Lyapunov Spectral Gap and Branch Splitting of Lyapunov Modes in a Diatomic System

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Lyapunov instability of a ''diatomic'' system of coupled map lattices is studied and the dynamics of Lyapunov modes (LMs) is compared with phonon dynamics. Similar to the phonon case mass differences between neighboring sites induce gaps in the Lyapunov spectrum and LMs split into two types correspondingly. An unexpected finding is that contrary to the phonon case a nontrivial threshold value for the mass difference is required for the occurrence of the spectral gap and the splitting of LMs. A possible origin of such a nontrivial threshold value of mass differences is suggested.

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Collective excitation is one of the most important concepts in modern physics. For instance, vibrational normal modes in a rigid crystal lattice, phonons, are known to play an essential role for many physical properties of solids [1]. In the past, encouraged by the success of that concept in solids, there have already been some attempts [2–4] to extend the concept of phonons and to find their counterpart in fluids. Such an idea may date back to Maxwell [2], who suggested that the dynamics of liquids at short times is similar to solids. One recent contribution to this line of research consists in the so-called *instantaneous normal modes* (INMs) [4], which are eigenvectors of the Hessian matrix evaluated from instantaneous states of liquids. The concept of INMs has been demonstrated successful in many respects in understanding liquids dynamics [4].

Recently, the study of hydrodynamic Lyapunov modes (HLMs) attracts a lot of interest [5–14] due to its potential to connect the reduced description of a many-body system to the microscopic information of its detailed dynamics [15]. HLMs are long wavelength collective structures in Lyapunov vectors (LVs) associated with near-zero Lyapunov exponents [5]. Questions on the connection of HLMs to other physical quantities were posed right after their discovery. It has already been noticed that the appearance of HLMs relies on the same mechanisms as phonons and INMs, i.e., the spontaneous breaking of certain symmetries of the system Hamiltonians [6,9]. Moreover, all three sets of modes, phonons, INMs, and HLMs, are related to the Hessian matrix. According to the geometric theory of Hamiltonian chaos [16], both phonons and HLMs represent certain eigendirections characterizing stabilities of geodesics of certain manifolds with suitable metrics. Similar to INMs the calculation of HLMs relies on Hessian matrices evaluated from instantaneous states of the system. HLMs, however, encode additional information on the time correlations among these instantaneous states. In view of these facts, it is natural to ask whether there are connections between these modes and whether HLMs are able to serve as the counterpart of phonons in systems with strong anharmonic dynamics [17]. As a step towards the understanding of such problems, we compare the dynamics of HLMs in a diatomic system with that of phonons. It is known that in diatomic crystal lattices the frequency spectrum of phonons has a gap and phonons split into two branches, acoustic and optical ones, respectively. Our current investigation demonstrates that, similar to the phonon case, mass imparity may induce a gap in the Lyapunov spectrum, and the two corresponding branches of Lyapunov modes [18] behave acoustic- and optical-like, respectively. A major difference between LMs and phonons is, however, that a large enough mass difference beyond a certain threshold value is necessary for the appearance of the gap in the Lyapunov spectrum and the splitting of the modes.

We use here a simple model system of coupled map lattices

$$v^l_{t+1} = v^l_t + \epsilon^l[f(u^{l+1}_t - u^l_t) - f(u^l_t - u^{l-1}_t)] \quad (1a)$$

$$u^l_{t+1} = u^l_t + v^l_{t+1}, \quad (1b)$$

where $f(z)$ is a nonlinear map, t is the discrete-time index, $l = \{1, 2, \ldots, L\}$ is the index of the lattice sites, and L is the system size. The skewed tent map,

$$f(z) = \begin{cases} z'/r & \text{for } 0 \le z' < r, \\ (1 - z')/(1 - r) & \text{for } r \le z' < 1, \end{cases} \quad (2)$$

with $z' = z \pmod 1$, is adopted in the following numerical simulations. Other choices of the function $f(z)$, for instance, the standard map $f(z) = \sin(z/2\pi)$, yield qualitatively the same results as shown here; i.e., the form of $f(z)$ is not an essential factor for the considered problem. The parameter ϵ^l, precisely the quantity $1/\epsilon^l$, plays the same role as mass in mechanical systems and it takes the values ϵ_1 and ϵ_2 for the odd and even lattice sites, respectively [19]. In the following simulations $\epsilon_2 = 1$ is fixed and the value ϵ_1 is tuned to study the influence of mass differences. We expect that the universal features of HLMs will be captured well by such a simple system [14] since it bears similar symmetries as other mechanical systems used in previous studies of HLMs [5,6,10,12]. The Lyapunov exponents and Lyapunov vectors are obtained via the so-called standard method [20].

In general, the tangent space dynamics of a Hamiltonian (lattice) system with continuous symmetries is formally similar to the lattice dynamics of harmonic crystals [7,17]. The force constant matrix for tangent space dynamics, i.e., the Hessian matrix, is, however, not constant and depends on instantaneous states of the system. Owing to the chaotic nature of the system dynamics, the force constant matrix fluctuates spatially and temporally. There are, however, limiting cases, where these fluctuations vanish and the correspondence between Lyapunov modes and phonons becomes exact. Two such limits for our system Eq. (1) are as follows. In the first, the case $r = 1$ in Eq. (2), the tangent space dynamics is just the discrete-time version of the lattice dynamics of one-dimensional harmonic crystals [21]; i.e., the Lyapunov modes are identical to phonons. In contrast to this integrable limit, the second case with $r = 0$ is fully chaotic and the force constant matrix becomes the negative of the discrete Laplacian. This implies that again the Lyapunov modes take the form of phonon modes, but in addition, the Lyapunov spectrum takes the form of the phonon spectrum of harmonic chains including the appearance of gaps. Detuning from these limiting cases, some features of the phonon modes persist in the Lyapunov modes, but also new and unexpected features appear due to the fluctuations of the force constant matrix along the chaotic trajectories.

We show in Fig. 1 the variation of Lyapunov spectra with the mass ratio $\kappa \equiv \epsilon_2/\epsilon_1$. For the Hamiltonian system considered, the Lyapunov spectrum has the symmetry $\lambda^{(2L-1-\alpha)} = -\lambda^{(\alpha)}$. As can be seen in the plot, gaps appear in the middle of each half of the spectrum as the mass imparity is large. With increasing κ, the spectral gap shrinks and disappears eventually. These facts imply that Lyapunov exponents play a similar role for Lyapunov modes as do the frequencies for phonons and the mass difference between neighboring sites does induce gaps in the Lyapunov spectrum.

The Lyapunov spectrum of an extended system is proven to be a continuous curve in the thermodynamic limit for many cases [22]. In the numerical simulation of a system of size L, the increments between neighboring Lyapunov exponents are not zero but of the order $1/L$. Thus one may suspect that the observed disappearance of the spectral gap in Fig. 1 is only a numerical artifact; i.e., the spectral gap just becomes too small to be detected in the simulation using a finite L. In order to clarify this point, we present in Fig. 2 the system size dependence of the spectral gap $\delta\lambda \equiv \lambda^{(L/2-1)} - \lambda^{(L/2)}$. Obviously, in the two regimes on each side of the threshold value κ_c [23], the spectral gap size $\delta\lambda$ behaves differently. For $\kappa < \kappa_c$, $\delta\lambda$ is independent of the system size L while $\delta\lambda$ vanishes for large L as L^{-1} for $\kappa > \kappa_c$. As for the κ dependence, $\delta\lambda$ decreases with increasing κ in the regime $\kappa < \kappa_c$ while it is nearly constant in the regime $\kappa > \kappa_c$. Thus one expects that in the thermodynamic limit the spectral gap size $\delta\lambda$ decreases gradually to zero as κ approaches κ_c from the side $\kappa < \kappa_c$ while it stays to be zero in the regime $\kappa > \kappa_c$. Figure 2(a) shows that data of $\delta\lambda$ from simulations with increasing system size L have the tendency to approach such a master curve. This indicates that the spectral gap does disappear at the threshold value κ_c and excludes the possibility of numerical artefacts. One can state now that a large enough mass difference between the two sorts of elements is required for the appearance of gaps in the Lyapunov spectrum of diatomic systems.

Moreover, as shown in Fig. 2(a), the critical behavior of the spectral gap size $\delta\lambda$ in the supercritical regime can be

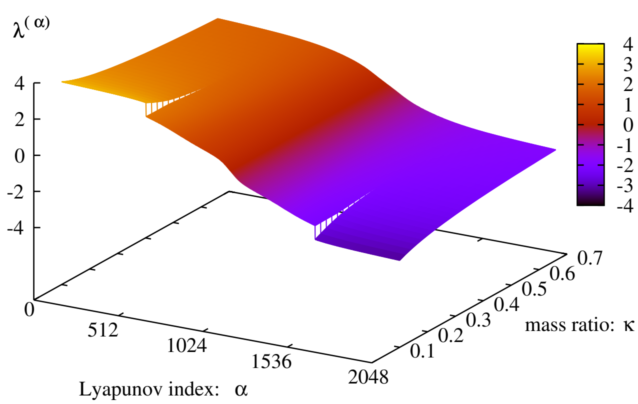

FIG. 1 (color online). Lyapunov exponents as function of the Lyapunov index α and the mass ratio $\kappa \equiv \epsilon_2/\epsilon_1$. Here $L = 1024$ and $r = 0.2$. Notice that the gaps in the Lyapunov spectra disappear as κ increases beyond a certain threshold value κ_c.

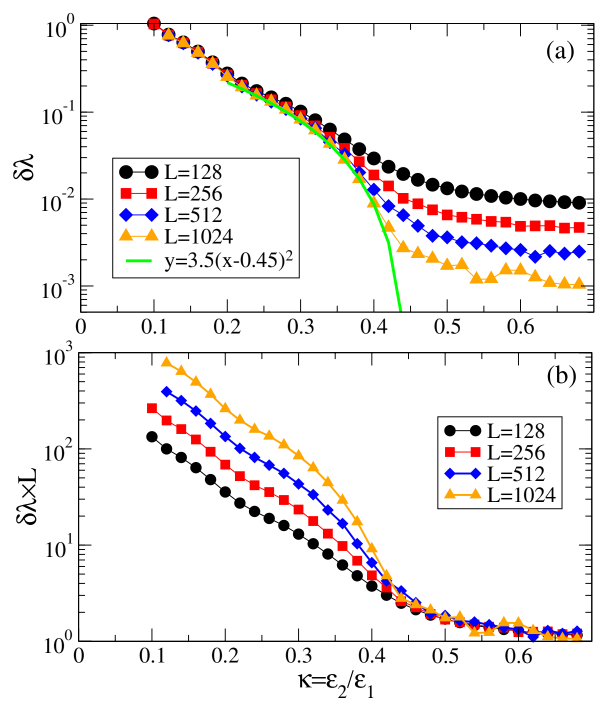

FIG. 2 (color online). The Lyapunov spectral gap size $\delta\lambda \equiv \lambda^{(L/2-1)} - \lambda^{(L/2)}$ vs the mass ratio κ with $r = 0.2$. Obviously, $\delta\lambda$ has different system size dependencies as κ is below or beyond the threshold value $\kappa_c \approx 0.45$.

fitted well by the function $\delta\lambda \sim (\kappa - \kappa_c)^2$ with a rough estimation of the threshold value $\kappa_c \approx 0.45$.

Now we turn to the study of the influence of mass imparity on Lyapunov modes. Inspired by the scenario of changes in phonons we expect to observe also two types of Lyapunov modes: acoustic and optical ones, respectively. To check this we consider the tangent space dynamics of neighboring sites for two Lyapunov modes belonging to the two branches, respectively. Results for an example with $\kappa = 0.125 < \kappa_c$ is shown in Fig. 3. Here $\delta u_1^{(\alpha)}$ denotes the coordinate component of the αth Lyapunov mode for the first lattice site and $\delta u_2^{(\alpha)}$ for the second site correspondingly. The plot of $\delta u_2^{(\alpha)}$ versus $\delta u_1^{(\alpha)}$ in Fig. 3 shows that the distribution of phase points is highly anisotropic and they tend to align along some directions. In a phonon context one would associate the two modes presented with the edge of the first Brillouin zone in a diatomic harmonic chain, i.e., with the wave number $\frac{\pi}{2a}$. The constant a denotes the equilibrium distance between neighboring particles. A similar plot as Fig. 3 for the corresponding quantities of phonons with identical wave number $\frac{\pi}{2a}$ in monatomic systems usually gives rise to circles. Mass difference in diatomic systems induces differences in oscillating amplitudes of the two sorts of particles. The dynamics of these zone-boundary phonons becomes quite simple; i.e., one or the other of the two sublattices is at rest [1]. We expect that the anisotropy observed in Fig. 3 has a similar origin as the corresponding zone-boundary phonon dynamics. To further quantify such anisotropy of tangent space dynamics, we evaluated the quantity $\theta(t) \equiv \frac{1}{\pi} \times \arctan(\delta u_2^{(\alpha)}/\delta u_1^{(\alpha)})$. The probability distributions of $\theta(t)$ for the two Lyapunov modes are presented in Fig. 3(c). Each distribution has a sharp dominant peak, which confirms the significance of the anisotropy in phase point distributions. As expected, the position θ_0 of the dominant peak is very close to 0 and $\pm\pi/2$ for the acoustic and optical Lyapunov modes, respectively [24]. A crucial observation is that, with increasing κ the peak in the probability distribution of $\theta(t)$ becomes gradually lower and broader, and it fades away eventually as κ approaches κ_c; i.e., the angular distribution of phase points becomes homogeneous then [see Fig. 3(c)]. Details will be given in a future publication. Simulations for other Lyapunov vectors show that the evolution of θ_0 with the Lyapunov index α, or the dominant wave number k of Lyapunov vectors, exhibits qualitatively the same behavior as phonons in diatomic systems.

By varying the parameter r in the skewed tent map Eq. (2), the curve of the threshold value $\kappa_c(r)$ divides the (r, k) parameter plane into two regimes, with and without gap in the Lyapunov spectrum, respectively. As shown in Fig. 4, the threshold value κ_c decreases with increasing r; i.e., the appearance of a spectral gap becomes more and more difficult to observe. We noticed in numerical simulations that for the cases with $\kappa = 1$, as r is small there are step structures in the near-zero regime of the Lyapunov spectra [see Fig. 4(b)]. Moreover, this regime shrinks in size with increasing r. Recently, we proposed to use the concept of *domination of the Oseledec splitting* to explain the appearance of these step structures in the Lyapunov spectrum and the significance of HLMs [25]. The basic idea is that for systems with small fluctuations, in the finite-time Lyapunov exponents a good separation between different unstable directions gives rise to these step structures and significant HLMs. With increasing r the increasing fluctuations in finite-time Lyapunov exponents induces the entanglement of the time evolution of unstable directions.

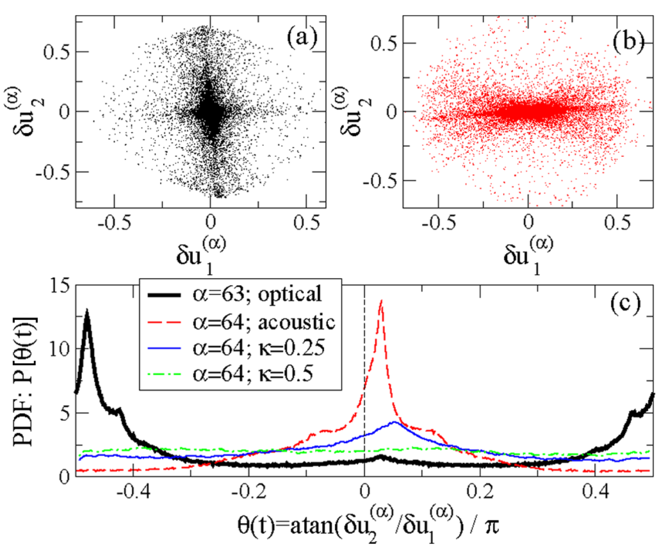

FIG. 3 (color online). Coordinate component of the offset vector for the first lattice site $\delta u_1^{(\alpha)}$ vs that for the second site $\delta u_2^{(\alpha)}$ for Lyapunov modes with (a) $\alpha = L/2 - 1$ and (b) $\alpha = L/2$, which belong to the acoustic and optical branch, respectively. Here $L = 128$, $\kappa = 0.125$, and $r = 0.3$. Note that the distributions of phase points are highly anisotropic for both LMs. (c) The probability distributions of the quantity $\theta(t) \equiv \frac{1}{\pi} \times \arctan(\delta u_2^{(\alpha)}/\delta u_1^{(\alpha)})$. Two additional cases with $\kappa = 0.25$ and 0.5 are also shown. Note that the peak in $P[\theta(t)]$ fades away gradually with increasing κ.

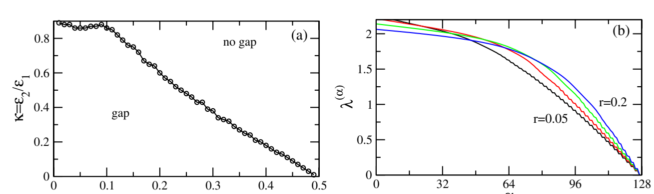

FIG. 4 (color online). (a) Phase diagram for the diatomic system Eq. (1). Appearance of spectral gaps is judged in a system with $L = 128$ by using the criterion $\delta\lambda > \lambda^{(L/2-2)} - \lambda^{(L/2-1)} + \lambda^{(L/2+1)} - \lambda^{(L/2+2)}$. Notice that the appearance of a gap in the Lyapunov spectrum becomes more difficult to observe with increasing r. (b) Lyapunov spectra for several cases with $\kappa = 1$, $r = 0.05$, 0.1, 0.15, and 0.2, respectively. See that the regime of the Lyapunov spectrum with step structures shrinks with increasing r.

In consequence, the regime of the Lyapunov spectrum with step structures shrinks. We believe that the same mechanism works here for the appearance of the spectral gap in diatomic systems. The entanglement of the evolution of unstable directions caused by the fluctuations of finite-time Lyapunov exponents works against the splitting effect caused by the mass difference. The existence of a nontrivial threshold value is the direct result of the competition between these two effects.

In summary, a simple system of coupled map lattices was used to study the influence of mass differences on Lyapunov exponents and the dynamics of Lyapunov vectors of extended systems with continuous symmetries. Our main finding is that the mass difference induces the appearance of gaps in the Lyapunov spectrum and the splitting of Lyapunov modes into acoustic and optical branches. Such a similarity in response to mass differences has its root in the similarity of the mathematical form of tangent space dynamics of our system and that of lattice dynamics of harmonic crystals. It suggests and partially confirms the existence of a certain correspondence between Lyapunov modes and phonons even in the strongly anharmonic regime. This finding on one hand is important for understanding the physical relevance of Lyapunov modes in relation to normal modes such as phonons. On the other hand, it suggests a potential relevance of Lyapunov modes for understanding strong anharmonic dynamics such as conformational transformations of proteins. Moreover, serving as a first step toward the study of disordered systems the implication of our finding for the glass transition in Lennard-Jones fluids will be worked out. Another important task is to discover further similarities between Lyapunov modes and INMs and to see whether one can connect macroscopic transport coefficients such as the diffusion coefficient with Lyapunov modes, especially HLMs, similar to what has been done for INMs [4].

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