Time-dependent mode structure for Lyapunov vectors as a collective movement in quasi-one-dimensional systems

Tooru Taniguchi and Gary P. Morriss

School of Physics, University of New South Wales, Sydney, New South Wales 2052, Australia

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Time dependent mode structure for the Lyapunov vectors associated with the stepwise structure of the Lyapunov spectra and its relation to the momentum auto-correlation function are discussed in quasi-one-dimensional many-hard-disk systems. We demonstrate mode structures (Lyapunov modes) for all components of the Lyapunov vectors, which include the longitudinal and transverse components of their spatial and momentum parts, and their phase relations are specified. These mode structures are suggested from the form of the Lyapunov vectors corresponding to the zero-Lyapunov exponents. Spatial node structures of these modes are explained by the reflection properties of the hard-walls used in the models. Our main interest is the time-oscillating behavior of Lyapunov modes. It is shown that the largest time-oscillating period of the Lyapunov modes is twice as long as the time-oscillating period of the longitudinal momentum auto-correlation function. This relation is satisfied irrespective of the particle number and boundary conditions. A simple explanation for this relation is given based on the form of the Lyapunov vector.

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I. INTRODUCTION

Statistical mechanics based on dynamical instability has drawn considerable attention in recent years. The dynamical instability is described as a rapid separation of two nearby trajectories, the so called Lyapunov vector, and causes the loss of memory or unpredictability of the dynamical system. The exponential rate of expansion or contraction of the magnitude of the Lyapunov vector is called the Lyapunov exponent, and its positivity, meaning that the system is chaotic, is a well known indicator of the dynamical instability. Many efforts have been devoted to connect the dynamical instability with statistical properties, like transport coefficients. Some works concentrated on specific effects of the dynamical instability in many-particle systems. Information on the dynamical instability in many-particle systems is given by the set of Lyapunov exponents (the Lyapunov spectrum) and their associated Lyapunov vectors, and their structures have been of much interest to the study of chaotic properties of many-particle systems. The conjugate pairing rule of Lyapunov spectra for thermostated systems, localized behaviors for Lyapunov vectors, and the thermodynamic limit of Lyapunov spectra and so on have been discussed from this point of view.

The stepwise structure of Lyapunov spectra is a typical chaotic property of many-particle systems, which was found recently. This stepwise structure appears in the Lyapunov exponents with smallest absolute value, and the dynamical structure of these Lyapunov exponents should reflect a slow and global behavior of the macroscopic system. Therefore, clarification of the stepwise structure of Lyapunov spectra (Lyapunov steps) is expected to make a bridge between the macroscopic statistical theory and the microscopic chaotic dynamics. Remarkably, the Lyapunov steps accompany wavelike structures in the associated Lyapunov vectors, namely the Lyapunov modes, which offer a useful tool to understand the origin of the stepwise structure of the Lyapunov spectrum. Originally, these structures were observed in many-hard-disk systems, but very recently numerical evidence for the Lyapunov modes was reported for many-particle system with soft-core particle interactions. Some theoretical arguments have been proposed to explain this phenomenon, for example, using random matrix theory, kinetic theory, and periodic orbit theory, etc.

The first step to understand the Lyapunov step and mode is in the zero Lyapunov exponents and the associated Lyapunov vectors. For instance, the two-dimensional system consisting of N particles with periodic boundary conditions has six zero-Lyapunov exponents, and the associated Lyapunov vectors are linear combinations of the six basis vectors $N^{-1/2}(1,0,0,0)$, $N^{-1/2}(0,1,0,0)$, $N^{-1/2}(0,0,1,0)$, $N^{-1/2}(0,0,0,1)$, $|p|^{-1}(p_x,p_y,0,0)$, and $|p|^{-1}(0,0,p_x,p_y)$ where $0$ is a N-dimensional null vector, $1$ is an N-dimensional vector with all $x$-component equal to 1, and $p \equiv (p_x,p_y)$ is the momentum vector with its $x$-component $p_x$ and $y$-component $p_y$. Here, the first (second) vector is associated with the translational invariance in the $x$-direction (y-direction), the third (fourth) vector with the conservation of the $x$-component (y-component) of the total momentum, the fifth vector with the time-translational invariance (deterministic nature of the orbit), and the last vector with the energy conservation. This means that the six sets of the Lyapunov vector components $\{\delta x_j^{(n)}\}_j$, $\{\delta y_j^{(n)}\}_j$, $\{\delta p^{(n)}_{xj}\}_j$, $\{\delta p^{(n)}_{yj}\}_j$, $\{\delta y_j^{(n)}/p_{yj}\}_j$, and $\{\delta p^{(n)}/p_{xj}, \delta p^{(n)}/p_{yj}\}_j$ can have equal components independent of the particle number index $j$ in zero-Lyapunov exponents. Here, we use the notation $\delta \Gamma^{(n)} = (\delta q^{(n)}, \delta p^{(n)})$ for the Lyapunov...
vector corresponding to Lyapunov exponents $\lambda^{(n)}$, and $\delta \mathbf{q}^{(n)} \equiv (\delta x_1^{(n)}, \delta x_2^{(n)}, \ldots, \delta x_N^{(n)}, \delta y_1^{(n)}, \delta y_2^{(n)}, \ldots, \delta y_N^{(n)})$ and $\delta \mathbf{p}^{(n)} \equiv (\delta p_{x_1}^{(n)}, \delta p_{x_2}^{(n)}, \ldots, \delta p_{x_N}^{(n)}, \delta p_{y_1}^{(n)}, \delta p_{y_2}^{(n)}, \ldots, \delta p_{y_N}^{(n)}$ are the spatial and the momentum part of the Lyapunov vector, respectively.

As the next step we regard the degeneracy of the zero-Lyapunov exponents and the structure of the corresponding Lyapunov vectors as the zero-th Lyapunov step and mode. This scenario was proposed first in Ref.~[18], and was also discussed very recently in Ref.~[20]. First of all, the Lyapunov steps for the two-dimensional system with periodic boundary conditions consist of two-point steps and four-point steps~[17, 18], namely the number of Lyapunov exponents for one set of Lyapunov steps is six, which is equal to the number of the zero-Lyapunov exponents. It is also known that the stepwise structure of Lyapunov spectra is changed by violating the spatial translational invariance and the total momentum conservation, which also change the number of zero-Lyapunov exponents~[13]. As a second point, some mode structures were observed in some of the above Lyapunov vector components, which should be constant in zero-Lyapunov exponents. For example, a mode structure in the Lyapunov vector component $\delta y_j^{(n)}$ (the transverse spatial translational invariance Lyapunov mode) is well known~[17]. This mode is stationary in time, and appears in one of the two types of the Lyapunov steps. Ref.~[18] showed another mode structure in $\delta y_j^{(n)}/p_{yj}$, (the transverse time translational Lyapunov mode). This mode depends on time, and appears in other types of the Lyapunov steps. These Lyapunov modes are enough to categorize all the Lyapunov steps. Ref.~[17, 18] also claim a moving mode structure in $\delta x_j^{(n)}$.

However, there has not been enough evidence yet to confirm the above scenario for the Lyapunov steps and modes. For example, the mode structure in the momentum part of Lyapunov vectors has not been reported explicitly. Besides, the phase relations of different modes, for example, the modes in $\delta y_j^{(n)}/p_{yj}$ and $\delta x_j^{(n)}$, have not been discussed. Another important point is the time scale specified by a time-dependent Lyapunov mode, like the time-oscillation for the mode in $\delta y_j^{(n)}/p_{yj}$. The time-oscillating period is usually much longer than the mean free time of the system, and it should correspond to a collective movement, but quantitative evidence for it has not been shown explicitly.

As an indicator for collective movements of many-particle systems, we can use the momentum auto-correlation functions, where collective movement may appear as a time-oscillation behavior~[27] as observed in many macroscopic models~[28, 29, 31, 32]. The auto-correlation functions are accessible experimentally using neutron and light scattering techniques~[32, 33, 34, 35]. As an essential aspect of auto-correlation functions is their role as response functions for the system. For example, linear response theory connects the time integral of the auto-correlation function with a transport coefficient~[36]. However it should be emphasized that the auto-correlation functions themselves provide much more detailed information about the system. Linear response theory requires the time-integral and the thermodynamic limit of the auto-correlation function to calculate transport coefficients, and in this process information about short time-scales and a finite size effects are lost. For instance, the time-oscillation of the auto-correlation functions is one of the finite size effects, which linear response theory does not treat. Information on short time-scales and finite size effects in the auto-correlation functions also plays an important role in the generalized hydrodynamics~[37] and generalized Fokker-Planck equation~[38].

The purposes of this paper are two-fold. First we calculate all components of the Lyapunov vectors associated with the stepwise structure of the Lyapunov spectrum. They include the longitudinal and transverse components of both the spatial and momentum parts of the Lyapunov vectors. We demonstrate the wave-like structures in the components of the Lyapunov vectors, and specify their phase relations. These results support the above explanation for the origin of the Lyapunov steps and modes based on the zero-Lyapunov exponents and the associated Lyapunov vectors. Spatial node structures of these Lyapunov modes are explained in terms of boundary conditions. It is emphasized that some of the Lyapunov modes show time-oscillating behaviors, and a particle number dependence in their time-oscillating periods. The second purpose of this paper is to discuss the connection between the time-oscillation of the Lyapunov modes and the momentum auto-correlation functions. Our central result is that the longest time-oscillating period of the Lyapunov modes is twice as long as that for the auto-correlation function for the longitudinal component of the momentum. This relation is satisfied irrespective of the number of particles in the system and the boundary conditions. We give a simple explanation for this relation. This result means that the time-oscillating behavior of the Lyapunov vectors is reflected by a collective movement within many-particle systems. This also gives some evidence to connect the Lyapunov mode, a tangent space property specified by Lyapunov vectors, to the auto-correlation function, which is a phase space property and is accessible experimentally.

We use a quasi-one-dimensional many-hard-disk system, as this model allows fast numerical calculation of the Lyapunov exponents and vectors, and shows clear Lyapunov steps and modes. In general the numerical calculation of the Lyapunov spectrum and vectors are very time-consuming, and it is often difficult to get clear Lyapunov mode structures, particularly for time-dependent Lyapunov modes. If the above picture of the Lyapunov steps and modes based on universal properties such as the translational invariances and the conservation laws can be justified, then a simple model should be sufficient to convince us of their origin. This system also exhibits a clear oscillatory behavior in the longitudinal
momentum auto-correlation function. A useful technique to get clear Lyapunov steps and modes is to use hard-wall boundary conditions. Although hard-wall boundary conditions destroy the spatial translational invariance and the total momentum conservation, and lead to different structure in the Lyapunov spectrum compared to periodic boundary conditions, it has been shown that there is a simple relation between the observed Lyapunov steps and modes and different boundary conditions \[18\]. Specifically, we use a quasi-one-dimensional system with hard-wall boundary conditions in the longitudinal direction and periodic boundary conditions in the transverse direction. Usually, the hard-wall boundary conditions make numerical calculation slower compared to periodic boundary conditions, but in our system only the two particles at each end of the system collide with the hard-walls so the effect is small.

The outline of this paper is as follows. In Sec. II the quasi-one-dimensional system is introduced. In Sec. III we discuss the Lyapunov steps and modes. In Sec. IV the momentum auto-correlation functions and their relation with the Lyapunov modes is discussed. Finally we give some conclusion and remarks in Sec. V.

II. QUASI-ONE-DIMENSIONAL SYSTEM

The model considered in this paper is a quasi-one-dimensional many-hard-disk system. It is a two-dimensional rectangular system consisting of many hard-disks with the width of the system so narrow that the disk positions are not exchanged, thus the disks can be numbered from left to right. We assume that the mass \( m \) and the radius \( R \) of each disk is the same. In this case the quasi-one-dimensional system has a width \( L_y \) that satisfies the condition \( 2R < L_y < 4R \). Figure 1 gives a schematic illustration of the quasi-one-dimensional system with the particles numbered \( 1, 2, \cdots, N \) (\( N \): particle number) from the left to right.

![FIG. 1: A schematic illustration of a quasi-one-dimensional system used in this paper. The system shape is so narrow that particles always remain in the same order. Here, \( L_x \) (\( L_y \)) is the length (width) of the system in the longitudinal (transverse) direction, and \( R \) is the radius of a particle. The dashed lines represent periodic boundary conditions and the solid lines represent hard-wall boundary conditions. The particles are numbered \( 1, 2, \cdots, N \) from the left to the right.](image)

Originally, the quasi-one-dimensional many-hard-disk system was introduced as a system to easily and clearly observe the stepwise structure of Lyapunov spectrum (which we call the “Lyapunov steps”) and the corresponding wave-like structure of Lyapunov vectors (the so called ”Lyapunov modes”) \[18\]. Numerical observation of the Lyapunov steps and modes is very time-consuming, and even at present the Lyapunov spectra is limited to about 1000 particles \[17\]. Therefore it is valuable to explore fast and effective ways to calculate them numerically. It is well known that the rectangular system has a wider stepwise region than a square system with the same area and number of particles. This quasi-one-dimensional system is the most rectangular two-dimensional system possible. Ref. \[18\] demonstrated that in the quasi-one-dimensional system we can clearly observe the structure of the Lyapunov modes. It is known that there are two kinds of Lyapunov modes: stationary modes and time-dependent modes. The stational Lyapunov modes are much more easily observed because of their stable structure, but generally the observation of the time-dependent Lyapunov modes is much harder because of large fluctuations in their structure and their intrinsic time-dependence. The quasi-one-dimensional system is the first system in which time-oscillating Lyapunov modes were demonstrated \[18\].

Another advantage of the quasi-one-dimensional system is that the particle interactions in this system are restricted to nearest-neighbor particles only, so we need much less effort to find colliding particle pairs numerically compared with the fully two-dimensional system in which each particle can collide with any other particle. This leads to faster numerical calculation of the system dynamics. Besides, in this system, particle movement in the narrow direction is suppressed, compared to the longitudinal direction, and roughly speaking the particle sequence corresponds to the particle position. This leads to a much simpler representation of Lyapunov modes, which must be investigated as functions of spatial coordinates and time. One may also notice that in the quasi-one-dimensional system the system size is proportional to the particle number \( N \), while for the square system it is proportional to \( \sqrt{N} \). This implies that in the quasi-one-dimensional system, many-particle effects are more evident than in the fully two-dimensional systems with the same number of particles.

Another important point in the quasi-one-dimensional system is the effect of boundary conditions. Different from the square system, in which the boundary length is proportional to the square root of the system size, in the quasi-one-dimensional system the boundary length is proportional to the system size itself, therefore we cannot neglect its effect even in the thermodynamic limit. Actually Ref. \[18\] showed that the Lyapunov steps and modes depend strongly on boundary conditions. Boundary conditions change, not only the structure of Lyapunov steps and modes, but also the clearness of Lyapunov mode structure. For example, a system with purely hard-wall boundary conditions has no stationary Lyapunov mode and its corresponding Lyapunov steps and show much clearer time-oscillating Lyapunov modes, compared to a system with the periodic boundary conditions. Roughly speaking, hard-wall boundary conditions pin the positions of the nodes and thus lead to...
clearer Lyapunov modes. On the other hand, the numerical calculation with the hard-wall boundary conditions is more time-consuming. This disadvantage is significant in the quasi-one-dimensional system with purely hard-wall boundary conditions. As another disadvantage of the system with purely hard-wall boundary conditions, we cannot investigate the stationary Lyapunov mode due to spatial translational invariance. As an optimal system we mostly consider a quasi-one-dimensional system with hard-wall boundary conditions in the longitudinal direction and periodic boundary conditions in the transverse direction. We use the notation (H,P) for this boundary condition throughout this paper. In Fig. we represent the boundary condition (H,P) as different types of lines on the boundaries: the bold solid lines signify hard-wall boundary conditions and the broken lines signify periodic boundary conditions. In this system we can get much clearer Lyapunov modes than for purely periodic boundary conditions and we observe both types of Lyapunov steps and modes.

Although the quasi-one-dimensional many-hard-disk system with the boundary condition (H,P) may be artificially introduced to investigate Lyapunov steps and modes in a fast and effective way, it is essential to note that the results from this system can be used to predict Lyapunov steps and modes in more general systems, such as a fully two-dimensional system with purely periodic boundary conditions. Details of the relation of the Lyapunov steps and modes in quasi-one-dimensional systems with different boundary conditions were given in Ref. [18]. For example, the step widths of the Lyapunov spectrum (the spatial and time periods of the corresponding Lyapunov modes) in the system with the boundary condition (H,P) are halves (twice) the ones in the system with the purely periodic boundary conditions (P,P). It is also known that the structure of Lyapunov steps for the quasi-one-dimensional system is the same as the fully two-dimensional system.

As we discussed above, the main reason to use the quasi-one-dimensional system with the boundary condition (H,P) is to get clear Lyapunov steps and modes in a fast numerical calculation. On the other hand, these advantages may not assist the calculation of the momentum auto-correlation function. In the quasi-one-dimensional system, collisions of a particle are restricted to its two nearest-neighbor particles only, so it may be supposed that specific types of collisions like the "back scattering effect" play an important role in this system. The back scattering effect, which comes from a reversal of the velocity of a particle by a collision with the nearest neighbor particle, can lead to a negative region of the momentum auto-correlation function. One may also suppose that in the quasi-one-dimensional system a collective motion may be enhanced, because the movement of particles in the narrow direction is very restricted. This may lead to a clear time-oscillation of the momentum auto-correlation function, as will be actually observed in Sect. IV of this paper. It may also be noted that boundary condition effects on the momentum auto-correlation function are not well known. Because we need to know about them to be able to guess the relation between the auto-correlation functions and Lyapunov modes in different boundary conditions, we will discuss boundary condition effects on momentum auto-correlation function briefly in Sect. IV C.

In this paper we use units where the mass m and the particle radius R are 1, and the total energy E is N (except in Sec. IV D). For the numerical calculations, the system lengths are chosen as \( L_x = 1.5N^2 + 2R \) and \( L_y = 2R(1 + 10^{-6}) \) for the quasi-one-dimensional system with the boundary condition (H,P).

### III. LYAPUNOV STEPS AND MODES

In this section we discuss the Lyapunov steps and modes in the quasi-one-dimensional system with boundary condition (H,P). Part of these results have already been presented in Ref. [18], and here we complete this presentation. Some of the discussions omitted in Ref. [18] were the relation between the time-oscillating Lyapunov mode proportional to the momentum and the longitudinal Lyapunov modes, the Lyapunov modes for the momentum parts of Lyapunov vectors, and the particle number dependence of the time-oscillating period of the Lyapunov modes.

We introduce the Lyapunov spectrum as the ordered set of the Lyapunov exponents \( \lambda^{(n)}, n = 1, 2, \ldots, 4N \), where \( \lambda^{(1)} \geq \lambda^{(2)} \geq \cdots \geq \lambda^{(4N)} \). The notations \( \delta q_j^{(n)} = (\delta x_j^{(n)}, \delta y_j^{(n)}) \) and \( \delta p_j^{(n)} = (\delta p_{xj}^{(n)}, \delta p_{yj}^{(n)}) \) are used for the spatial and momentum components, respectively, of the \( j \)-th particle Lyapunov vector corresponding to the \( n \)-th Lyapunov exponent \( \lambda^{(n)} \).

For a numerical calculation of the Lyapunov spectrum and the Lyapunov vectors, we used the numerical algorithm developed by Benettin et al. [32] and Shimada et al. [40] (Also See Refs. [41, 42]). This algorithm is characterized by regular re-orthogonalizations and renormalization of set of Lyapunov vectors, which can be done after each particle collision in a many-hard-disk system. Usually the Lyapunov steps and modes appear after a long trajectory calculation, and we typically calculated trajectories of more than \( 5 \times 10^5 \) particle collisions to get the Lyapunov spectra and vectors shown here.

The main purpose in this section is to investigate the time-oscillating structures in the transverse and longitudinal Lyapunov modes. As we mentioned in Sect. IV the numerical calculation of Lyapunov spectra and Lyapunov vectors for many-particle systems is time-consuming even in the quasi-one-dimensional system, and in this paper we present results of 100 particle systems. In such a rather small system the structure of the Lyapunov modes has large fluctuations in space and time, which prevents the appearance of clear mode structures. Another problem appears in the investigation of the Lyapunov modes.
Ruelle}. The stepwise structure of the Lyapunov spectrum in this system is one and two-point steps. These two kinds of Lyapunov steps accompany different mode structures in the Lyapunov vectors: one is the stationary modes, as discussed in subsections III B and the other is time-oscillating modes, as discussed in the subsection III C. Here we count the sequence of Lyapunov steps from the zero Lyapunov exponents, so $\lambda^{(200)}$ and $\lambda^{(199)}$ are the zero exponents, $\lambda^{(198)}$ is the first one-point step, $\lambda^{(197)}$ and $\lambda^{(196)}$ are the first two-point step, $\lambda^{(195)}$ is the second one-point step, and $\lambda^{(194)}$ and $\lambda^{(193)}$ are the second two-point step, see Fig. 2.

**B. Stationary Lyapunov modes**

First we discuss the Lyapunov mode corresponding to the first and second one-point steps in Fig. 2. Fig. 3 shows the graph of the Lyapunov vector components corresponding to the first and second one-point step as a function of the collision number $n_t$ and the normalized local time average $(x_j)/L_x$ of the $x$-component of the particle position. Here, Fig. 3(a) is for the local time-averages of $\langle \delta x_j^{(198)} \rangle_t$ and $\langle \delta y_j^{(198)} \rangle_t$ for the first one-point step $\lambda^{(198)}$, and Fig. 3(b) is a similar graph for the second one-point step $\lambda^{(195)}$. These one-point steps are indicated by arrows in Fig. 2. Both graphs have the same collision number interval $[524000, 569600]$. On the base of each of Figs. 3(a) and (b) we give contour-plots of the transversal modes $\langle \delta y_j^{(198)} \rangle_t$ and $\langle \delta y_j^{(195)} \rangle_t$, respectively, in which the dotted lines, the solid lines, and the broken lines correspond to the levels -0.08, 0, and +0.08, respectively.

![FIG. 2: Stepwise structure of the Lyapunov spectrum normalized by the largest Lyapunov exponent for the quasi-one-dimensional many-hard-disk system with 100 particles with (H,P) boundary condition. The entire positive branch of the Lyapunov spectrum is shown in the inset to this figure. In a Hamiltonian system, the negative branch of the Lyapunov spectrum takes the same absolute value as the positive branch of the Lyapunov spectrum from the conjugate pairing rule: $\lambda^{(4N-n+1)} = -\lambda^{(n)}$, $n = 1, 2, \ldots, 2N/4$, so they are omitted in Fig. 2.](image-url)

This system has 4 zero-Lyapunov exponents, which come from the conservation of the $y$-component of the total momentum and the center of mass, energy conservation, and the deterministic nature of the orbit. Note that the $x$-component of the total momentum and the center of mass are not conserved, because of the hard-wall boundary condition in the $x$-direction. Half of these 4 zero-Lyapunov exponents appear in Fig. 2.

The stepwise structure of the Lyapunov spectrum in this system is one and two-point steps. These two kinds of Lyapunov steps accompany different mode structures in the Lyapunov vectors: one is the stationary modes, as discussed in subsections III B and the other is time-oscillating modes, as discussed in the subsection III C. Here we count the sequence of Lyapunov steps from the zero Lyapunov exponents, so $\lambda^{(200)}$ and $\lambda^{(199)}$ are the zero exponents, $\lambda^{(198)}$ is the first one-point step, $\lambda^{(197)}$ and $\lambda^{(196)}$ are the first two-point step, $\lambda^{(195)}$ is the second one-point step, and $\lambda^{(194)}$ and $\lambda^{(193)}$ are the second two-point step, see Fig. 2.

**B. Stationary Lyapunov modes**

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**FIG. 3: Local time averages of $\langle \delta x_j \rangle_t$ and $\langle \delta y_j \rangle_t$ for the first two-point step (exponent 198) in (a), and for the second two-point step (exponent 195) in (b). These are shown as functions of the collision number $n_t$ and the normalized local time average $(x_j)/L_x$ of the $x$-component of the $j$-th particle position (with the system length $L_x$). The corresponding Lyapunov exponents $\lambda^{(198)}$ and $\lambda^{(195)}$ are indicated by arrows in Fig. 2. The base of each graph are the contour plots of the transverse Lyapunov modes at the levels -0.08 (broken lines), 0 (solid lines), and +0.08 (dotted lines).**

In Fig. 3 we recognize spatial wave-like structures in the transverse components of $\langle \delta y_j^{(n)} \rangle_t$ for $n = 198$ and 195 which are stationary in time (at least in a time interval of more than $45 \times 10^6$ collisions as shown in this figure). These wave-like structures are very nicely fitted by sinusoidal functions. Note that in the calculation of Lyapunov vectors we used the numerical algorithm which
imposed renormalization of the Lyapunov vectors at every collision, so that the amplitudes of any component of the Lyapunov vector must be less than 1. It should be emphasized that anti-nodes in the modes appear at the end of the system in the $x$-direction. By comparison the amplitudes of the longitudinal components of $(\delta x_j^{(n)})_t$ for $n = 198$ and 196 are extremely small. These observations suggest that the Lyapunov mode corresponding to the $k$-th one-point Lyapunov step is approximately represented by

$$
\delta x_j^{(\mu(k))} \approx 0,
$$

$$
\delta y_j^{(\mu(k))} \approx \alpha_k \cos \left( \frac{\pi k}{L_x} x_j \right), \tag{2}
$$

$j = 1, 2, \ldots, N$, corresponding to the Lyapunov exponents $\lambda^{(\mu(k))}$, in which $\alpha_k$ is a constant and $\mu(k)$ is the Lyapunov index corresponding to the $k$-th one-point step of the Lyapunov spectrum. Here we take the origin of the $x$-component of the spatial coordinate to be $x_j = 0$, so that an ambiguity in spatial phase can be removed in Eq. (4).

C. Time-oscillating Lyapunov modes

Now we discuss the remaining Lyapunov modes, which correspond to the two-point steps of the Lyapunov spectrum. Figure 4 shows the graphs of the local time averages of $\langle \delta x_j^{(197)} \rangle_t$, $\langle \delta x_j^{(197)}/p_{xj} \rangle_t$, $\langle \delta y_j^{(197)} \rangle_t$, and $\langle \delta y_j^{(197)}/p_{yj} \rangle_t$ as functions of the collision number $n_t$ and normalized local time averaged position $\langle x_j \rangle_t/L_x$ of the $j$-th particle. The number of particles is $N = 100$, and the four graphs are for the same collision number interval $n_t \in [535200, 569600]$. These correspond to the first exponent on the first two-point step, exponent 197, in Fig. 2. In these figures, we draw a contour plot on the base of each three dimensional graph at levels $-0.08$ (dotted lines), $0$ (solid lines), and $+0.08$ (broken lines).

We can easily recognize spatial wave-like structures with time-oscillations in Figs. 4(a) and (d). In Fig. 4(a), the longitudinal Lyapunov vector component $\langle \delta x_j^{(197)} \rangle_t$ has nodes at the ends of the quasi-one-dimensional system, and the wave-length is given by $2L_x$. On the other hand, in Fig. 4(d), the transverse Lyapunov vector component $\langle \delta y_j^{(197)}/p_{yj} \rangle_t$ has anti-nodes at the end of the system and has a node at the middle, although its wave-length is given by $2L_x$ as for the longitudinal modal of Fig. 4(a).

There is also a time-oscillating wave-like structure in the longitudinal Lyapunov vector component $\langle \delta x_j^{(197)}/p_{xj} \rangle_t$, as shown in Fig. 4(b). This structure is different from the one shown in Fig. 4(a) associated with the same longitudinal Lyapunov vector component $\delta x_j^{(197)}$. It has anti-nodes at the ends of the system, and has a node in the middle. Its wave-length is $2L_x$. These characteristics suggest that although there are large fluctuations in the middle of the system, the time-oscillating wave-like structure in Fig. 4(b) is the same as that in Fig. 4(d). In Fig. 4(c) it is rather difficult to recognize any structure. Roughly speaking, it is just random fluctuations, in middle of the system but the amplitude of such fluctuations is small compared to region at the end of the system. However such small amplitude fluctuations are required for consistency with Fig. 4(d), namely the fact that in this region the value of $\delta y_j^{(197)}/p_{yj}$ is small, so that the value of $\delta y_j^{(197)}$ itself should be small with an almost position independent momentum $p_{yj}$.

Next we discuss the phase relations for the Lyapunov modes of the first two-point steps, corresponding to exponents $\lambda^{(196)}$ and $\lambda^{(197)}$ (the black-filled circles with brace underneath in Fig. 2). Figure 5 shows the contour plots of the local time averages of $\langle \delta x_j \rangle_t$, $\langle \delta x_j/p_{xj} \rangle_t$, and $\langle \delta y_j/p_{yj} \rangle_t$, and for $\lambda^{(196)}$ and $\lambda^{(197)}$ as functions of the collision number $n_t$ and the normalized local time average $\langle x_j \rangle_t/L_x$ of the position of the $j$-th particle at levels $-0.08$, $0$, and $+0.08$, for a 100-particle system. The six graphs in Fig. 5 have the same collision number interval [535200, 569600], and Figs. 5(a), (c), and (e) correspond to Figs. 4(a), (b), and (d), respectively.

FIG. 4: Local time averages of $\langle \delta x_j \rangle_t$, $\langle \delta x_j/p_{xj} \rangle_t$, $\langle \delta y_j \rangle_t$, and $\langle \delta y_j/p_{yj} \rangle_t$ for the Lyapunov modes corresponding to the first exponent of the first two-point step ($\lambda^{(197)}$), as functions of the collision number $n_t$ and the normalized local time average $\langle x_j \rangle_t/L_x$ of the $x$-component of the position of the $j$-th particle. The base of each graph is a contour plot of the three dimensional graph at the levels $-0.08$ (dotted lines), $0$ (solid lines), and $+0.08$ (broken lines).

FIG. 5: Contour plots of the local time averages of $\langle \delta x_j \rangle_t$, $\langle \delta x_j/p_{xj} \rangle_t$, $\langle \delta y_j/p_{yj} \rangle_t$, for the first two-point steps ($\lambda^{(197)}$ (a,c,e) and $\lambda^{(196)}$ (b,d,f)), as functions of the collision number $n_t$ and the normalized local time average $\langle x_j \rangle_t/L_x$ of the position of the $j$-th particle in the same collision number interval [535200, 569600]. The dotted lines, the solid lines, and the broken lines are contour lines at the levels $-0.08$, $0$, and $+0.08$, respectively.

Figure 5 shows that the two Lyapunov exponents for the same two-point step have the same structure of Lyapunov modes, but they are orthogonal in time, namely node lines of the Lyapunov modes corresponding to the Lyapunov exponent $\lambda^{(197)}$ correspond to anti-node lines of the ones of $\lambda^{(196)}$. We also notice that the node lines of the Lyapunov modes in $\langle \delta x_j^{(n)} \rangle_t/p_{xj}$ and $\langle \delta y_j^{(n)} \rangle_t/p_{yj}$ coincide with each other in space and time ($n = 197, 196$),

...
on the other hand the Lyapunov modes in $\langle \delta x_j^{(n)} \rangle_t$ and $\langle \delta x_j^{(n)}/p_{xj} \rangle_t$ are orthogonal in space and time at the same Lyapunov index.

The above discussions based on Figs. 4 and 5 (and similar observations of Lyapunov modes in the other two-point steps of the Lyapunov spectrum) lead to the conjecture that the spatial part of Lyapunov vector components $\delta x_j^{(\nu(k))}$ and $\delta y_j^{(\nu(k)-1)}$ corresponding to the Lyapunov exponents constructing the $k$-th two-point step are approximately expressed as

$$
\delta x_j^{(\nu(k))} \approx \alpha_k' p_{xj} \cos \left( \frac{\pi k}{L_x} x_j \right) \cos \left( \frac{2\pi k}{T_{lya}} n_t + \beta_k' \right) + \hat{\alpha}_k' \sin \left( \frac{\pi k}{L_x} x_j \right) \sin \left( \frac{2\pi k}{T_{lya}} n_t + \beta_k' \right)
$$

$$
\delta x_j^{(\nu(k)-1)} \approx \alpha_k'' p_{xj} \cos \left( \frac{\pi k}{L_x} x_j \right) \sin \left( \frac{2\pi k}{T_{lya}} n_t + \beta_k' \right) + \hat{\alpha}_k'' \sin \left( \frac{\pi k}{L_x} x_j \right) \cos \left( \frac{2\pi k}{T_{lya}} n_t + \beta_k' \right)
$$

$$
\delta y_j^{(\nu(k))} \approx \alpha_k' p_{yj} \cos \left( \frac{\pi k}{L_x} x_j \right) \cos \left( \frac{2\pi k}{T_{lya}} n_t + \beta_k' \right)
$$

$$
\delta y_j^{(\nu(k)-1)} \approx \alpha_k'' p_{yj} \cos \left( \frac{\pi k}{L_x} x_j \right) \sin \left( \frac{2\pi k}{T_{lya}} n_t + \beta_k' \right)
$$


\[ j = 1, 2, \cdots, N \] with constants $\alpha_k'$, $\alpha_k''$, $\hat{\alpha}_k'$, $\hat{\alpha}_k''$ and $\beta_k'$. It should be noted that large fluctuations in the Lyapunov mode represented in middle of Figs. 1(b), 5(c), and 5(d) can come from the second terms on the right-hand sides of Eqs. 8 and 9. On the other hand the effect of the first terms on the right-hand side of Eqs. 3 and 4 does not appear explicitly in Figs. 2(a), 5(a) and 2(b), because the factor $p_{xj}$ in these terms distributes their contributions randomly and these terms disappear after taking local time averages.

### D. Energy dependence of Lyapunov mode amplitudes

In the expressions 3, 4, 5 and 6 for the time-oscillating Lyapunov modes, the quantities $\alpha_k'$, $\alpha_k''$, $\hat{\alpha}_k'$ and $\hat{\alpha}_k''$ are introduced simply as coefficients of the linear combination of the longitudinal spatial translational invariance Lyapunov mode and the time translational invariance Lyapunov mode. However it is important to note that these coefficients are related to each other through the normalization of the Lyapunov mode.

We consider the condition that the Lyapunov mode vector $(\delta x_1^{(\nu)}, \delta x_2^{(\nu)}, \cdots, \delta x_N^{(\nu)}, \delta y_1^{(\nu)}, \delta y_2^{(\nu)}, \cdots, \delta y_N^{(\nu)}), \nu = \nu(k), \nu(k) - 1$ is normalizable. This leads to the approximate relations

$$
|\alpha_k'| \sim \frac{|\hat{\alpha}_k'|}{\sqrt{2mE/N}}
$$

$$
|\alpha_k'| \sim |\alpha_k''|
$$

$$
|\hat{\alpha}_k'| \sim |\hat{\alpha}_k''|
$$

with the mass $m(=1)$, the total energy $E$ and the number of particles $N$.

In Fig. 7 we show the amplitudes $|\alpha_k'|$ and $|\hat{\alpha}_k'|$, which are obtained by fitting the Lyapunov modes $(\delta x_j^{(2N-3)})_t$, $(\delta y_j^{(2N-3)})_t$ to sinusoidal functions multiplied by constants, as functions of $\sqrt{2mE/N}$. To get the data for this figure we used the quasi-one-dimensional system of 50 hard-disks with (H,P) boundary condition. The broken line is a fit of the amplitude $|\alpha_k'|$ to a constant function $y = \xi$ with a fitting parameter $\xi$, and the solid line is given by $y = \xi x$.

In Fig. 6 we fitted the amplitude $|\alpha_k'|$ for the mode $(\delta x_j^{(2N-3)})_t$ (circles) to a constant function $y = \xi$ (the broken line) with a fitting parameter value $\xi \approx 0.179$, and the solid line is given by $y = \xi x$ using this value of $\xi$. The amplitudes $|\alpha_k'|$, $|\hat{\alpha}_k'|$ for the modes $(\delta x_j^{(2N-3)})_t$, $(\delta y_j^{(2N-3)})_t$ (triangles), and $(\delta y_j^{(2N-3)})_t$ (squares) are reasonably on the line $y = \xi x$, and these results support the relation 7, and also suggest that the amplitude $|\hat{\alpha}_k'|$ for the mode $(\delta x_j^{(2N-3)})_t$ is independent of $\sqrt{2mE/N}$. The amplitude $|\alpha_k'|$ for $(\delta x_j^{(2N-3)})_t$ (triangles) and $(\delta y_j^{(2N-3)})_t$ (squares) in Fig. 6 almost coincide with each other, and it gives support to the claim that the coefficients $\alpha_k'$ (in the first term) on
the right-hand side of Eqs. 5 and 6 coincide.

It may be noted that the normalization procedure in the Benettin’s algorithm, which we used to calculate the Lyapunov exponents and vectors in this paper, requires the normalization of Lyapunov vectors including both their spatial part and momentum part, but in the above argument we assumed the normalizability of the spatial part only of the Lyapunov vectors. This can be justified by the fact that as shown in Sec. III B the spatial part and momentum part of Lyapunov vectors constructing Lyapunov modes show almost the same mode structure, so each of them should be independently normalizable.

E. Spatial node structures of the Lyapunov modes and reflections in the hard-walls

The spatial node structure of the Lyapunov modes can be explained using the collision rule for particles with hard-walls.

For (H,P) boundary condition the particle collisions with the hard-walls in the x-direction cause a change in the sign of the x-component of the momentum with the remaining components of the phase space vector unchanged:

\[
x_j \rightarrow x_j, \quad y_j \rightarrow y_j, \quad p_{xj} \rightarrow -p_{xj}, \quad p_{yj} \rightarrow p_{yj},
\]

Similarly, in this type of collision the x-components of the Lyapunov vector change their signs while the remaining components unchanged:

\[
\delta x_j \rightarrow -\delta x_j, \quad \delta y_j \rightarrow \delta y_j, \quad \delta p_{xj} \rightarrow -\delta p_{xj}, \quad \delta p_{yj} \rightarrow \delta p_{yj}.
\]

Note that in the x components of Lyapunov vector \(\delta x_j\) changes its sign as well as \(\delta p_{xj}\), which is different from the phase space vector.

The important point is that a system with hard-wall boundaries is equivalent to an infinite system generated by reflecting the positions and velocities of all particles (in the hard wall) and by changing the signs of all x-components of the Lyapunov vectors at the hard-wall. That is explicitly incorporating the reflection symmetries for the phase space vector and the Lyapunov vector at hard walls. If the modes of the entire system are connected smoothly sinusoidal functions at the hard walls, then this condition requires that the mode for the quantity \(\delta x_j\) has a node at a hard wall, because it changes sign there. On the other hand, the quantities \(\delta x_j/p_{xj}\) and \(\delta y_j/p_{yj}\) do not change their signs at hard walls, so these modes should have anti-nodes at hard walls. These results explain the spatial node structures shown in Fig. 5. The spatial node structure of the stationary Lyapunov modes in \(\delta y_j\) corresponding to the one-point steps can be explained in this way. Because \(\delta y_j\) varies sinusoidally and must satisfy the reflection symmetry, it must be either a node (if the sign changes) or an anti-node (if the sign is invariant). Hence, in this case the Lyapunov mode in \(\delta y_j\) should have an anti-node at the hard-walls.

F. Lyapunov modes in momentum components of Lyapunov vectors

So far, we have discussed only the spatial components of the Lyapunov vectors. In this subsection we discuss briefly the Lyapunov modes appearing in the momentum parts of Lyapunov vectors.

One of the few differences between spatial and momentum components of Lyapunov vectors is that the amplitudes of the momentum components are often much smaller than those of the corresponding spatial components. This makes Lyapunov modes for the momentum parts of the Lyapunov vectors less clear than the corresponding spatial components. However, basically the structure of the Lyapunov mode for the momentum part of the Lyapunov vector is quite similar to the corresponding spatial component. For this reason, in this subsection we omit a detailed discussion of the phase relations of multiple Lyapunov modes for the momentum parts of Lyapunov vectors, and just show that there are certain modes structures in the momentum components of Lyapunov vectors corresponding to the Lyapunov steps.

Figure 7 shows mode structure of \(\delta p_{yj}^{(n)}\) corresponding to the first three one-point steps \((n = 198, 195\) and \(192\)) as functions of the normalized global time average \((x_j)/L_x\) of the position of the j-th.

Figure 8 shows contour plots of time-oscillating Lyapunov modes for \((\delta p_{xj}^{(197)})_t\), \((\delta p_{xj}^{(197)}/p_{xj})_t\), and \((\delta p_{yj}^{(197)}/p_{yj})_t\) as functions of the collision number \(n_t\) and the normalized local time average \((x_j)/L_x\) in the first two-point step. We used the same collision number interval [535200, 569600] in Fig. 8 as in Fig. 6. The mode
structures in Figs. S(a), (b) and (c) are almost the same as Figs. S(a), (c) and (e) for the corresponding spatial components $\langle \delta x_j^{(n)} \rangle_t$, $\langle \delta x_j^{(n)}/p_{xj} \rangle_t$, and $\langle \delta y_j^{(n)}/p_{yj} \rangle_t$, respectively, although their oscillating amplitudes are much smaller than those of the corresponding spatial components.

The spatial mode structures of the momentum components of Lyapunov vectors are explained by the same reflection property at hard-walls, which was discussed in the previous subsection [11].

G. Particle number dependence of the oscillating periods

In Sect. III C we showed that the quantities $\langle \delta x_j^{(n)} \rangle_t$, $\langle \delta x_j^{(n)}/p_{xj} \rangle_t$, and $\langle \delta y_j^{(n)}/p_{yj} \rangle_t$ corresponding to the two-point Lyapunov steps show time-oscillating behavior. Now we consider how the time-oscillating period of those Lyapunov modes depends on the number of particles $N$ for the quasi-one-dimensional system.

We evaluate the collision number interval for the time-oscillation of Lyapunov modes as follows. As shown in the proceeding subsection III C the Lyapunov modes related to the quantity $\langle \delta x_j^{(n)} \rangle_t$ (the quantities $\langle \delta x_j^{(n)}/p_{xj} \rangle_t$ and $\langle \delta y_j^{(n)}/p_{yj} \rangle_t$) have an anti-node in the middle (at the end) of the system in the $x$-direction ($n = 2N - 3$ and $2N - 4$) for (H,P) boundary condition. Using these properties we took 6 data points for the quantity $\langle \delta x_j^{(n)} \rangle_t$ (the quantities $\langle \delta x_j^{(n)}/p_{xj} \rangle_t$ and $\langle \delta y_j^{(n)}/p_{yj} \rangle_t$) ($n = 2N - 3$) in the middle (at the end) of the system with (H,P) boundary condition. These data are fitted to a sinusoidal function $y = a \sin \{2\pi x/T_{lya} \} + b$ with fitting parameters $a$, $h$ and $T_{lya}$, which leads to a numerical estimation of the period $T_{lya}$ of the time-oscillation of the Lyapunov modes. The collision number interval $T_{lya}$ can be translated into a real time interval by multiplying by the mean free time $\tau$, if necessary.

Figure 9 is the graph of the period $T_{lya}$ of the time-oscillations of $\langle \delta x_j^{(197)} \rangle_t$ (circles), $\langle \delta x_j^{(197)}/p_{xj} \rangle_t$ (triangles), and $\langle \delta y_j^{(197)}/p_{yj} \rangle_t$ (squares) in the quasi-one-dimensional system with (H,P) boundary condition, as functions of the number of particles $N$. Spatial and temporal behavior of these quantities has already been shown in Fig. 4(a), (b), and (d) for $N = 100$. Figure 4 shows that the three time-oscillations associated with $\langle \delta x_j^{(197)} \rangle_t$, $\langle \delta x_j^{(197)}/p_{xj} \rangle_t$, and $\langle \delta y_j^{(197)}/p_{yj} \rangle_t$ all have the same period. In Fig. 4 the data is fitted to a quadratic function $y = \alpha + \beta x^2$ with the fitting parameter values $\alpha \approx 17.9$ and $\beta \approx 1.65$. The inset to this figure shows the mean free time $\tau$ as a function of the number of particles $N$. The dependence of $\tau$ is nicely fitted to the function $y = \gamma/x$ with the value $\gamma \approx 1.91$ of the fitting parameter $\gamma$. Noting that the period, in real time, is given by $\tau T_{lya}$ approximately, these results suggest that the period of the Lyapunov modes is proportional to the number of particles $N$, namely the system size.

Now, we investigate the time-oscillating period of the Lyapunov modes in a different way. Figure 10 shows the quantity $L_x/(\tau T_{aut})$ as a function of the number of particles $N$. Here, $T_{lya}$ is the collision number interval given by the average of the three collision number intervals $T_{lya}$ for time-oscillations of the Lyapunov vector components $\langle \delta x_j^{(2N-3)} \rangle_t$, $\langle \delta x_j^{(2N-3)}/p_{xj} \rangle_t$, and $\langle \delta y_j^{(2N-3)}/p_{yj} \rangle_t$ in the first two-point step of the Lyapunov spectrum. The line is given by $y = 1$, which is the thermal velocity $\sqrt{E/(MN)}$.

IV. AUTO-CORRELATION FUNCTIONS

In this section we discuss another property of the quasi-one-dimensional system, namely the time-oscillation behavior of the momentum auto-correlation function. This is a typical measure of the collective behavior of many-particle systems. We connect this behavior with the
time-oscillating behavior of the Lyapunov modes, suggesting that the time-oscillating behavior of the Lyapunov modes can also be regarded as a collective mode.

We calculate numerically the auto-correlation functions \( C_\eta(t) \) for the \( \eta \)-component of the momentum based on the normalized expression \( \hat{C}_\eta(t) \equiv \frac{\tilde{C}_\eta(t)}{\tilde{C}_\eta(0)} \), in which \( \tilde{C}_\eta(t) \) is defined by

\[
\tilde{C}_\eta(t) = \lim_{t \to +\infty} \frac{1}{(N_2 - N_1 + 1)T} \sum_{j=N_1}^{N_2} \int_0^T ds \ p_{\eta j}(s + t) p_{\eta j}(s),
\]

\( \eta = x \) or \( y \). Eq. (18) includes a time-average and an average over some of particles (from the \( N_1 \)-th particle to the \( N_2 \)-th particle) in the middle of the system. (Note that number the particles 1, 2, \ldots, \( N \) from left to right in the system, as shown in Fig. 11.) In actual calculations we choose \( N_1 = [(N + 1)/2] - 5 \) and \( N_2 = [(N + 1)/2] + 5 \) with \( [x] \) as the integer part of the real number \( x \). This means that we take into account only 11 particles in the middle of the system in the calculation of the auto-correlation function \( C_\eta(t) \). (In this paper we consider the case \( N \geq 40 > 11 \).) It should be noted that using \((H,P) \) boundary condition the auto-correlation function for particles near hard-walls are different from the ones for particles in the middle of the system, as discussed in Appendix A. Especially, the momentum auto-correlation function of particles near hard-walls do not show clear time-oscillating behavior. To get the clearest time-oscillating behavior for the auto-correlation function \( C_\eta(t) \) and to get less hard-wall boundary condition effects, we exclude the auto-correlation functions of particles near hard-walls in the calculation of \( C_\eta(t) \).

If the system is ergodic, the value of the auto-correlation function (18) will be independent of the initial condition. To get the results for the auto-correlation function in this section we take a time-average of the auto-correlation function over more than \( 2 \times 10^6 \) collisions. For convenience, in figures the auto-correlation functions are shown as functions of the collision number \( n_\tau \), it can always be translated into the real time \( t \) by multiplying by the mean free time \( \tau \).

A. Momentum auto-correlation functions and their direction dependence

Figure 11 contains the momentum auto-correlation functions \( C_x \) and \( C_y \) for the momentum components in the \( x \)- and \( y \)-directions, respectively, as a function of the collision number \( n_\tau \) in the quasi-one-dimensional system with \( N = 100 \) and \((H,P) \) boundary condition. The main figure in Fig. 11 is a linear-linear plot of the auto-correlation functions \( C_x \) and \( C_y \), while its inset is a log-log plot of the graph of the absolute values \( |C_x| \) and \( |C_y| \) of the momentum auto-correlation functions. In this system the mean free time is given by \( \tau \approx 0.0188 \). From Fig. 11 it is clear that the momentum auto-correlation function has a strong direction dependence and shows a time-oscillating behavior in \( C_x \).

FIG. 11: The auto-correlation function \( C_x \) and \( C_y \) for the \( x \)- and \( y \)-components of momentum, respectively, as functions of the collision number \( n_\tau \). Main figure: Linear-linear plots of \( C_x \) and \( C_y \) as functions of \( n_\tau \). The inset: Log-log plots of the absolute values \( |C_x| \) and \( |C_y| \) of the auto-correlation functions as functions of \( n_\tau \). Here, the broken line is a fit of the graph of \( |C_x| \) to an exponential function, and the line is a fit of the graph of \( |C_y| \) to a \( \kappa \)-exponential function (defined by Eq. (21)).

In the beginning, the auto-correlation function \( C_x \) for the \( x \)-component of momentum decays exponentially in time. To show this point, in the inset to Fig. 11 we fitted the beginning of the graph of \( |C_x| \) to an exponential function

\[
G_1(x) = \exp(-\alpha' x)
\]

with the fitting parameter value \( \alpha' \approx 0.0385 \).

FIG. 12: The time-oscillating part of auto-correlation function \( C_x \) for the \( x \)-component of momentum as functions of the collision number \( n_\tau \). Here, the line is the fit to the product of a sinusoidal and an exponential function.

The significant point about the auto-correlation function \( C_x \) is its time-oscillating behavior. To show this behavior explicitly we show Fig. 12 as an enlarged graph of the time-oscillating part of \( C_x \), which is already shown in Fig. 11. This time-oscillating accompanies a time decay, so we fitted this graph to the product of a sinusoidal and an exponential function \( G_2(x) \), namely

\[
G_2(x) = A \ e^{-\beta' x} \sin\left(\frac{2\pi}{T_{acf}} x + \xi\right)
\]

with fitting parameters \( A, \beta', T_{acf}, \) and \( \xi \). The time oscillating part of the auto-correlation function \( C_x \) is nicely fitted to this function with the parameter values \( A \approx 0.0209, \beta' \approx 5.17 \times 10^{-5}, T_{acf} \approx 8.29 \times 10^3, \) and \( \xi \approx 1.62 \). This also gives us a way of numerically evaluating the oscillation period \( T_{acf} \) of the auto-correlation function \( C_x \). We note the quasi-one-dimensional system shows a much clearer time-oscillating behavior of the momentum auto-correlation function than a fully two- (or
three-) dimensional system. One may ask whether the damping behavior of the envelope of time-oscillation of \( C_x \) is best fitted to a power-law function, like the slow damping of the long time behavior of \( C_y \), rather than to an exponential function as assumed in Eq. (20). (Actually the data in Fig. 12 is not sufficient to decide between exponential and power decay.) This point is discussed further in Appendix 13.

On the other hand, the auto-correlation function \( C_y \) for the \( y \)-component of momentum shows a significantly different behavior from \( C_x \). This comes from the specific shape of the system and the boundary condition. As shown in Fig. 11 the damping of the momentum auto-correlation function \( C_y \) in the \( y \)-direction is much slower than in the \( x \)-direction. This is simply explained by the fact that in the quasi-one-dimensional system particle collisions occur mostly as head-on collisions, so that the change in the \( y \)-component of momentum in a collision can be much smaller than the change of the \( x \)-component of momentum. In the inset to Fig. 11 the graph of the auto-correlation function for the \( y \)-component of momentum is fitted to the "\( \kappa \)-exponential function" \( F_\kappa(x) \), which is defined by

\[
F_\kappa(x) \equiv \left[ 1 + (\alpha'' \kappa x)^2 - \alpha'' \kappa x \right]^{1/\kappa}, \quad (21)
\]

in \( x \geq 0 \) with fitting parameters \( \alpha'' \) and \( \kappa \). In the collision number region shown in Fig. 11 the auto-correlation function \( C_y \) in the \( y \)-direction is positive, so this fitting can be for \( C_y \) as well as for \( |C_y| \). From the definition, in the limit as \( \kappa = 0 \) the function \( F_\kappa(x) \) becomes the exponential function: \( \lim_{\kappa \to 0} F_\kappa(x) = \exp(-\alpha'' x) \), noting \( F_\kappa(0) = 1 \) and \( \partial F_\kappa(x)/\partial x = -\alpha'' F_\kappa(x)/\sqrt{1 + (\alpha'' \kappa x)^2} \), so this function is a one-parameter deformation of the exponential function. The important properties of this function are that it is approximated by an exponential function at small \( x \) and is approximately a power function in a large \( x \).

\[
F_\kappa(x) \sim \begin{cases} e^{-\alpha'' x} & \text{in } x \ll 1 \\ (2\kappa \alpha'' x)^{-1/\kappa} & \text{in } x \gg 1 \text{ and } \kappa \alpha'' x > 0 \end{cases} \quad (22)
\]

The fitting of the numerical data for the auto-correlation function \( C_y \) to the \( \kappa \)-exponential function with parameter values \( \alpha'' \approx 0.00358 \) and \( \kappa \approx 1.44 \) is very satisfactory, and this implies that this auto correlation function decays exponentially in the beginning, (like the auto correlation function in the \( x \)-direction), and decays as a power function after that, at least in the time scale shown in Fig. 11. (This does not mean that the auto-correlation function \( C_y \) decays as a \( \kappa \)-exponential function in any time-scale. See Appendix 13 about the auto-correlation function \( C_y \) at much longer time-scales than shown in Fig. 11.)

\section{Particle number dependence of the auto-correlation function and a relation with the time-oscillation of the Lyapunov modes}

We have shown the two kinds of time-oscillation behaviors in the quasi-one-dimensional system: one for the Lyapunov mode and another for the momentum auto-correlation function. Now we show numerical evidence to connect these two behaviors.

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{fig13.png}
\caption{The period \( T_{\text{lya}} \) (in collision numbers) of the time-oscillation of the Lyapunov mode as a function of the period of time-oscillation of the longitudinal momentum auto-correlation function \( T_{\text{acf}} \). Data points are obtained from numerical calculation of the quasi-one-dimensional system with \((H,P)\) boundary condition for different numbers of particles \( N = 40, 50, 60, \ldots, 100 \). The line is given by the function \( T_{\text{lya}} = 2T_{\text{acf}} \).}
\end{figure}

Fig. 13 is the graph of the time-oscillating period \( T_{\text{lya}} \) of the Lyapunov modes as a function of the time-oscillating period \( T_{\text{acf}} \) of the momentum auto-correlation function \( C_x \). Here, the time-oscillating periods are calculated for \( N = 40, 50, 60, \ldots, 100 \), and the time-oscillating periods \( T_{\text{lya}} \) are calculated as the average of the collision number interval \( T_{\text{lya}} \) for time-oscillations of the Lyapunov vector components \( (\delta x_j^{(2N-3)})(t), (\delta x_j^{(2N-3)}/p_y)(t), \) and \( (\delta y_j^{(2N-3)}/p_y)(t) \) in the first two-point step of the Lyapunov spectra. (As shown in Sect. 11 these three oscillating periods \( T_{\text{lya}} \) of the Lyapunov modes take almost the same values.) In Fig. 13 we also show the line given by the function \( T_{\text{lya}} = 2T_{\text{acf}} \). The numerical data for the time-oscillations in Fig. 13 is nicely fitted to the function,

\[
T_{\text{lya}} \approx 2T_{\text{acf}}. \quad (23)
\]

This is the main result of this paper.

In Table II we summarize, not only the values of the time-oscillating periods \( T_{\text{lya}} \) and \( T_{\text{acf}} \) of the Lyapunov modes and the momentum auto-correlation function in real time, but also the data about the \( N \)-dependences of the damping properties of the auto-correlation functions \( C_x \) and \( C_y \). They include the mean free time \( \tau \), the exponential damping times \( \tau/\alpha' \) and \( \tau/\beta' \) (for \( C_x \)) and \( \tau/\alpha'' \) (for \( C_y \)), and the power \( 1/\kappa \) of the damping of \( C_y \) at long time. Here, values of \( \alpha', \beta' \) and \( T_{\text{acf}} \) \( \alpha'' \) and \( \kappa \) are derived by fitting the auto-correlation function \( C_x \) \( C_y \) to Eqs. (19) and (20) (Eq. (21)). From this table it is clear that the exponential damping times \( \tau/\alpha' \) and \( \tau/\alpha'' \), and the power \( 1/\kappa \) are almost independent of the particle number \( N \). On the other hand, the exponential damping
the beginning of the longitudinal momentum auto-correlation function $C_x$ as a function of the collision number $n_t$ to an exponential function $y = \exp\{-\alpha' t\}$. The parameters $\beta'$ and $T_{acf}$ are given by fitting the time-oscillating part of the same function $C_y$ to the function $y = A \exp\{-\beta' t\} \sin\{2\pi/T_{acf}\} + \xi$. The parameters $\alpha''$ and $\kappa$ are given by fitting the transverse momentum auto-correlation function $C_y$ as a function of the collision number $n_t$ to the $\kappa$-exponential function $y = (\sqrt{1 + (\alpha'' \kappa t)^2} - \alpha'' \kappa t)^{1/\kappa}$ (Eq. 5).

### Table I: Time-oscillating periods and decay factors for the Lyapunov modes and the momentum auto-correlation functions.

| $N$ | Lyapunov mode | $\tau$ | $\bar{T}_{lya}$ | $\tau/\alpha'$ | $\tau/\beta'$ | $T_{acf}$ | $\tau/\alpha''$ | $C_y$ | $1/\kappa$ |
|-----|----------------|-------|-----------------|----------------|-------------|-----------|-----------------|------|------------|
| 40  | $\alpha$      | 0.0489| 123.5           | 0.493          | 74.2        | 63.9      | 5.33            | 0.732|
| 50  | $\beta$       | 0.0380| 154.7           | 0.483          | 102.5       | 76.0      | 5.26            | 0.716|
| 60  | $\gamma$      | 0.0326| 197.3           | 0.505          | 156.1       | 96.6      | 5.37            | 0.675|
| 70  | $\delta$      | 0.0275| 223.1           | 0.493          | 196.1       | 107.9     | 5.26            | 0.608|
| 80  | $\epsilon$    | 0.0238| 256.7           | 0.487          | 204.5       | 125.0     | 4.74            | 0.577|
| 90  | $\zeta$       | 0.0210| 283.3           | 0.487          | 252.0       | 139.9     | 4.89            | 0.624|
| 100 | $\eta$        | 0.0188| 305.7           | 0.488          | 302.7       | 155.5     | 5.27            | 0.693|

C. Boundary condition effects

So far, we have concentrated into the quasi-one-dimensional system with hard-wall boundary conditions in the $x$-direction and periodic boundary conditions in the $y$-direction, namely the (H,P) boundary condition, for technical convenience in the analysis of the Lyapunov modes. On the other hand, in Ref. 18 we have already discussed and compared Lyapunov steps and modes in the different boundary conditions: the purely periodic boundary conditions (P,P), the purely hard-wall boundary conditions (H,H), and periodic boundary conditions in the $x$-direction and hard-wall boundary conditions in the $y$-direction (P,H) as well as the boundary condition (H,P). In this section we carry out a similar discussion for the momentum auto-correlation functions $C_x$ in these different boundary conditions. Figure 14 contains schematic illustrations of these boundary conditions.

For meaningful comparisons between the different boundary conditions we use the same mass $m$ and radius $R$ for the particles, and the same number of particles ($N = 50$). Using the set of the lengths $(L_x, L_y)$ to define the size of the system in the $x$ and $y$ directions for (H,P) boundary conditions, then we use $(L_x - 2R, L_y)$ for (P,P) boundary conditions $(L_x - 2R, L_y + 2R)$ for (P,H) boundary conditions, and $(L_x, L_y + 2R)$ for (H,H) boundary conditions. This gives the same effective area for particles to move in each of the four systems. This also means that the mean free time $\tau$ in these four types of the boundary conditions will be the same (Concrete numerical values of $\tau$ are given in Table I).

FIG. 14: Schematic illustrations of the four boundary conditions (P,P), (P,H), (H,P) and (H,H) used in quasi-one-dimensional systems. Here, (P,P) is the purely periodic boundary conditions, (P,H) is periodic boundary conditions in the $x$-direction and hard-wall boundary conditions in the $y$-direction, (H,P) is hard-wall boundary conditions in the $x$-direction and periodic boundary conditions in the $y$-direction, and (H,H) is the purely hard-wall boundary conditions. The dashed lines and the solid lines on the boundaries represent periodic boundary conditions and hard-wall boundary conditions, respectively.

FIG. 15: Auto-correlation functions $C_x$ for the $x$-component of the momenta as functions of the collision number $n_t$ for the boundary conditions (P,P), (P,H), (H,P) and (H,H). The systems are quasi-one-dimensional systems consisting of 50 hard-disks. We observe: (a) Exponential decay region in the beginning of the damping of the auto-correlation function $C_x$ as a linear-linear plot. The dotted line and the broken line are the fits for the cases (P,P) and (H,P) and the cases (P,H) and (H,H) to exponential functions, respectively. (b) Time-oscillating region of the auto-correlation functions $C_x$ as a linear-linear plot. The four graphs of the auto-correlation functions $C_x$ are fitted to the functions $y = A \exp\{-\beta' t\} \sin\{2\pi/T_{acf}\} + \xi$ with the fitting parameters $A$, $\beta'$, $T_{acf}$ and $\xi$. Fig. 15 shows the auto-correlation functions $C_x$ for the $x$-component of the momenta in quasi-one-dimensional systems consisting of 50 hard-disks with boundary conditions (P,P), (P,H), (H,P) and (H,H) as functions of the
collision number $n_t$. Here, Fig. 15(a) is the beginning part of the autocorrelation functions $C_x$, and is given as a linear-log plot to show their exponential decay as straight lines. In this figure the fits to the exponential function (19) with the fitting parameter $\alpha$' are given for the cases (P,P) and (H,P) and the cases (P,H) and (H,H) separately. The dotted line is the fit for the cases (P,P) and (H,P) with the fitting parameter values $\alpha' \approx 0.0765$, and the broken line is for the cases (P,H) and (H,H) with the fitting parameter values $\alpha' \approx 0.0597$. Fig. 15(b) is the time-oscillating part of $C_x$ in the four different boundary conditions. In this figure, each auto-correlation function is fitted to a function (20) with the fitting parameters $A$, $\beta'$, $T_{acf}$, and $\xi$. The values of these fitting parameters are $(A, \beta', T_{acf}, \xi) \approx (0.0422, 0.00108, 1.00 \times 10^3, 1.37)$ for (P,P), $(A, \beta', T_{acf}, \xi) \approx (0.0447, 0.000803, 1.24 \times 10^3, 1.33)$ for (P,H), $(A, \beta', T_{acf}, \xi) \approx (0.0398, 0.000369, 2.04 \times 10^3, 1.56)$ for (H,P), and $(A, \beta', T_{acf}, \xi) \approx (0.0403, 0.000246, 2.53 \times 10^3, 1.56)$ for (H,H).

Finally, we show a relation between the time-oscillating periods of the Lyapunov mode and the momentum auto-correlation function for different boundary conditions. In Table II we summarize the mean free time $\tau$, the averages of the longest time-oscillating time period $T_{lya}$ for the Lyapunov vector, and the time-oscillating time period $T_{acf}$ of the longitudinal momentum auto-correlation function $C_x$ for the different boundary conditions (P,P), (P,H), (H,P) and (H,H) in a quasi-one-dimensional system consisting of 50 hard-disks. $T_{lya}$ is the average over three collision number intervals of $T_{lya}$. Here, $T_{lya}$ is the average of the time-oscillations of the three components ($\langle \delta x_j^{(k)} \rangle_t$, $\langle \delta x_j^{(k)} / p_{xj} \rangle_t$, and $\langle \delta y_j^{(k)} / p_{yj} \rangle_t$), for the first Lyapunov step which has time-oscillating Lyapunov modes ($k = 2N-5$ for (P,P), $k = 2N-2$ for (P,H), $k = 2N-3$ for (H,P), and $k = 2N-1$ for (H,H)).

![Table II](https://example.com/table2.png)

**Table II:** The mean free time $\tau$, the averages of the longest time-oscillating time period $T_{lya}$ for the Lyapunov vector, and the time-oscillating time period $T_{acf}$ of the longitudinal momentum auto-correlation function $C_x$ for the different boundary conditions (P,P), (P,H), (H,P) and (H,H) in a quasi-one-dimensional system consisting of 50 hard-disks. $T_{lya}$ is the average over three collision number intervals of $T_{lya}$. Here, $T_{lya}$ is the average of the time-oscillations of the three components ($\langle \delta x_j^{(k)} \rangle_t$, $\langle \delta x_j^{(k)} / p_{xj} \rangle_t$, and $\langle \delta y_j^{(k)} / p_{yj} \rangle_t$), for the first Lyapunov step which has time-oscillating Lyapunov modes ($k = 2N-5$ for (P,P), $k = 2N-2$ for (P,H), $k = 2N-3$ for (H,P), and $k = 2N-1$ for (H,H)).

D. An explanation for the relation of time-oscillation periods of the Lyapunov mode and the momentum auto-correlation function

As we have shown, the relation $T_{lya} = 2T_{acf}$ (Eq. (23)) between the largest time-oscillating period $T_{lya}$ of the Lyapunov modes and the time-oscillating period $T_{acf}$ of the momentum auto-correlation function is independent of the number of particles $N$ and the boundary conditions. In this subsection we discuss a possible explanation for this relation, which is a physical argument rather than a strict mathematical proof.

We consider a momentum component $\tilde{p}_x(t)$, like the $x$-component of the momentum in the quasi-one-dimensional system, which shows a time-oscillating behavior in its auto-correlation function with a frequency $\omega_{acf}$:

$$\tilde{p}_x(t) \sim \phi(t) e^{i\omega_{acf} t}$$

where we use the notation $X(t)\bar{X}(0)$ for the auto-correlation function for any complex quantity $X(t)$ with complex conjugate $X(t)^*$. Here $\phi(t)$ is the damping envelope of the auto-correlation function $\tilde{p}_x(t) \tilde{p}_x(0)$, which can be an exponential decay, $\phi(t) \sim \exp\{-\alpha t\}$ with a positive constant $\alpha$ (See Appendix B).
tor, like the first terms on the right-hand sides of Eqs. \(\text{38}\) and \(\text{41}\), as

\[
\delta q_x(t) \sim \psi_1(t) \bar{p}_x(t) e^{i \omega_{lya} t}
\]

(25)

with a frequency \(\omega_{lya}\), where \(\psi_1(t)\) is the decay envelope of the amplitude of \(\delta q_x\), and may show an exponential divergence (or contraction) following the corresponding Lyapunov exponent. Now, we assume that if the quantity \(\delta q_x\) oscillates persistently in time, then its auto-correlation function \(\delta q_x(t)^* \delta q_x(0)\) should oscillate in time with the same frequency \(\omega_{lya}\), namely

\[
\delta q_x(t)^* \delta q_x(0) \sim \psi_2(t) e^{i \omega_{lya} t}
\]

(26)

with a new envelope function \(\psi_2(t)\).

It follows from Eqs. \(\text{24}\), \(\text{28}\) and \(\text{26}\) that

\[
\psi_2(t) e^{i \omega_{lya} t} \sim \psi_1(t)^* \psi_1(0) \bar{p}_x(t)^* \bar{p}_x(0) e^{-i \omega_{lya} t}
\]

\[
\sim \psi_1(t)^* \psi_1(0) \phi(t) e^{i (\omega_{acf} - \omega_{lya}) t},
\]

which immediately leads to

\[
\psi_2(t) \sim \psi_1(t)^* \psi_1(0) \phi(t)
\]

(27)

\[
\omega_{lya} \sim \omega_{acf}/2.
\]

(28)

The time-oscillating periods \(T_{acf}\) and \(T_{lya}\) of the momentum auto-correlation function and the Lyapunov mode are given by \(T_{acf} \sim 2\pi/(\tau \omega_{acf})\) and \(T_{lya} \sim 2\pi/(\tau \omega_{lya})\). Using this point and Eq. \(\text{28}\) we obtain our relation \(\text{28}\).

Note that the above explanation for \(T_{lya} = 2T_{acf}\) is independent of the number of particles \(N\) and the boundary conditions.

Here, the Lyapunov index \(n = 2N - 3\) of the Lyapunov vector component \(\delta x_j^{(n)}\) is chosen so that the corresponding Lyapunov step is the first two-point step associated with a time-oscillating Lyapunov mode. In Fig. \(\text{16}\) the numerical data is fitted to a sinusoidal function multiplied by an exponential function, namely the function \(\psi_2(t)\), with the fitting parameter values \(A \approx 0.967\), \(\beta' \approx 1.03 \times 10^{-5}\), \(T_{acf} = T_{lya} \approx 4.12 \times 10^3\), and \(\zeta \approx 1.54\). This time-oscillating period \(T_{acf}\) for the auto-correlation function for the longitudinal Lyapunov vector component coincides almost exactly with the time-oscillating period \(T_{acf} \approx 4.07 \times 10^3\) of the corresponding Lyapunov mode. This coincidence of the time-oscillating periods supports our assumption \(\text{20}\) \(\text{15}\).

V. CONCLUSION AND REMARKS

In this paper we have discussed the relation between the wave-like structure of Lyapunov vectors and the time-oscillating behavior of the momentum auto-correlation functions in quasi-one-dimensional many-hard-disk systems. The quasi-one-dimensional system is a narrow rectangular system in which the \(x\) components of the particle positions remained in the same order. This system was proposed as a many-particle system which shows clear stepwise structure of the Lyapunov spectrum (the Lyapunov steps) and wave-like structure of the associated Lyapunov vectors (the Lyapunov modes). Using this system, we showed that there are two types of Lyapunov modes in the spatial and momentum components of the Lyapunov vectors corresponding to the two kinds of steps in the Lyapunov spectrum: one is stationary in time and the other involves a time-oscillation. Here, the time-oscillating Lyapunov vectors consist of a simple time-oscillating part plus a momentum proportional time-oscillating part in the longitudinal components, while the transverse time-oscillating Lyapunov vectors consist of a momentum proportional time-oscillating part only.

We revealed the phase relation for these time-oscillating Lyapunov modes. It was shown that the system length divided by the time-oscillating period of the Lyapunov modes is independent of the number of particles at the same density, and is of order of the thermal velocity. After discussing these wave-like structures of the Lyapunov vectors, we connected them to the time-oscillation of the momentum auto-correlation. The time-oscillation of the auto-correlation function appears in the longitudinal component of the momentum, and its envelope decays exponentially in time. The main point is that the largest time-oscillating period of the first time-oscillating Lyapunov modes is twice as long as the time-oscillating period of the momentum auto-correlation function. We showed that this relation is independent of the number of particles and the boundary conditions (constructed from combinations of periodic and hard-wall boundary conditions). A simple explanation is given for this relation. It was also shown that the auto-correlation function for the

FIG. 16: The normalized auto-correlation function \(C_{lya,x}^{(2N-3)}\) for the longitudinal Lyapunov vector component \(\delta x_j^{(2N-3)}\) as a function of the collision number \(n_t\). The system is a quasi-one-dimensional system consisting 50 particles with boundary condition \((H,P)\). The numerical data is well fitted to a sinusoidal function multiplied by an exponential function.

In the above explanation, the assumption \(\text{20}\) is crucial, so it may be useful to demonstrate this behavior numerically. Figure \(\text{16}\) shows that the auto-correlation function \(C_{lya,x}^{(2N-3)}\) for the longitudinal Lyapunov vector component \(\delta x_j^{(2N-3)}\) normalized by its initial value (about 0.0203) in a quasi-one-dimensional system of 50 particles with \((H,P)\) boundary condition. In the auto-correlation function \(C_{lya,x}^{(2N-3)}\) its mean value is subtracted, and an average over the auto-correlation functions of 11 particles in the middle of the system is taken.
transverse component of the momentum is nicely fitted to the $\kappa$-exponential function, implying that it decays exponentially at the beginning and decays as a power after that.

In this paper we considered mainly a specific boundary condition for the quasi-one-dimensional system: (H,P) hard-wall boundary conditions in the longitudinal direction and periodic boundary conditions in the transverse direction. The system with this boundary condition exhibit a much clear wavelike-like structure of Lyapunov modes than the purely periodic boundary conditions (P,P), which is a big advantage for quantitative discussions of the Lyapunov modes. Using the (H,P) boundary condition, the spatial translational invariance in the longitudinal direction is violated, and it leads to a different Lyapunov step structure and auto-correlation functions, compared with the (P,P) boundary conditions. For example, in (H,P) the step widths of the Lyapunov spectrum are half of the ones in (P,P), and individual particles can have different momenta auto-correlation functions due to the back scattering effect of the hard-wall (See Appendix IV.C) while the momentum auto-correlation function is particle-independent for the (P,P) boundary condition. However, as discussed in Ref. 18 for the Lyapunov modes and in Sec. IV.C for the auto-correlation functions, there is a simple relation connecting the results obtained from different boundary conditions, so we can predict some of the results of the other boundary conditions from the results for (H,P).

The mode structure of Lyapunov vectors discussed in this paper is related to the structure of the Lyapunov vectors associated with zero-Lyapunov exponents. As explained in the introduction of this paper, there are sets of Lyapunov vector components which take a constant value independent of the particle index, and that these quantities corresponding to the stepwise structure of the Lyapunov spectrum have wavelike structures. These are connected with the spatial and time translational invariances and the energy and momentum conservation laws. However we need to be careful when making a connection between the conservation laws (or the translation invariances) and the Lyapunov modes. For example, in a system with hard-wall boundary conditions the spatial translational invariance is violated, but even in such systems the mode structure in the Lyapunov vector component $\delta x_j^{(n)}$ (or $\delta y_j^{(n)}$), can be observed. However, a scenario which suggests that translational invariance is only evident when it is observed in the zero-Lyapunov exponent modes, will not predict these observed longitudinal modes.

It should be noted that a time-dependence of the Lyapunov modes may not always appear as a time-oscillating behavior. Ref. 19 claim that the spatial wave of the Lyapunov vector "moves" at a specific speed in the square system consisting of many hard-disks. It is interesting to know how these different behaviors, one oscillating in time and another moving with a speed, can appear.

In some papers, an understanding of the Lyapunov modes was attempted based on an analogy with the hydrodynamic modes 19. Actually, in both cases the conservation laws like the total momentum conservation and the energy conservation play an essential role, and the longitudinal mode shows a time-dependent behavior. However it is important to know that the deterministic nature of orbits also plays one of the essential roles in the Lyapunov modes and leads to momentum-proportional time-oscillating components of Lyapunov vectors, although such a characteristic does not appear explicitly in the hydrodynamic mode. In this sense, it is still an open question to see how hydrodynamic modes, which have no concept of a phase space trajectory, can incorporate time translational invariance.

From results of this paper, it is suggested that there is a connection between existence of the stepwise structure of Lyapunov spectra and the time-oscillations of momentum auto-correlation functions. It is well known that the stepwise structure of the Lyapunov spectra appears clearly in rectangular systems rather than in square systems at the same density. It is possible to get a similar result for the time-oscillation of the momentum auto-correlation function? For example, in a square system with a small number of hard-disks we cannot observe the stepwise structure of the Lyapunov spectrum, and in this case the time-oscillation of the momentum auto-correlation function does not appear. Therefore, the time-oscillations of the auto-correlation function may be useful to understand the condition for existence of the Lyapunov steps and modes. In this sense, for example, it may be interesting to investigate the time-correlation function in systems with soft-core particle interactions in which the observation of the Lyapunov steps is much harder, and less direct than in systems with hard-core interactions.

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APPENDIX A: MOMENTUM AUTO-CORRELATION FUNCTION OF INDIVIDUAL PARTICLE

In this appendix we discuss the momentum auto-correlation function of individual particles in the quasi-one-dimensional system with hard-wall boundary conditions in the longitudinal direction and periodic boundary conditions in the transverse direction (the boundary condition (H,P)). Different from purely periodic boundary conditions, the hard-wall boundary in (H,P) violates the translation invariance in the longitudinal $x$-direction,
and this implies that different particles can have different momentum auto-correlation functions.

We introduce the auto-correlation function \(c^{(j)}_{\eta}(t)\) of the \(j\)-th particle in the \(\eta\)-direction at time \(t\) \((j = 1, 2, \cdots, N\) and \(\eta = x, y)\) based on the normalized expression \(c^{(j)}_{\eta}(t) \equiv c^{(j)}_{\eta}(t)/c^{(j)}_{\eta}(0)\) with \(c^{(j)}_{\eta}(t)\) defined by

\[
\tilde{c}^{(j)}_{\eta}(t) \equiv \lim_{T \to +\infty} \frac{1}{T} \int_0^T ds \, p_{kj}(s + t)p_{kj}(s). \tag{A1}
\]

Using this quantity \(\tilde{c}^{(j)}_{\eta}(t)\), the auto-correlation function \(\tilde{C}_{\eta}(t)\) defined by Eq. (18) is simply given by \(\tilde{C}_{\eta}(t) = [1/(N_2 - N_1 + 1)] \sum_{j=N_1}^{N_2} \tilde{c}^{(j)}_{\eta}(t)\). In this appendix we show graphs of \(\tilde{c}^{(j)}_{\eta}(t)\) as a function of the collision number \(n_t \approx t/\tau\) in the quasi-one-dimensional system consisting of 100 hard-disks. We number the particles \(1, 2, \cdots, N\) from the left to right, as shown in Fig. 1, so, for example, the 1st and \(N\)-th particles are closest to the hard-walls.

**FIG. 17:** Auto-correlation functions for \(c^{(1)}_x\), \(c^{(20)}_x\) and \(c^{(50)}_x\) for the \(x\)-components of momenta of the 1st, 20-th, and 50-th particle, respectively, as functions of the collision number \(n_t\). The system is a quasi-one-dimensional system of 100 hard-disks with (H,P) boundary condition. The inset: Enlarged graphs in the small magnitude part of the auto-correlation functions.

The first important point of the individual auto-correlation functions is that the time-oscillation in the \(x\)-direction is weak for particles near the walls. This is shown in Fig. 17 in which we plot the auto-correlation function \(c_x^{(j)}\) for the \(j\)-th particle in the \(x\)-direction for \(j = 1\) (the nearest particle to the left hard-wall), \(j = 50\) (the particle most distant from the hard-walls), and \(j = 20\) (a particle between these two extremes). In Fig. 17 the main figure is the full data for these auto-correlation functions, and its inset is an enlarged graph to emphasize the time-oscillating part. This figure shows that we cannot recognize a time-oscillating behavior in the auto-correlation function \(c_x^{(1)}\) of the particle nearest to the hard-wall, although a clear time-oscillation can be recognized in \(c_x^{(50)}\) of the particle in the middle of the system. We can see a time-oscillating behavior in the auto-correlation function \(c_x^{(20)}\), but its amplitude is smaller than that of \(c_x^{(50)}\). The positions of the nodes of the time-oscillations of \(c_x^{(20)}\) and \(c_x^{(50)}\) almost coincide with each other.

Another difference between individual particle auto-correlation functions appears in the short time scale. Figure 18 shows the momentum auto-correlation functions \(c^{(j)}_{\eta} = 1, 2\) and 50, as functions of the collision number \(n_t\) showing the initial damping behavior (\(\eta = x, y\)).

These auto-correlation functions show an exponential decay, which we present as a linear-log plot (straight lines imply exponential decay). This figure shows that the \(x\)-component \((y\)-component) of the auto-correlation function of the particle nearest the hard-wall decays faster (slower) than the ones of other particles, while in any of them the damping behavior is nicely fitted to an exponential function.

**FIG. 18:** Exponential decay region of the auto-correlation functions \(c^{(1)}_x\) (circles), \(c^{(2)}_x\) (triangles), and \(c^{(50)}_x\) (squares) for the \(x\)-components of momenta, as functions of the collision number \(n_t\) on a linear-log plot. The solid line (the dotted-broken lines) is a fit of the graph of \(c^{(1)}_x\) (the graphs of \(c^{(2)}_x\) and \(c^{(50)}_x\)) to an exponential function. Similar graphs are given for the auto-correlation functions for the \(y\)-component of momenta: \(c^{(1)}_y\) (inverted triangles), \(c^{(2)}_y\) (pluses), and \(c^{(50)}_y\) (crosses). The broken line (the dotted line) is a fit of the graph of \(c^{(1)}_y\) (the graphs of \(c^{(2)}_y\) and \(c^{(50)}_y\)) to an exponential function.

The inset: Absolute values of the same auto-correlation functions, and its inset is an enlarged graph showing the initial damping behavior of the auto-correlation function. (In Fig. 18 the graphs are fitted to the exponential function \(e^{-\alpha t}\) with the fitting parameter values \(\alpha' \approx 0.0457\) for \(c^{(1)}_x\) (solid line), \(\alpha' \approx 0.0369\) for \(c^{(2)}_x\) and \(c^{(50)}_x\) (dotted-broken line), \(\alpha' \approx 0.00184\) for \(c^{(1)}_y\) (broken line), and \(\alpha' \approx 0.00368\) for \(c^{(2)}_y\) and \(c^{(50)}_y\) (dotted line)). This difference may come from the different types of collisions experienced. For the particle nearest the wall, half of the collisions will be with the wall and the other half with the neighboring particle. The \(x\)-component of the momentum is drastically changed (namely it changes the sign of \(p_{kj}\)), so it may cause a faster decay of the auto-correlation function in the \(x\)-direction than for other particles. On the other hand, collisions with the wall effect the \(y\)-component of the momentum much less, because it is invariant under wall collisions, and does not cause loss of memory of \(p_{kj}\), and this can also explain a slower decay of the momentum auto-correlation for the 1st (and \(N\)-th) particle in the \(y\)-direction compared to other particles.

**FIG. 19:** The negative region of auto-correlation functions \(c^{(1)}_x\), \(c^{(3)}_x\), \(c^{(5)}_x\), and \(c^{(10)}_x\) for the \(x\)-components of momenta, as functions of the collision number \(n_t\) as a log-log plot.

Another point of difference of the auto-correlation functions of individual particles is a negative region which appears after their initial exponential decay. It may be meaningful to mention that a negative region of momentum auto-correlation function has drawn attention.
in some previous works \cite{46, 47, 48}. To discuss such a negative region, in Fig. 19 we show the collision number \(n_t\) dependence of the auto-correlation functions \(c_x^{(1)}, c_x^{(3)}, c_x^{(5)}, \) and \(c_x^{(10)}\). To emphasize such a negative region of the auto-correlation function, we show a log-log plot of the absolute values of the same quantities as functions of \(n_t\) in the inset to Fig. 20. As shown in this figure, a negative region of the auto-correlation functions appears after the initial exponential decay and before the time-oscillates appear. The collision number (or time) at the bottom of this negative region of the auto-correlation function increases, and the amplitude of the bottom decreases, as the particle is further from the hard-wall (namely as the particle index \(j\) in \(c_x^{(j)}\) increases from \(j = 1\) to 10 in Fig. 21). This phenomenon can be explained by the backscattering effect of the hard-walls. Such a backscattering effect is stronger (so the amplitude of the negative region is stronger) in a particle closer to a hard-wall, as well, the time interval to react to the presence of the wall is longer (so the time at the bottom of the negative region is later) in a particle far from the hard-wall. This kind of behavior is not observed in a system in which the boundary conditions in the \(x\)-direction are periodic.

After such a negative region of the auto-correlation function the time-oscillating part appears. Figure 20 shows the collision number \(n_t\) dependence of the auto-correlation functions for \(c_x^{(10)}, c_x^{(20)}, c_x^{(35)}\) and \(c_x^{(50)}\) in the collision number region before the time-oscillation of the auto-correlation starts (about \(n_t \approx 6000\) in Fig. 20). The negative peak of the auto-correlation function (discussed in the previous paragraph and indicated by the arrows in Fig. 20) moves to a longer collision number \(n_t\) as the particle index \(j\) increase from \(j = 10\) to 35 in Fig. 20. On the other hand, the time oscillation of the auto-correlation function starts from about \(n_t \approx 6000\) which is independent of the particle index, although the amplitude of the time-oscillation is large for a particle far from the hard-walls. Moreover the time-oscillating period of the auto-correlation function is almost independent of the particle index. These characteristics of the time-oscillation of the auto-correlation function suggest that the time-oscillating behavior of the auto-correlation function reflects a collective movement of the system.

FIG. 20: The region before the start of the time-oscillation of auto-correlation functions for \(c_x^{(10)}, c_x^{(20)}, c_x^{(35)}\) and \(c_x^{(50)}\) as functions of the collision number \(n_t\).

APPENDIX B: DAMPING BEHAVIOR OF MOMENTUM AUTO-CORRELATION FUNCTION IN A LONG TIME INTERVAL

In this appendix we discuss two points about the momentu-autocorrelation function in the long time interval: (i) The shape of the envelop of the time-oscillation in the auto-correlation function \(C_x\) for the \(x\)-component of the momentum, and (ii) The behavior of the auto-correlation function \(C_y\) of the \(y\)-component of the momentum on a much longer time scale than that shown in the text of this paper.

![Figure 21](image-url) shows the absolute values of \(|C_x|\) and \(|C_y|\) of the auto-correlation functions for the \(x\)-component and the \(y\)-component of the momentum, respectively, as functions of the collision number \(n_t\) presented as a log-log plot. The solid line is a fit of the envelop of the time-oscillating part of the auto-correlation function \(C_x\) to an exponential function. The dotted line is a fit of the auto-correlation function \(C_y\) to a \(\kappa\)-exponential function (Eq. (21)) and the dotted broken line is a fit of the envelop of the time-oscillating part of the auto-correlation as a graph of the absolute value \(|C_x|\) as a function of the collision number \(n_t\) presented as a linear-log plot. The broken line is a fit to a sinusoidal function multiplied by an exponential decay function (Eq. (20)), and the solid line is its envelop, which is the same as the solid line in Fig. (a). The system is a quasi-one-dimensional system consisting of 50 hard-disks with (H,P) boundary condition.

Figure 21 shows the absolute values of \(x\) and \(y\) auto-correlation functions \(|C_x|\) as functions of the collision number \(n_t\) in a quasi-one-dimensional system of 50 hard-disks with (H,P) boundary condition. In Fig. 21(a) these graphs are plotted as log-log plots, while in Fig. 21(b) the graph for \(|C_x|\) is plotted as a linear-log plot. The collision number interval in this figure is about ten times as long as the previous ones in this paper, and we took a much longer time-average (eg. over \(10^9\) collisions) to get this data.

As shown in Sec. IV.A the auto-correlation function \(C_x\) for the \(x\)-component of the momentum decays exponentially initially. After the initial decay, the time-oscillating region of \(C_x\) starts. We fitted this region of \(C_x\) to a sinusoidal function multiplied by an exponential function, namely Eq. (20), with the fitting parameters \(A \approx 0.0402, \beta' \approx 0.000368, T_{osc} \approx 2.03 \times 10^3\) and \(\xi \approx 1.53\) as the broken lines in Fig. 21(b). The solid lines in Fig. 21(a) and (b) are the envelope \(y = A \exp\{-\beta't\}\) of this function. In order to see its exponential behavior we show, in Fig. 21(b), the linear-log plot of \(|C_x|\) for the time-oscillating region of \(C_x\), in which the exponential decay is represented as a straight line. In this linear-log plot the local maximum points of \(|C_x|\) are clearly on a
straight line. In Sec. IV A we also showed that the auto-correlation function $C_y$ for the $y$-component of the momentum is nicely fitted to a $\kappa$-exponential function \cite{21}. This is also shown in Fig. 21(a) as the fit line to the $\kappa$-exponential function with fitting parameter values $\alpha'' \approx 0.00746$ and $\kappa \approx 1.48$ (dotted line). However, Fig. 21(a) shows that there is a deviation from this functional form on a long time scale. Such a deviation is significant in the collision number region $n_t > 10000$ in this graph. We fitted the auto-correlation function $C_y$ to an exponential function $y = \mathcal{A}' \exp\{-\alpha'' x\}$ with fitting parameter values $\mathcal{A}' \approx 0.0369$ and $\alpha'' \approx 6.25 \times 10^{-5}$ (the dotted-broken in Fig. 21(a)) in the region where $C_y$ deviates from the $\kappa$-exponential.

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