Karhunen-Loève local characterization of spatiotemporal chaos in a reaction-diffusion system

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By computing the Karhunen-Loève decomposition (KLD) correlation length ξ_{KLD} of a reaction-diffusion system in the extensive chaos regime, we show that it is a sensitive measure of spatial dynamical inhomogeneities. It reveals substantial spatial nonuniformity of the dynamics at the boundaries and can also detect slow spatial variations in system parameters. The intensive length ξ_{KLD} can be easily computed from small local subsystems and is found to have a similar parametric dependence as the two-point correlation length computed over the full system size.

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A poorly understood issue in nonequilibrium physics is the space-time characterization of spatiotemporal chaos [1,2]. These states exhibit a lack of correlation in both space and time and are found in many physical systems including reacting and diffusing chemical flows [3], convective transport of heat [4], and charge transport in semiconductors [5–7]. These states have been characterized using two-point correlation functions [8] and dimension correlation lengths [9], though both are global measures of the dynamics that assume uniform homogeneous chaos. However, averages of spatiotemporal chaos in experiment [10–12] and simulation [13] have demonstrated that the dynamics can be strongly effected by the boundaries. Further, system parameters can often vary spatially (an example being the concentration of a chemical species in a spatially-extended reaction-diffusion system), so a means to quantify parametric variations in the system can be important in making comparison with experiment. Recently, the Karhunen-Loève decomposition (KLD) correlation length [14] was used to characterize extensive chaos *locally* in small subsystems of the larger dynamics based on the extensive growth of the KLD dimension [15]. Since the KLD correlation length is defined in a subsystem, it allows a dynamical measure of nonuniformities in space. Further, this length scale was shown to be an independent quantity, which behaves similarly to the dimension correlation length [14] but has a different parametric dependence than the two-point correlation length ξ_2 in coupled map lattices [14] and convection data [16]. These results suggest that the KLD correlation length is a useful independent length scale in spatiotemporal chaotic systems.

In this paper, we present an application of the KLD correlation length to a reaction-diffusion model, which describes charge transport in a semiconductor with bistable current-voltage characteristics [17]. This model has an advantage over the Kuramoto-Sivashinsky equation on which the KLD correlation length was originally computed in that there are tunable parameters in the partial differential equations making it a more general model of spatiotemporal chaos. For a sufficiently large system size, the model exhibits long transients, which are extensively chaotic [6], i.e., the number of positive Lyapunov exponents grows in proportion to the system volume [7]. If one defines the KLD dimension D_{KLD} as the number of KLD eigenmodes needed to approximate the space-time data with a certain accuracy, this number also scales extensively with subsystem volume. A KLD local correlation length ξ_{KLD} is then derived from the rate of growth of the KLD dimension with subsystem volume V. This KLD correlation length is used to quantify dynamical inhomogeneity near boundaries. We demonstrate the existence of a long-range spatial nonuniformity in the KLD correlation length similar to the average patterns of spatiotemporal chaos [13]. Further, we vary a system parameter in the model and confirm that the KLD correlation length can detect parametric changes. Finally, we demonstrate that the KLD correlation length computed on small subsystems is proportional to the two-point correlation length computed over the entire system volume.

The Karhunen-Loève decomposition, also called the method of empirical orthogonal functions or proper orthogonal decomposition, is a classical statistical method to represent complex space-time data $U(t_i,\mathbf{x}_j)$ by a minimum number of space and time eigenmodes [15]. This decomposition proceeds by organizing the discretized data into a space-time matrix,

$$A_{ij}=U(t_i,\mathbf{x}_j)-\langle U(t_i,\mathbf{x}_j)\rangle, \tag{1}$$

where $\langle U(t_i,\mathbf{x}_j)\rangle$ is the space-time-average of the field $U(t_i,\mathbf{x}_j)$. The space-time matrix is of dimensions $T\times X$ where T is the number of observation times t_i, and X is the number of observation sites $\mathbf{x}_j$ within the subsystem. A singular value decomposition of this matrix provides an optimal 2-norm variance decomposition of the space-time matrix $\mathbf{A}$ in the sense that the expansion of

$$A_{ij}\approx\sum_{k=1}^{p} a_k(t_i)\sigma_k^2\Phi_k(\mathbf{x}_j) \tag{2}$$

in terms of spatial eigenmodes $\Phi_k(\mathbf{x}_j)$ and normalized mode amplitudes $a_k(t_i)$ has a minimum squared error for a fixed number of expansion terms p [15]. The weight of the different expansion terms is given by their variances σ_k^2, which correspond to the eigenvalues of the positive semidefinite

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covariance matrix $\mathbf{A}^T\mathbf{A}$, ordered in decreasing size, $\sigma_1^2 \geqslant \sigma_2^2 \geqslant \cdots \geqslant \sigma_X^2$, and $\Phi_k(\mathbf{x}_j)$ are the eigenvectors of $\mathbf{A}^T\mathbf{A}$. The KLD dimension [18] of the matrix A_{ij}

$$D_{\mathrm{KLD}} = \max\left\{ p: \frac{\Sigma_{k=1}^{p} \sigma_k^2}{\Sigma_{k=1}^{X} \sigma_k^2} \leqslant f \right\} \tag{3}$$

represents the number of linear eigenmodes needed to approximate some fraction $0<f<1$ of the total variance of the data [14,18,19].

The relation of the KLD decomposition to Fourier analysis depends on the symmetries of the matrix $\mathbf{A}$ [15]. If the data is homogeneous, i.e., periodic in time or translationally invariant in space, then the autocorrelation matrix $\mathbf{A}^T\mathbf{A}$ becomes translationally invariant and then the KLD modes are Fourier modes. In most physical situations, dynamics will not be homogeneous or space-translationally invariant due to the boundaries and varying system parameters. Therefore, in spatiotemporally chaotic systems the KLD modes most likely will not trivially correspond to Fourier modes of the data.

The KLD *local* correlation length is based on the computation of $D_{\mathrm{KLD}}(\mathbf{x_j})$ for concentric subsystems of volume V centered at the point $\mathbf{x_j}$ in space. The dimension $D_{\mathrm{KLD}}(\mathbf{x_j})$ typically depends on the point $\mathbf{x_j}$ and so provides a measure of spatial dynamical inhomogeneity. For extensive chaotic systems the KLD dimension $D_{\mathrm{KLD}}(\mathbf{x_j})$ will increase linearly with subsystem volume V with a slope δ_{KLD}. This indicates that the KLD dimension density $\delta_{\mathrm{KLD}} = D_{\mathrm{KLD}}/V$ is a more useful measure, as it is an intensive property of the subsystem. To derive a characteristic length scale, the KLD correlation length ξ_{KLD} is defined to be $\delta_{\mathrm{KLD}}^{-1/\mathrm{d}}$ where d is the spatial dimensionality of the data. The advantage of the KLD correlation length over dimension correlation length [20] or two-point correlation length [8] is that it is computed directly from data in small localized spatial subsystems of larger space-time data sets. This locality has allowed the detection of smooth spatial dynamical nonuniformities of a system parameter of a coupled map lattice [14] and of experimental spatial inhomogeneities in convection data [16]. Further, in the study of an Ising-like phase-transition, the KLD correlation length ξ_{KLD} was shown [14] to have a different critical parametric dependence than the commonly computed two-point correlation length, indicating at least for some cases that ξ_{KLD} is an independent length scale of spatiotemporal chaos. It is not understood whether these properties hold for systems described by partial differential equations with boundaries and tunable parameters where continuity smoothes out inhomogeneities.

To study the behavior of the KLD correlation length in a physically relevant partial differential equation model, we consider the spatially extended reaction-diffusion system of activator-inhibitor type [17]

$$\frac{\partial u(x,t)}{\partial t} = \alpha(j_0 - (u-a)) + D\frac{\partial^2 u}{\partial x^2} \tag{4}$$

$$\frac{\partial a(x,t)}{\partial t} = \frac{u-a}{(u-a)^2+1} - \mathcal{T}a + \frac{\partial^2 a}{\partial x^2}, \tag{5}$$

which models charge transport in layered semiconductor structures with bistable current-voltage characteristics, as observed experimentally, e.g., in *pin* diodes [21], *pnpn*-diodes [22], or heterostructure hot electron diodes [23]. Here $u(x,t)$ is the normalized voltage across the device and $a(x,t)$ is the activator variable representing a normalized interface charge density. The parameter $\mathcal{T}$ controls the size of the bistability regime, α is the ratio of time scales between u and a, D is the squared ratio of the effective length scales of $u(x,t)$ and $a(x,t)$, and j_0 is the driving current that represents an easily accessible control parameter. We restrict ourselves to one spatial dimension x in the layer plane perpendicular to the current flow, and use Neumann boundary conditions

$$\left.\frac{\partial a(x,t)}{\partial x}\right|_{x=0,L} = \left.\frac{\partial u(x,t)}{\partial t}\right|_{x=0,L} = 0, \tag{6}$$

where L is the system size. In our dimensionless units, the current density $j(x,t) = u(x,t) - a(x,t)$ is the physical quantity of interest. Equation (4) describes the dielectric relaxation of the voltage, while Eq. (5) is a nonlinear charge continuity equation.

The bistability gives rise to current filaments where the cross section of the current flow exhibits a region of high-current density embedded within a low-conductivity phase. It has been shown that the system exhibits both a Turing and a Hopf bifurcation, and near the codimension-two Turing-Hopf point a subharmonic mixed mode corresponding to spatiotemporal spiking of the current density with very long chaotic transients [6,24]. The mean transient times increase exponentially with the system size, and may be so long that the asymptotic periodic state is not reached during realistic observation times. A Karhunen-Loève decomposition of the transient spatiotemporally chaotic pattern has shown that the variance σ_k^2 decreases very slowly with increasing mode index k [7].

We consider a system in a range of sizes $L=1000$ to $L=2750$ and parameter values corresponding to transient spatiotemporal chaos. The model is integrated using a second-order midpoint Runge-Kutta integrator with a time step $\Delta t=0.1$ and a second-order spatial discretization with $0.25 \leqslant \Delta x \leqslant 0.5$. We record the spatial field $j(x,t) - \langle j(x,t) \rangle$ at each mesh point in a concentric subsystem of length S at intervals of 5 time units (corresponding to 50 time steps). To eliminate the influence of initial conditions, the first 250 time units are discarded. The resulting KLD dimension D_{KLD} is shown as a function of subsystem size S in Fig. 1. For most cases in the following, the KLD dimension D_{KLD} is computed with a relative total variance corresponding to $f=99.999\%$. This results in keeping roughly 1/5 of the number of eigenmodes of the covariance matrix A^TA. The KLD correlation length $\xi_{\mathrm{KLD}} = (D_{\mathrm{KLD}}/S)^{-1}$ is computed from the linear growth of the KLD dimension D_{KLD} with subsystem size S, and at least five subsystem sizes S are chosen to extract the slope δ_{KLD}. We have checked that it agrees to good accuracy with the slope determined by varying the *total* system size L. When the total system is made larger, the change in D_{KLD} is equivalent to adding more homogeneous center subsystems. The qualitative behavior of ξ_{KLD} remains similar for fractions f between 85% to 99.9999%. For frac-

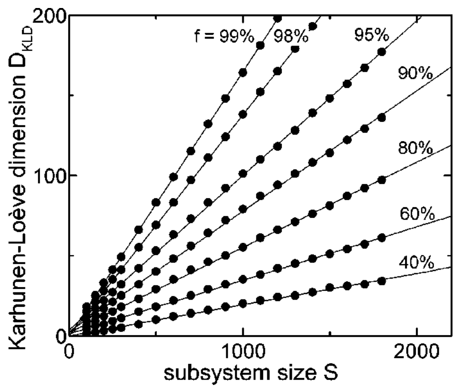

FIG. 1. KLD dimension D_{KLD} versus subsystem size S for different fractions f of the reconstruction ($L=2200$, $\Delta x=0.5$, $T=4000$ time snap shots). Numerical parameters are: $\mathcal{T}=0.05$, $j_0=1.218$, $D=8$, $\alpha=0.02$. All quantities, including length and time, are dimensionless.

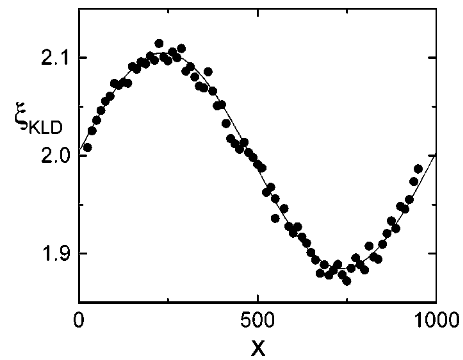

FIG. 3. Local KLD correlation length ξ_{KLD} versus position for a nonuniform modulation of the parameter $\mathcal{T}=0.05+0.0025\cdot\sin(2\pi x/1000)$ over a system size $L=1000$. Subsystems of size $S=15,20,25,30$, and a reconstruction of $f=99.999\%$ are used to compute the KLD correlation length ($\Delta x=0.5$, $T=4000$ time snap shots sampled every 5 time units, parameters as in Fig. 1). The continuous line is a guide to the eye.

tions $f<85\%$ the scaling of D_{KLD} becomes coarse due to the small number of modes required to satisfy smaller fractions of data variance.

First, we study a system of size $L=1000$ to perform a high-resolution ($\Delta x=0.25$) investigation of the dynamical inhomogeneity induced by the boundaries. This is motivated by recent calculations of mean patterns of spatiotemporally chaotic systems exhibiting complicated patterns that persist over a large distance into the interior of the system [11,12]. In our reaction-diffusion model, for the parameter regime considered, the two-point correlation length ξ_2, which is computed from the inverse full width at half maximum of the main peak of the power spectrum $P(k)\sim\exp[-(4\ln 2)\xi_2^2(k-k_0)^2]$ with respect to the wave vector k, is approximately 4.0 and so the system length is approximately equal to $250\xi_2$. We compute various KLD correlation lengths ξ_{KLD} centered at a distance x from the boundary, with $0<x<50\xi_2$. Figure 2 demonstrates that the KLD correlation length ξ_{KLD} oscillates and decays to its bulk value of approximately $\xi_{\mathrm{KLD}}\approx 2$ over the range of x from 0 to $50\xi_2\approx 200$. The oscillations indicate that the system of size $L=1000$ is still relatively far from the limit of homogeneous extensive chaos. These oscillations are fingerprints of interference effects induced by the Neumann system boundaries.

A second problem often encountered in experiment is that system parameters can vary nonuniformly in space or vary over time. To evaluate whether the KLD correlation length can detect small spatial parameter changes in partial differential equations we vary the parameter $\mathcal{T}$ spatially in the $L=1000$ system. Physically this could be achieved, e.g., by modulating the layer thickness of the semiconductor structure and thus the tunneling rate. We wish to test whether in a more strongly coupled spatiotemporally chaotic system the KLD correlation length is able to detect changes in parameters, similar to what was shown for weakly coupled systems of iterated chaotic maps [14]. The parameter $\mathcal{T}$ is modulated periodically according to $\mathcal{T}=0.05+0.0025\sin(2\pi x/1000)$ (this corresponds to a 5% change in a system parameter). Figure 3 shows that the KLD correlation length ξ_{KLD} has a sinusoidal form and is clearly able to predict the parametric dependence of the variation in $\mathcal{T}$. The noise in the data could be reduced by performing additional averages in time. The local nature of KLD allows a determination of dynamical inhomogeneity.

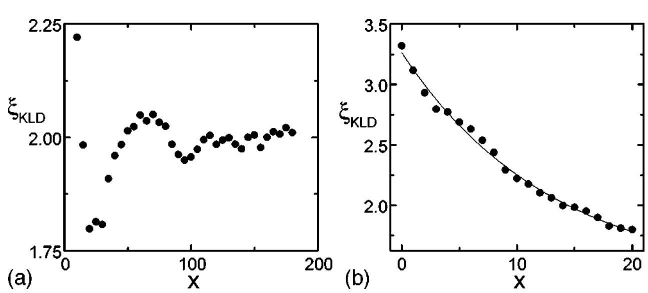

FIG. 2. (a) Local KLD correlation length ξ_{KLD} versus position x measured from the boundary of the system. (b) shows the same data close to the boundary with a higher spatial resolution. Subsystems of size $S=3,4,5,6,7,8$, and a reconstruction of $f=99.999\%$ are used (system size $L=1000$, $\Delta x=0.25$, $T=2000$ time snap shots, parameters as in Fig. 1).

Next, we consider whether the KLD correlation length has a different parametric dependence than the more commonly used two-point correlation length. For the case of a lattice of weakly coupled one-dimensional iterated maps it was shown by Zoldi and Greenside [14] that near a nonequilibrium Ising-like phase transition the KLD correlation length ξ_{KLD} varies in a similar way as the fractal dimension correlation length $\xi_\delta=(D/V)^{-1/d}$, where D is the fractal dimension, but differently than the two-point correlation length. Here, we consider a system of length $L=2750$ and vary $\mathcal{T}$ from 0.048 to 0.052. We have been unable to extend this range of $\mathcal{T}$ because the dynamics qualitatively changes outside this window of $\mathcal{T}$ and becomes non-chaotic. Note that the two-point correlation length ξ_2 is computed over the *entire* system size $L=2750$. Figure 4 demonstrates that within the errors in calculating the KLD correlation lengths ξ_{KLD} and the two-point correlation lengths ξ_2 both are proportional. Therefore, we suggest that in the reaction-diffusion model in this range of $\mathcal{T}$ the two-point and the KLD correlation lengths are related. Given the relationship between the KLD correlation length and the fractal-dimension correlation length [14], we expect that the fractal-dimension correlation

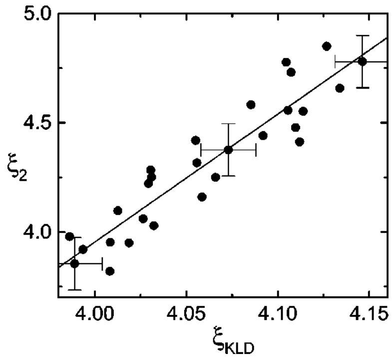

FIG. 4. Plot of the KLD correlation length ξ_{KLD} vs the two-point correlation length ξ_2 corresponding to the range of $\mathcal{T}$ from 0.048 to 0.052. The system size is $L=2750$. To compute the KLD correlation length ξ_{KLD}, $T=4000$ snap shots separated by 5 time units are used in subsystems of size $S=45$, 60, 75, and 90 with a reconstruction of $f=99.999\%$ $(\Delta x=0.5)$. In computing the two-point correlation length, we use the entire system size of $L=2750$ and the power spectra are averaged over 2000 realizations. Error estimates for ξ_{KLD} and ξ_2 are $\Delta\xi_2=0.12$ and $\Delta\xi_{\mathrm{KLD}}=0.015$. The line is a guide to the eye and is of the form $\xi_2=-19.5+5.9\xi_{\mathrm{KLD}}$. Parameters as in Fig. 1.

length is also proportional to the two-point correlation length. This is similar to the proportionality relationship between the dimension correlation length and the two-point correlation length found for the magnitude of the order parameter of the complex Ginzburg Landau equation [20]. However, we cannot exclude that near parameter values where the dynamics changes critically and abruptly, the KLD correlation length may exhibit different behavior. Moreover, since the KLD correlation length is much more readily accessible from small data sets than the other two types of correlation lengths, it appears to be more suitable for quantitative investigations.

In conclusion, we have utilized the KLD correlation length to characterize dynamical inhomogeneities of spatiotemporal chaos in a system of partial differential equations of reaction-diffusion type. We have confirmed that the KLD correlation length is able to detect dynamical inhomogeneities in both space and time due to boundaries or variations in a system parameter. The KLD correlation length ξ_{KLD} can be computed on small localized subsystems allowing quantification of spatial dynamical nonuniformities. Further, the KLD correlation length is based only on spatiotemporal data, and therefore can be easily applied to both experiment and computer simulation. Since spatiotemporal chaotic spiking of the current density $j(x,t)$ has been observed experimentally, e.g., in Si *pnpn* diodes [22], an analysis of such experimental data would provide potentially very interesting insights into inhomogeneities in the physical system.

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