | 0.1823 0.3791 | 0.1823 0.3791 | 0.1823 0.3791 | 0.1823 0.3791 |
work systematically ensuring orthogonality with all previous modes. Thus, for example, to Gram-Schmidt the 3rd $T$ mode it should be explicitly made orthogonal to the centre space, the 1st and 2nd $T$ modes and any $LP$ modes with lower value exponents.

In conclusion, we have shown that the Lyapunov exponents for all types of modes can be calculated using an inside-out Gram-Schmidt procedure and a complete knowledge of the functional form of the modes. The simplified Gram-Schmidt procedure is only accurate 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. Thus we see that the same information that is encoded in the modes is also encoded in the values of the exponents.

In all numerical calculations of Lyapunov modes there are a set of modes which are stable below some maximum mode number $n_{\text{max}}$. Here we require that $\epsilon$ in the dynamics of equation (9) is less than some threshold $\epsilon_{\text{max}}$ which we can estimate from the numerics used to generate table 1. For a system of $N = 200$ disks we find that $n_{\text{max}} \sim 24$, and for the QOD system $x_{ij}$ is positive and bounded by $\sqrt{1 - L^2/4} < x_{ij} < 1$. Therefore $\epsilon_{\text{max}} \sim 0.35 x_{ij}$ which corresponds to about 8 particles per half wavelength. If the initial Lyapunov vector is mode-like for a particular $n$ then the dynamics will preserve its mode-like character for $n < n_{\text{max}}$ and it will be unstable for $n > n_{\text{max}}$. The question of the stability or otherwise of a particular mode is a different level of stability for this system.

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