Lyapunov modes in extended systems

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Hydrodynamic Lyapunov modes, which have recently been observed in many extended systems with translational symmetry, such as hard sphere systems, dynamic XY models or Lennard–Jones fluids, are nowadays regarded as fundamental objects connecting nonlinear dynamics and statistical physics. We review here our recent results on Lyapunov modes in extended system. The solution to one of the puzzles, the appearance of good and ‘vague’ modes, is presented for the model system of coupled map lattices. The structural properties of these modes are related to the phase space geometry, especially the angles between Oseledec subspaces, and to fluctuations of local Lyapunov exponents. In this context, we report also on the possible appearance of branches splitting in the Lyapunov spectra of diatomic systems, similar to acoustic and optical branches for phonons. The final part is devoted to the hyperbolicity of partial differential equations and the effective degrees of freedom of such infinite-dimensional systems.

Keywords: Lyapunov modes; hyperbolicity; branch splitting; effective degrees of freedom

1. Introduction

The modern theory of nonlinear dynamics is of great importance for the understanding of the fundamentals of statistical mechanics. This idea already dates back to the pioneering work of Krylov (1979), where the connection between the exponential instability of the system dynamics and the mixing properties needed by statistical mechanics was pointed out. The latter was studied by adopting the mathematical results for the instability of geodesic flows on compact manifolds with negative curvatures. Following such a geometric point of view, the ergodic theory of smooth dynamical systems has been developed and is making ongoing progress, mainly for abstract dynamical systems (Sinai 2000). Complementary to this, the geometric theory of Hamiltonian chaos for many-body systems of concrete physical relevance has been developed recently, taking advantage of the progress in Riemannian geometry (Pettini et al. 2005). In the meantime, relations between quantities characterizing the microscopic dynamics of systems, for instance, the Kolmogorov–Sinai entropy and Lyapunov exponents, and quantities used in the macroscopic description of the same dynamics, for instance, the transport coefficients, have been worked out (Dorfman 1999).

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In view of these developments, the recent discovery of hydrodynamic Lyapunov modes (HLMs) by Posch & Hirschl (2000) is of potential importance, since it provides a new possibility to connect the reduced description of a many-body system to the microscopic information of its detailed dynamics. HLMs are long-wavelength collective structures in Lyapunov vectors (LVs) associated with near-zero Lyapunov exponents. They were originally reported in many-particle systems with hard-core interactions. Since then, HLMs were suspected, for a long time, to exist only in hard-core systems because no clear global structures were identified in other systems (Hoover et al. 2002; Forster et al. 2004). This numerical fact is in contrast to intuitive expectations and to results of theoretical attempts, indicating that continuous symmetries and conserved quantities are essential ingredients for HLMs. So far, by using the spectral analysis of LV correlation functions (Radons & Yang 2004; Yang & Radons 2005), the existence of HLMs has been demonstrated to be a common feature of a large class of systems with continuous symmetries and conserved quantities, including many-particle systems with hard-core (Posch & Hirschl 2000; Taniguchi & Morriss 2003, 2005; Forster et al. 2004; Eckman et al. 2005) or soft-potential interactions (Forster & Posch 2005; Yang & Radons 2005), coupled map lattices (Yang & Radons 2006a–c), Hamiltonian lattice models (Yang & Radons 2006a,d; 2008b) and the Kuramoto–Sivashinsky equation (Yang & Radons 2006a).

In this paper, we review briefly our current results on the Lyapunov instabilities of extended dynamical systems. In §2, the numerical method used to calculate Lyapunov exponents and vectors are explained and the correlation functions used to characterize the spatio-temporal structures of LVs are defined. In §3, we show, in model systems of coupled map lattices, that the hyperbolicity of the system, especially the angle between the LVs crucially determines the significance of Lyapunov modes. In §4, we show that, in a diatomic coupled map lattices system, the Lyapunov spectrum and the corresponding LVs split into two branches similar to the splitting of phonons in a diatomic crystal lattice. In §5, we show that the information of the hyperbolicity of a partial differential equation (PDE) can be used to infer the number of effective degrees of freedom (d.f.) involved in such an infinite-dimensional system. Details of these studies and our previous results on the Lennard–Jones system can be found in Yang & Radons (2007, 2008a,c) and Yang et al. (2009).

2. Numerical algorithms and Lyapunov vectors correlations

As usual, the standard method (Benettin et al. 1976) is used to calculate the orthogonal LVs and the corresponding Lyapunov exponents. For this purpose, an ensemble of linear equations, governing the evolution of the offset vectors, are integrated simultaneously with the original nonlinear evolution equations. The offset vectors have to be re-orthogonalized periodically, by means of either Gram–Schmidt orthogonalization or QR decomposition. To obtain scientifically useful results, one needs large system sizes and long integration times for the calculation of certain long time averages. This enforces the use of parallel implementations of the corresponding algorithms.

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In addition to this, a recently proposed algorithm allows us to calculate the so-called covariant LVs (CLVs; Ginelli et al. 2007). These quantities provide useful information about the hyperbolicity of the investigated system. The main idea of this method is based on the fact that almost every randomly selected vector inside a subspace spanned by the first $n$ orthogonal LVs will evolve backwards in time asymptotically to the $n$th CLV. The essential ingredient of this algorithm is the effective dynamics restricted to the mentioned subspace, which is obtained from the Gram–Schmidt orthogonalization or QR decomposition performed in the standard method.

In the spirit of molecular hydrodynamics, we introduced in Radons & Yang (2004) and Yang & Radons (2005) a dynamical variable called the LV fluctuation density

$$u^{(\alpha)}(r, t) = \sum_{j=1}^{N} \delta x^{(\alpha)}_j(t) \delta(r - r_j(t)), \quad (2.1)$$

where $\delta(z)$ is Dirac’s delta function, $r_j(t)$ is the position coordinate of the $j$th particle and $\{\delta x^{(\alpha)}_j(t)\}$ is the coordinate part of the $\alpha$th LV at time $t$. The spatial structure of LVs is characterized by the static LV structure factor, defined as

$$S^{(\alpha\alpha)}_u(k) = \int \langle u^{(\alpha)}(r, 0) u^{(\alpha)}(0, 0) \rangle e^{-jk r} dr, \quad (2.2)$$

which is simply the spatial power spectrum of the LV fluctuation density. Information on the dynamics of LVs can be extracted via the dynamic LV structure factor, which is defined as

$$S^{(\alpha\alpha)}_u(k, \omega) = \int \int \langle u^{(\alpha)}(r, t) u^{(\alpha)}(0, 0) \rangle e^{-jk r} e^{j\omega t} dr dt. \quad (2.3)$$

3. Hyperbolicity and the significance of Lyapunov modes

We know that HLMs were originally reported in many-particle systems with hard-core interactions (Posch & Hirschl 2000). Even though the controversy over the existence of HLMs in systems with soft-potential interactions has been successfully resolved (Forster & Posch 2005; Yang & Radons 2005) by using the spectral method invented in Radons & Yang (2004) and Yang & Radons (2005), there are still some important questions left open. For instance, the long-wavelength global structures in LVs of hard-core systems can be easily identified visually and they can be fitted well to a sinusoidal function directly (Posch & Hirschl 2000; Taniguchi & Morriss 2003; Forster et al. 2004; Eckmann et al. 2005), whereas such collective structures in soft-potential systems can only be detected indirectly via spectral analysis (Forster & Posch 2005; Yang & Radons 2005). One then asks naturally: what specific nature of a system determines the significance of HLMs?

In the past, the hyperbolicity of hard-core systems was considered as being relevant for the appearance of significant HLMs (Eckmann et al. 2005). The resulting (good) separation between stable and unstable manifolds, however, is too coarse and obviously not sufficient, since LVs provide a splitting of the tangent space on a very fine scale. Previous numerical investigations indicate
that large fluctuations in finite-time Lyapunov exponents may cause entanglement among unstable subspaces corresponding to different Lyapunov exponents, which damages HLMs. In order to have good HLMs, these unstable subspaces with different Lyapunov exponents should separate uniformly in the same manner as unstable and stable manifolds of hyperbolic sets. A useful concept is the domination of the Oseledec splitting (DOS), saying that each Oseledec subspace is uniformly more/less expanding than the next subspace corresponding to a larger/smaller Lyapunov exponent (Bochi & Viana 2005). Our hypothesis is that partial DOS with respect to subspaces associated with near-zero Lyapunov exponents is crucial for observing good HLMs. The results for a simple system of coupled map lattices are presented to support our proposal.

The model system used is a lattice of coupled maps. It reads

\[ v_{l+1}^i = v_i^l + \epsilon [f(u_{l+1}^i - u_l^i) - f(u_l^i - u_{l-1}^i)] \] (3.1a)

and

\[ u_{l+1}^i = u_i^l + v_{l+1}^i, \] (3.1b)

where the local map \( f(z) \) has the properties of the skewed tent (T) or Bernoulli shift map (B)

\[
  f_{B,T}(z) = \begin{cases} 
  z'/r & \text{for } 0 < z' \leq r, \\
  (z' - r)/(1 - r) & \text{for } r < z' < 1 \text{(B)}, \\
  (1 - z')/(1 - r) & \text{for } r < z' < 1 \text{(T)},
  \end{cases}
\] (3.2)

with \( z' = z \pmod 1 \). In this section, we concentrate on a homogeneous case with \( \epsilon^l = \epsilon \). A splitting parameter \( p_{\text{split}} \) was defined in Yang & Radons (2007) to characterize the fluctuations in the local Lyapunov exponents \( \lambda^{(a)}(t) \) corresponding to the CLVs,

\[ p_{\text{split}}^i \equiv \max_t \{p_{\text{split}}(t)\}, \] (3.3)

where \( p_{ij}(t) \) is defined as \( \lambda_j(t)/\lambda_i(t) \) or \( \lambda_i(t)/\lambda_j(t) \) for \( j > i \) or \( i > j \), respectively. The case \( p_{\text{split}} < 1 \) indicates the satisfaction of the DOS, a situation where the hyperbolic splitting among Oseledec subspaces (LVs) enables the appearance of good Lyapunov modes.

Figure 1 depicts the numerical results for a skewed tent map case \( f_T(z) \). Strong fluctuations in local Lyapunov exponents \( \lambda^{(a)} \), indicated by the standard deviations of \( \lambda^{(a)} \), show that the chaoticity of the dynamics of this system is not uniform. The splitting parameter \( p_{\text{split}} \) increases gradually as the Lyapunov exponents \( \Lambda^{(a)} \) increase from zero and it crosses the line \( p_{\text{split}} = 1 \) at \( i_c/L \approx 0.4 \). Consistently with this, the fraction of DOS violation time \( \nu^i \) is constantly 0 in the regime \( i > i_c \).

Let us see how the dynamics and the significance of HLMs change with the splitting parameters \( p_{\text{split}} \) and \( \nu \). To characterize the entanglement among Lyapunov modes, we use the quantity \( \theta^i \), which is defined as the smallest angle between the \( i \)th Lyapunov mode (Oseledec subspace) and any other Lyapunov modes (subspaces) with different Lyapunov exponents. As can be seen from figure 1c, in the regime \( p_{\text{split}}(1, \text{i.e. } i) > i_c \), the angle \( \theta^i \) stays close to \( \pi/2 \) and it decreases with increasing \( p_{\text{split}} \). An interesting point is that the value of \( \theta^i \)
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fluctuates strongly in the regime $i_2 < i < i_c$ and experiences a sudden fall to near-zero values at $i_1$, the boundary for the regime of the steep increase in the violation of DOS. Taking into account that $\theta^i = 0$ implies the presence of tangencies or entanglements among Oseledec subspaces, the observation that $\theta^i$ is bounded away from zero in the regime $i > i_c$ confirms that the DOS prevents the presence of tangencies. Surprisingly, the minimal angle $\theta^i$ for decreasing $i$ becomes zero in a regime near $i_1$, far below the threshold value $i_c$ for the DOS. The reason for the delayed response of $\theta^i$ to the violation of DOS is discussed in Yang & Radons (2007). To measure the significance of HLMs, we use a quantity $S^{(a)}(k_{\text{max}})/S^{(a)}_{\text{total}}$, where $S^{(a)}(k)$ is the static LV structure factor equation (2.2), $k_{\text{max}}$ is the wavenumber of the dominant peak in $S^{(a)}(k)$ and $S^{(a)}_{\text{total}} = \sum_k S^{(a)}(k)$. The significance measure attains a value 1 if the HLM is a pure Fourier mode. As can be seen from figure 1d, in the regime $p^{\text{split}} < 1$, the measure $S^{(a)}(k_{\text{max}})/S^{(a)}_{\text{total}}$ always stays very close to one. It decreases monotonically with increasing $p^{\text{split}}$ in the regime $i_2 < i < i_c$ and drops drastically to zero in a regime around $i_2$, the boundary value for nearly permanent violation of DOS. To further quantify the change in the significance of HLMs, we use $s^{(a)}_{\text{min}} = \min_t \{s^{(a)}(k_{\text{max}}, t)/S^{(a)}_{\text{total}}(t)\}$, the minimal value of the instantaneous LV structure factor $s^{(a)}(k_{\text{max}}, t)$. We find that the time evolution of $s^{(a)}(k_{\text{max}}, t)$ is also strongly fluctuating for $i_2 < i < i_c$. Moreover, as shown in figure 1d that corresponds to the sudden fall of the variable

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θ^i, a sudden jump in \( s^{(α)}_{\text{min}} \) occurs at \( i_1 \). The strong correlation in the evolution of the two quantities implies that entanglement among Oseledec subspaces, as indicated by the minimal angle \( θ^i \), is the origin for the steep decrease of the significance of HLMs, as demonstrated by the variation of \( S^{(α)}(k_{\text{max}})/S^{(α)}_{\text{total}} \) and \( s^{(α)}_{\text{min}} \). Note that even the fluctuations of the minimal angle \( θ^i \) are reflected in the instantaneous spatial structure of the LVs, as indicated by \( s^{(α)}_{\text{min}} \) (cf. figure 1c,d). These findings show that \( p_{\text{split}} \) and \( ν \) indicate faithfully the tendency of change in the significance of HLMs. Moreover, the significance of HLMs is quite sensitive to the change in the values of the splitting parameters, especially in the regime \( i_2 < i < i_c \). Our results thus show that DOS can be used successfully to explain the variation in the significance of HLMs as the Lyapunov exponents increase from zero.

We also studied how the significance of HLMs changes with the splitting parameter \( p_{\text{split}} \) in the regime \( p_{\text{split}} > 1 \). As shown in figure 2, for all cases considered, the significance measure \( S^{(α)}(k_{\text{max}})/S^{(α)}_{\text{total}} \) decreases monotonically with increasing \( ν \), the fraction of time for which the DOS is violated. The monotonic decrease of \( S^{(α)}(k_{\text{max}})/S^{(α)}_{\text{total}} \) with increasing \( ν \) shows that HLMs are more significant the less the DOS is violated.

These numerical results demonstrate clearly the existence of an essential relation between the hyperbolicity of the system dynamics and the significance of coherent structure in LVs, i.e. the relevance of the DOS for observing good HLMs.

4. Lyapunov spectral gap and branch splitting of Lyapunov modes in a ‘diatomic’ system

Collective excitation is one of the most important concepts in modern physics. For instance, vibrational normal modes in a crystal lattice, phonons, are known to play an essential role for many physical properties of solids. In the past, encouraged by the success of that concept in solids, there have already been some attempts to extend the concept of phonons and to find their counterpart in
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Figure 3. Lyapunov exponents as function of the Lyapunov index $\alpha$ 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 $\kappa$ increases beyond a certain threshold value $\kappa_c$.

fluids. Such an idea may date back to Maxwell, who suggested that the dynamics of liquids at short times is similar to solids. One recent contribution to this line of research consists of the so-called instantaneous normal modes (INMs; Keyes 1997), which are eigenvectors of the Hessian matrix evaluated from instantaneous states of liquids.

On the other hand, questions on the connection of the recently found 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 (de Wijn & van Beijeren 2004; Forster et al. 2004). Moreover, all three sets of modes, phonons, INMs and HLMs, are related to the Hessian matrix. According to the geometric theory of Hamiltonian chaos, both phonons and HLMs represent certain eigendirections characterizing the 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. 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 behave acoustic- and optical-like, respectively. A major difference between Lyapunov modes 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.
The coupled map lattices equation (3.1) with \( f(z) \) being the skewed tent map is investigated in this section. The quantity \( \frac{1}{\epsilon^l} \) plays the same role as mass in mechanical systems and \( \epsilon^l \) takes the values \( \epsilon_1 \) and \( \epsilon_2 \) for the odd and even lattice sites, respectively. In the following simulations, \( \epsilon_2 = 1 \) is fixed and the value \( \epsilon_1 \) is tuned to study the influence of mass differences. The Lyapunov exponents and LVs are obtained via the so-called standard method (Benettin et al. 1976).

We show, in figure 3, 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 if the mass imparity is large. With increasing \( \kappa \), 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 neighbouring sites does induce gaps in the Lyapunov spectrum.

The Lyapunov spectrum of an extended system is proved to be a continuous curve in the thermodynamic limit for many cases. In the numerical simulation of a system of size \( L \), the increments between neighbouring Lyapunov exponents are not zero but of the order \( 1/L \). Thus, one may suspect that the observed disappearance of the spectral gap in figure 3 is only a numerical artefact, 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 figure 4, 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 \( \kappa_c \), 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 \( \kappa \)-dependence, \( \delta \lambda \) decreases with increasing \( \kappa \) 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 \( \kappa \) approaches \( \kappa_c \) from the side \( \kappa < \kappa_c \), while it stays zero in the regime \( \kappa > \kappa_c \). Figure 4a 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 \( \kappa_c \) and excludes the possibility of numerical artefacts.

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 also observe two types of Lyapunov modes, acoustic and optical ones. To check this, we consider the tangent space dynamics of neighbouring sites for two Lyapunov modes belonging to the two branches, respectively. Results for an example with \( \kappa = 0.125 < \kappa_c \) is shown in figure 5. Here, \( \delta u^{(a)}_1 \) denotes the coordinate component of the \( \alpha \)th Lyapunov mode for the first lattice site and \( \delta u^{(a)}_2 \) is for the second site. The plot of \( \delta u^{(a)}_2 \) versus \( \delta u^{(a)}_1 \) in figure 5 shows that the distribution of phase points is highly anisotropic and they tend to align along different directions for the two Lyapunov modes. In a phonon context, one would associate the two modes presented with the edge of the first Brillouin zone in a diatomic harmonic chain. Mass difference in diatomic systems induces differences in oscillating amplitudes of the two sorts of particles. The dynamics of these zone-boundary phonons then becomes quite simple, i.e. one or the other of the two sublattices is at rest. We expect that the anisotropy observed in figure 5 has a similar origin as the corresponding zone-boundary phonon dynamics. The anisotropy

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Figure 4. (a, b) The Lyapunov spectral gap size $\delta \lambda \equiv \lambda^{(L/2-1)} - \lambda^{(L/2)}$ versus the mass ratio $\kappa$ with $r = 0.2$. Obviously, $\delta \lambda$ has different system-size dependencies as $\kappa$ is below/beyond the threshold value $\kappa_c \approx 0.45$. Circles, $L = 128$; squares, $L = 256$; diamonds, $L = 512$; triangles, $L = 1024$; thick line, $y = 3.5(x - 0.45)^2$.

of tangent space dynamics may be further evidenced by the sharp peak in the probability distributions of $\theta(t) = 1/\pi \arctan(\delta u^{(a)} / \delta u^{(a)})$. Simulations for other LVs show that, despite the chaotic nature of the system, the evolution also exhibits qualitatively, in many respects, the same behaviour as phonons in diatomic systems.

Our main finding in this section 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 the 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.

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Figure 5. \( \delta u^{(w)}_1 \) versus \( \delta u^{(w)}_2 \) 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 \( \tau = 0.3 \). (c) The probability distributions of \( \theta(t) \). Black, \( \alpha = 63 \), optical; red, \( \alpha = 64 \), acoustic; blue, \( \alpha = 64 \), \( \kappa = 0.25 \); green, \( \alpha = 64 \), \( \kappa = 0.5 \).

5. Hyperbolicity and the effective degrees of freedom of partial differential equations

It is well known that, despite an underlying discreteness, many phenomena in nature and in the laboratory are well described by PDEs. Examples include the Navier–Stokes equation for fluid dynamics, the complex Ginzburg–Landau equation and the Kuramoto–Sivashinsky equation for pattern formation and space–time chaos.

An immediate difficulty for studying the dynamics of PDE systems is that the number of d.f. involved is infinite. For instance, numerical simulation of such systems, which is usually the only available way to obtain information of their complex behaviour, often starts from discretizing space and time. The infinite-dimensional nature of PDE systems seems to demand an infinitesimal discretization step, which is obviously impossible for any computer. Fortunately, owing to the strong dissipative nature, such infinite-dimensional systems often possess a finite-dimensional global attractor. Thus, a finite-dimensional smooth manifold, the inertial manifold, is assumed to exist for many interesting examples of PDE systems (Foais et al. 1988). All essential dynamics of these systems is believed to take place just inside the inertial manifold, which thus opens up the possibility to model an infinite-dimensional PDE system by a finite-dimensional one. Although conceptually important for understanding many issues of PDE systems, the application of the inertial manifold to the investigation of nonlinear systems is yet very limited, partially owing to the absence of a practical method to determine it accurately.
On the other hand, in the study of space–time chaos in extensive dynamical systems, it was recognized that not all information about the dynamics of each d.f. is relevant for macroscopic features of such systems (Cross & Hohenberg 1993). Instead, the extensive nature of space–time chaotic systems suggests that distant parts of such systems are uncorrelated and that the whole system could further be viewed as consisting of many such uncorrelated components. Therefore, a probabilistic description in the spirit of statistical mechanics or a reduced description based on coarse-grained models would be a better choice. To this aim, seeking the effective d.f. entering such descriptions becomes an essential step.

In a pioneering work, Ruelle (1982) conjectured the existence of a large-volume limit of the Lyapunov spectrum of extensive chaotic systems. It implies the existence of an intensive quantity, namely the Lyapunov dimension density $\delta \equiv D/V$, where $D$ is the attractor dimension and $V$ the system volume. A length scale can be defined correspondingly as $\xi_\delta \equiv \delta^{-1/d}$, where $d$ is the dimensionality of the considered system. The physical significance of this length scale is that regions of size $\xi_\delta$ contain, on average, one non-trivial d.f.

In this section, the Lyapunov instability of a one-dimensional PDE system is investigated. In contrast to most works in the literature, we attempt to see how the spatial resolution of simulations influences the obtained Lyapunov characteristics. Our simulations show that the Oseledec splitting of the tangent space dynamics of a PDE system is highly hyperbolic. This provides strong evidence for the isolated nature of a manifold corresponding to the smooth part of the Lyapunov spectrum, which is thought to be associated with non-trivial active d.f. for the underlying system. Moreover, the dimension of this manifold shows a stepwise increase with system size. These features are expected to be common for a large class of PDEs.

Our results were obtained from simulations of the one-dimensional Kuramoto–Sivashinsky equation in the form

$$\partial_t u = -\partial_x^2 u - \partial_x^4 u - (\partial_x u)^2, \quad x \in [0, L], \quad (5.1)$$

and by applying periodic boundary conditions. It is known that the system size $L$ is the only control parameter of this system and, for $L \geq 50$, the system becomes spatio-temporally chaotic. The algorithm proposed in Ginelli et al. (2007) is used to calculate CLVs $e^{(\alpha)}$ and the corresponding local Lyapunov exponents $\lambda^{(\alpha)}$.

Figure 6 shows how the spatial resolution of simulations influences the Lyapunov spectrum. Several cases with the same $L$ but different space resolutions $\delta x \equiv L/N$ are presented in the main panel, where $N$ is the number of space grid points used. Improving space resolution means more d.f. entering the simulated dynamics and therefore more Lyapunov exponents are obtained. As can be seen clearly from the enlargement of spectra in the left inset, the Lyapunov spectrum of this system splits naturally into a smoothly varying part for $\alpha < \alpha_c$ and a part consisting of size-two step structures. Note that the threshold value $\alpha_c$ lies deeply in the regime of negative Lyapunov exponents. Moreover, the smooth part of the Lyapunov spectrum and the threshold value $\alpha_c$ of the splitting are not influenced by the variation of the spatial resolution, as demonstrated by the data collapse in this regime. In contrast, the number of Lyapunov exponents in the other part and the value of these Lyapunov exponents do change with varying the spatial resolution. The pairing nature

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of Lyapunov exponents is, however, not influenced by the variation of space resolution. These numerical results suggest that the dynamics associated with the smooth part of the Lyapunov spectrum does not depend on the simulation detail and thus would be more interesting than that corresponding to the discrete part.

To characterize the detailed hyperbolicity, we use the quantities $p_{\text{split}}$ and $\theta_{\min}$ (Yang et al. 2009). The former $p_{\text{split}}$ measures the fluctuations of finite-time Lyapunov exponents $\lambda_\tau$ and the latter $\theta_{\min}$ denotes the minimal angle between a selected Oseledec subspace (or the corresponding CLVs) and all the other Oseledec subspaces (the corresponding CLVs). For simplicity, we have $p_{\text{split}}^{(\alpha)}(\tau) = \max_{\beta \neq \alpha} \{ p_{\alpha\beta}^{(\tau)}(t) \}$ and $p_{\alpha\beta}^{(\tau)}$ is defined as $p_{\alpha\beta}^{(\tau)}(t) = \lambda_\tau^{(\alpha)}(t) - \lambda_\tau^{(\beta)}(t)$ for $\beta > \alpha$ and $p_{\beta\alpha}^{(\tau)} = p_{\alpha\beta}^{(\tau)}$. Notice that the definition of $p_{\text{split}}$ used here is slightly different from in §3 and instead negative values of $p_{\text{split}}$ and corresponding non-zero values of $\theta_{\min}$ indicate the fulfillment of the DOS. Figure 7 shows the variation of the hyperbolicity measures $p_{\text{split}}$ and $\cos(\theta_{\min})$ with Lyapunov index $\alpha$ for several cases with the same $L$ but different $\delta x$ and $\tau$. Look first at the case $\delta x = 0.52$ and $\tau = 0.4$, which is denoted by filled circles in the plot. Obviously, the behaviour of both quantities $p_{\text{split}}$ and $\cos(\theta_{\min})$ is clearly distinct in the two regimes separated by a threshold value $\alpha_c$, corresponding to the splitting of the Lyapunov spectrum shown in figure 6. One can easily see that $p_{\text{split}}$ always attains positive values in the regime $\alpha \leq \alpha_c$, whereas for $\alpha > \alpha_c$ it is always negative and its value decreases with increasing $\alpha$. Correspondingly, $\cos(\theta_{\min})$ stays close to 1 for $\alpha \leq \alpha_c$ and it departs
from 1 gradually with increasing $\alpha$ beyond $\alpha_c$. This indicates the fulfilment of the (partial) DOS with respect to the LVs with $\alpha \geq \alpha_c$. And the dynamics in the manifold spanned by CLVs with $\alpha \leq \alpha_c$ is hyperbolically isolated from that along CLVs with $\alpha > \alpha_c$.

Now let us specify more clearly the meaning of this isolation and/or the implication of the claimed strong hyperbolicity. The quantity $\theta_{\min}$ being non-zero for $\alpha > \alpha_c$ means that, during the time evolution, any one of the CLVs with $\alpha > \alpha_c$ has no chance to be tangent to any other CLV associated with a different Lyapunov exponent. Combined with their covariant nature, one can thus easily see that each of these CLVs evolves just freely. Imagine adding to the system dynamics a small perturbation along some CLV, with $\alpha > \alpha_c$. The amplitude of this perturbation will decay exponentially to zero, as indicated by the negative value of $\Lambda(\alpha)$. Moreover, perturbations along this specified direction would not induce perturbations along other directions with different $\Lambda(\alpha)$ and vice versa. In contrast, zero values of $\theta_{\min}$ for $\alpha \leq \alpha_c$ indicate the appearance of tangencies between CLVs in that regime. Therefore, perturbations initially introduced along some CLVs with $\alpha \leq \alpha_c$ may eventually induce activity along all other directions with $\alpha \leq \alpha_c$. In particular, perturbations introduced along CLVs with negative Lyapunov exponents in the regime $\alpha \leq \alpha_c$ are able to induce motions along directions with positive Lyapunov exponents and eventually lead to a drastic change of the dynamical evolution. In this sense, the dynamics along CLVs with $\alpha \leq \alpha_c$ is highly entangled while decoupled from the decaying dynamics along the directions with $\alpha > \alpha_c$, and therefore the manifold spanned by CLVs with $\alpha \leq \alpha_c$ is called dynamically isolated.

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Figure 8. Stepwise increasing of the dimension $D_{IM}$ of the isolated manifold with system size $L$. Numerical fitting yields $D_{IM} = 0.39L + 0.88$. Moreover, numerical data agree well with a function $D_{IM} = 1 + 2\lfloor L/\xi_{IM}\rfloor$ with $\xi_{IM} \approx 4.98$ and $\lfloor x\rfloor$ denoting the integer part of $x$. Dashed line, $y = 0.88 + 0.39x$; thick line, $y = 1 + 2\lfloor x/4.98\rfloor$.

Other cases with the same $\delta x$ and different $\tau$ and one case with smaller $\delta x$ shown in figure 7 demonstrates that the existence of an entangled manifold is an intrinsic property of the underlying PDE system and simulation details have no or ignorable influence on it.

As noticed already in figure 6, the dimension of the isolated manifold is much larger than the Kaplan–Yorke dimension of the attractor. Thus, a new characteristic length that is different from the dimension length $\xi_{S}$ may be defined. For this purpose, one needs to study the system-size dependence of the isolated manifold and to check its extensivity. Figure 8 shows a stepwise increase of $D_{IM}$ with system size $L$ as expected. Moreover, the value of $D_{IM}$ jumps by two between nearest neighbouring steps, which is related to the double degeneration of Lyapunov exponents and is assumed to result from the spatial translational invariance of the system. Remarkably, the variation of $D_{IM}$ follows perfectly a function $D_{IM} = 1 + 2\lfloor L/\xi_{IM}\rfloor$ with $\lfloor x\rfloor$ denoting the integral part of $x$. The extension of the steps $\xi_{IM} \approx 4.98$ may be defined as a new length scale for characterizing space–time chaos.

We conclude the section with some comments. First, our proposition of Lyapunov instability analysis provides a practical method to probe information on the number of the effective d.f. (the dimension of the inertial manifold) of PDEs. Secondly, although the numerical results presented here were obtained for the Kuramoto–Sivashinsky equation, similar results were found for the complex Ginzburg–Landau equation (Yang et al. 2009). We expect our discovery to hold for a large class of dissipative PDE systems. Finally, we would like to emphasize that, besides the conceptual importance for understanding features of PDE systems, our method for an accurate estimation of $D_{IM}$ may also provide helpful hints to continuum system-related practical applications.

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References


