Spatiotemporal Chaos: The Microscopic Perspective

Nicolas B. Garnier
Laboratoire de Physique, CNRS UMR 5672, Ecole Normale Supérieure de Lyon, 46 allée d'Italie, 69364 Lyon Cedex 07, France

Daniel K. Wójcik*
Department of Neurophysiology, Nencki Institute of Experimental Biology, 3 Pasteur Strasse, 02-093 Warsaw, Poland
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Extended nonequilibrium systems can be studied in the framework of field theory or from the dynamical systems perspective. Here we report numerical evidence that the sum of a well-defined number of instantaneous Lyapunov exponents for the complex Ginzburg-Landau equation is given by a simple function of the space average of the square of the macroscopic field. This relationship follows from an explicit formula for the time-dependent values of almost all the exponents.

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The search for connections between theories and quantities at different scales is the essence of statistical physics and condensed matter theory. In the past decade, there has been a lot of interest in relating the dynamical characteristics of the system, e.g., Lyapunov exponents, Kolmogorov-Sinai entropy, and fractal dimensions, with macroscopic properties, such as transport coefficients or entropy production, in both classical and quantum systems [1–6]. An important quantity studied in this context is the phase space contraction rate, which in many cases can be directly connected to the entropy production in a nonequilibrium system [2–4]. The central goals of this new trend are providing a better understanding of irreversibility of microscopically reversible systems and obtaining a general theory of systems far from equilibrium. So far, all deterministic systems studied within this perspective have been finite-dimensional. A natural question arises as to whether similar results can be obtained for spatially extended systems. For instance, one would like to know the statistical properties of the fluctuations of the phase space contraction rate and of the entropy production in driven fluid systems [7,8].

Also, in studies of turbulence and spatiotemporal chaos, there is interest in connecting dynamical characteristics of the system with the statistics of macroscopic quantities such as correlation lengths; however, the emphasis here is put mostly on quantifying the complexity of the dynamics. Such connections, if found, have not only a theoretical value but also important practical consequences, because it is much easier to study macroscopic quantities than to obtain dynamical characteristics, especially in experiments [9,10].

These considerations prompted us to consider the complex Ginzburg-Landau equation (CGL) and study the fluctuation properties of its phase space contraction. The CGL is a paradigmatic model of spatiotemporal chaos which in a sense is intermediate between thermostated molecular dynamics models and realistic fluid systems. Because of its strong dissipative properties, infinite-dimensional CGL has a finite-dimensional attractor which can be appropriately described in terms of low spatial frequency Fourier modes [11].

In this Letter, we show that, even though the phase space contraction rate in the CGL is infinite, one can consider the contraction rate of volumes restricted to the inertial manifold, which is finite-dimensional. This rate is equal to the sum of a finite number of instantaneous Lyapunov exponents. It turns out to be proportional to the macroscopic mass of the field. Thus, we have found a direct relation between the "microscopic" sum of a finite number of instantaneous Lyapunov exponents and the "macroscopic" mass of the field. We explore the structure of the spectrum of Lyapunov exponents and instantaneous Lyapunov exponents and show an approximate formula for a large part of the spectrum of instantaneous Lyapunov exponents. The statistical properties of the fluctuations of phase space contraction rates and its relations to other macroscopic entropylike quantities will be reported in a follow-up article [12].

We consider a one-dimensional cubic complex Ginzburg-Landau equation on an interval of length L with periodic boundary conditions

$$A_t = \varepsilon A + (1 + ic_1)\Delta A - (1 + ic_2)|A|^2 A, \qquad (1)$$

where ε, c_1, c_2 are real and we set $\varepsilon = 1$. For convenience, let us restrict to a finite-dimensional truncation in a Fourier base with $N = 2K$ modes and write

$$A(x, t) = \sum_{n=-K}^{K} A_n(t) e^{i2\pi n x/L}.$$

From Eq. (1), we obtain

$$\dot{A}_n = \varepsilon A_n - \left(\frac{2\pi n}{L}\right)^2 (1 + ic_1) A_n - (1 + ic_2) \sum_{k+l-m=n} A_k A_l A_m^*. \qquad (2)$$

Note that $A_K = A_{-K}$ due to periodicity. Writing $A_n = B_n + iC_n$, where B_n and C_n are real, we derive a formula for the phase space contraction rate $\sigma = \mathrm{div}_A \dot{A} = \sum_n (\partial \dot{B}_n / \partial B_n) + (\partial \dot{C}_n / \partial C_n)$ as well as the normalized phase space contraction rate $\tilde{\sigma} := \sigma / N_{\mathrm{modes}}$. Here $N_{\mathrm{modes}} = 2N = 4K$ is the number of real modes under examination:

$$\tilde{\sigma} = \frac{\sigma}{2N} = \varepsilon - 2\langle \varrho \rangle - \left(\frac{2\pi}{L}\right)^2 \frac{N^2 + 1}{12}, \tag{3}$$

where $\langle \varrho \rangle = (1/L) \int_0^L dx |A|^2 = \sum_k |A_k|^2$. Using $a = L/N$, we get

$$\tilde{\sigma} = \varepsilon - 2\langle \varrho \rangle - \frac{\pi^2}{3a^2}\left(1 + \frac{1}{N^2}\right) \approx \varepsilon - 2\langle \varrho \rangle - \frac{\pi^2}{3a^2}.$$

The beauty of this result connecting the average macroscopic field $\langle \varrho \rangle$ to the microscopic normalized phase space contraction rate $\tilde{\sigma}$ is jeopardized by the last term, which diverges when the spatial resolution N is increased. However, increasing the resolution only adds high frequency modes which are strongly damped. We show below that their contribution can be isolated and removed, as in the case of zero-temperature entropy in spin systems.

We conjecture that there is a distinguished dimension such that the contraction rate of volumes restricted to this dimension is always finite and connected to the space averaged ϱ in a simple manner. These volumes are defined by the sum of an appropriate number of instantaneous Lyapunov exponents. Before supporting these claims, let us recall the definitions of Lyapunov exponents and instantaneous Lyapunov exponents and show how they connect to the volume contraction rates.

Consider a continuous time dynamical system defined by a set of differential equations $\dot{x} = F(x)$, $x \in \mathbb{R}^n$. The solution of the system is given by the flow $x_t = \Phi^t(x_0)$, $t \in \mathbb{R}$. Then the growth of an infinitesimal perturbation δx_0 around x_0 is governed by the linearization of the flow $\delta x_t = D_{x_0} \Phi^t \delta x_0 = M(t, x_0) \delta x_0$. The *fundamental matrix* $M(t, x_0)$ governing this growth is the solution of the equation $\dot{M}(t, x_0) = J(t, x_0) M(t, x_0)$, where $J(t, x_0) = \frac{\partial F}{\partial x}(x_t)$ is the Jacobi matrix of partial derivatives of the field velocity. The *Oseledec matrix* $(M(x_0, t)^\dagger M(x_0, t))^{1/2t}$ has n positive eigenvalues $\Lambda_i(x_0, t)$, which we order by size $\Lambda_1 \geq \Lambda_2 \geq \ldots \geq \Lambda_n$. *Lyapunov exponents* $\lambda_i(x_0)$ are defined as logarithms of eigenvalues of a long time limit of the Oseledec matrix $\lambda_i(x_0) := \lim_{t \to \infty} \ln \Lambda(x_0, t)$. For an ergodic system, they are the same for almost every initial point [13,14].

To define *instantaneous Lyapunov exponents* [15] μ_i, consider volume $V_k(t)$ of a parallelogram $u_1(x_0, t) \wedge u_2(x_0, t) \wedge \ldots \wedge u_k(x_0, t)$, spanned initially by k orthogonal vectors $\tilde{u}_i$ attached at x_0, traveling along the trajectory $u_i \in \mathbb{R}^n$. Its evolution is given by the fundamental matrix, i.e., $u_i(x_0, t) = M(x_0, t) \tilde{u}_i$. Then the $k \times n$ matrix $U = [u_1, \ldots, u_k]$ can be uniquely decomposed into a product of a $k \times n$ orthogonal matrix Q and an upper-diagonal $k \times k$ matrix R (*QR decomposition*)

$$U = QR = [Q_1, \ldots, Q_k] \begin{bmatrix} R_{11} & R_{12} & \ldots & R_{k1} \\ 0 & R_{22} & \ddots & \vdots \\ \vdots & \ddots & \ddots & R_{kk-1} \\ 0 & \ldots & 0 & R_{kk} \end{bmatrix}.$$

The product of the diagonal elements of R gives the volume spanned by u_i. Its contraction rate is

$$\sigma_k(t) := \lim_{dt \to 0} \frac{1}{dt} \ln \frac{V_k(t + dt)}{V_k(t)} = \frac{\dot{V}_k(t)}{V_k(t)}.$$

We define instantaneous Lyapunov exponents by $\mu_k(t) := \sigma_k(t) - \sigma_{k-1}(t)$. They depend on the initial point and on the initial vectors $\tilde{u}_i$. However, for almost all initial vectors, the first vector with time aligns along the most unstable direction, the first two vectors span the fastest stretching $2d$ volumes, and so on. After some time, the vectors become almost independent of the initial directions modulo degeneracy, and, consequently, the instantaneous Lyapunov exponents characterize the trajectory.

In practice, we propagate the vectors by finite time steps at each time reorthogonalizing the set. Thus, starting from $Q_0 \equiv U$ we move to $U_1 = M(dt) Q_0 \equiv Q_1 R_1$. Then $U_{n+1} = M(dt, x(ndt, x_0)) Q_n \equiv Q_{n+1} \tilde{R}_{n+1}$. Thus, we have $R(ndt) = \tilde{R}_n \ldots \tilde{R}_1$ and $\mu_k(ndt) \approx \frac{1}{dt} \ln [\tilde{R}_n]_{kk}$. Time averages of μ_i are sorted in decreasing order and equal to the usual Lyapunov exponents λ_i [13,14].

To estimate the values of the instantaneous Lyapunov exponents, consider an initial perturbation δA_n tangent to a single mode A_n^0

$$\partial \delta A_n / \partial t = (\varepsilon - (1 + ic_1) q^2 - 2(1 + ic_2)\langle \varrho \rangle) \delta A_n + (1 + ic_2)(\alpha_n + i\beta_n) A_n^* + f(\delta A))\}, \tag{4}$$

where $q := 2\pi n / L$, $f(\delta A)$ is a linear function of $\{\delta A\}$ independent of δA_n or δA_n^*, and $\alpha_n, \beta_n \in \mathbb{R}$ stand for the real and imaginary parts of the time-dependent sum $\alpha_n + i\beta_n = \sum_{j=-(K-|n|)}^{K-|n|} A_{n-j} A_{n+j}$. Rewriting Eq. (4) in terms of real and imaginary parts of $\delta A_n = \delta B_n + i\delta C_n$, we obtain a short time evolution of tangent vectors

$$\begin{bmatrix} \delta B_n(dt) \\ \delta C_n(dt) \end{bmatrix} = [a_0 I + a_i \sigma_i] \begin{bmatrix} \delta B_n(0) \\ \delta C_n(0) \end{bmatrix},$$

where σ_i are the Pauli matrices [16] and $a_0 = 1 + (\varepsilon - q^2 - 2\langle \varrho \rangle) dt$, $a_x = \beta_n + c_2 \alpha_n$, $a_y = i(c_1 q^2 + 2c_2 \langle \varrho \rangle)$, $a_z = \alpha_n - c_2 \beta_n$. Then the eigenvalues of $M^\dagger M(dt)$ are $\Lambda_\pm = 1 + 2(\varepsilon - q^2 - 2\langle \varrho \rangle) \pm \sqrt{1 + c_2^2} \times |\sum_{j=-(K-|n|)}^{K-|n|} A_{n-j} A_{n+j}|$, which gives extreme possible values of instantaneous Lyapunov exponents

$$\mu_{n\pm} = \varepsilon - q^2 - 2\langle \varrho \rangle \pm \sqrt{1 + c_2^2} \left| \sum_{j=-(K-|n|)}^{K-|n|} A_{n-j} A_{n+j} \right|.$$

Numerically observed values depend on an initial vector $[\delta B_n \delta C_n]^T$ and are between $\mu_{n\pm}$. To find out what the contraction rate of the $2d$ volumes in δA_n plane is, we can consider the action of $M(dt)$ restricted to δA_n on a pair of initially orthogonal vectors $[v_1, v_2]$ in this plane. The volume of $M(dt)[v_1, v_2]$ is given by the determinant, and, since $\det[v_1, v_2] = 1$, we have

$$\frac{1}{2}(\mu_{n1} + \mu_{n2}) = \lim_{dt\to 0} \frac{1}{dt} \ln \det M(dt) = \varepsilon - q^2 - 2\langle \varrho \rangle. \tag{5}$$

Therefore, at any time we predict that the sum of the two instantaneous Lyapunov exponents for perturbations in the plane tangent to any Fourier mode should be given by the formula above.

It is not *a priori* obvious that this prediction should hold for *any* exponents calculated for volumes evolved over a long time span, since we have considered the evolution along (A_n, A_n^*) only. With time, all the modes get mixed via the nonlinear term in (1), and evolved vectors can align arbitrarily in phase space. However, our numerical simulations show that only a finite number of modes W, which we call "active," disobey the above prediction (Fig. 1). The remaining exponents oscillate around (5), and at every instant the sum of the four modes for $\pm n$ is given by (5). To find this division, we label each exponent $\mu_k(t)$ with integer k so that their time averages λ_k are ordered: $\lambda_1 \geq \lambda_2 \geq \ldots$ (see Fig. 2). Then for some number W of the form $4n + 2$, the Lyapunov exponents λ_k for $k > W$ come in quadruplets given by the time average of (5) $\lambda_k = \varepsilon - q^2 - 2\langle \bar{\varrho} \rangle$, and for $k \leq W$ λ_k are different from this prediction.

In all the cases we have checked, independently of the chaoticity of the solution, we observe that W is the smallest number of the form $4n + 2$ greater or equal to L, i.e., $W = 2 + 4\lceil (L-2)/4 \rceil$. This size dependence suggests that W measures some extensive geometric structure in the phase space. We are aware of only two such structures for the CGL: the inertial manifold and the attractor. But W is *larger* than the Kaplan-Yorke dimension of the attractor. This is why we believe that our procedure probes the fluctuations of volumes on the inertial manifold, not on the attractor, which is its subset.

These conjectures were verified in several regimes of the CGL (Benjamin-Feir line, phase chaos, defect chaos, and intermediate regime), for different lengths of the system and truncations to 32, 64, 128, and 256 Fourier modes or equivalent numbers of spatial points. We used pseudospectral code and an implicit Gauss-Seidel Cranck-Nicholson scheme to integrate the CGL. Fundamental matrix M was calculated in both real and Fourier space representations. For all four combinations, the obtained time-dependent spectra were almost exactly the same in the interesting part; noticeable differences were visible in part of the spectrum corresponding to high frequency modes.

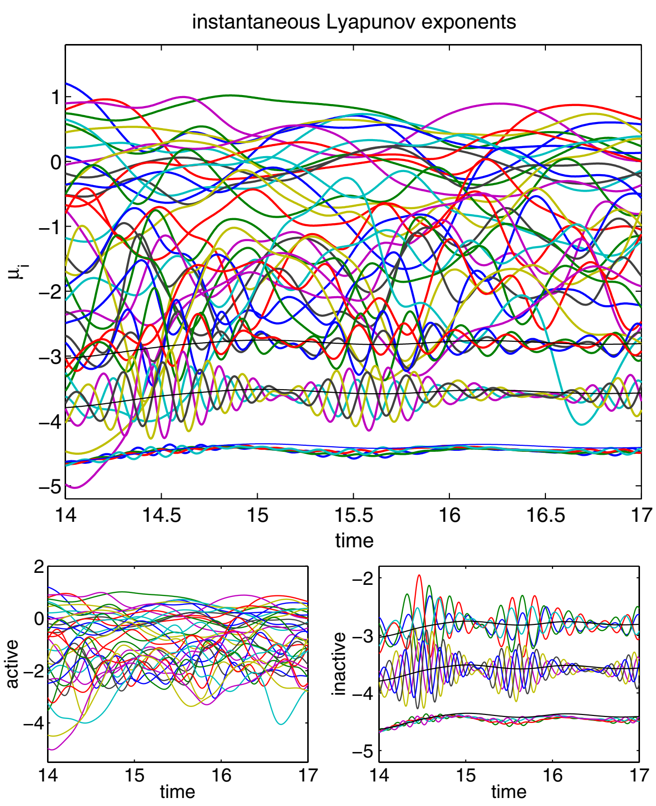

FIG. 1 (color online). Time dependence of all 34 "active" and the largest 12 inactive instantaneous Lyapunov exponents for the CGL with $L = 10\pi$, $c_1 = 4$, $c_2 = -4$. The bottom figures show two subsets of curves from the upper plot, the first 34 (left) and the next 12 exponents (right). Prediction (5) is also plotted.

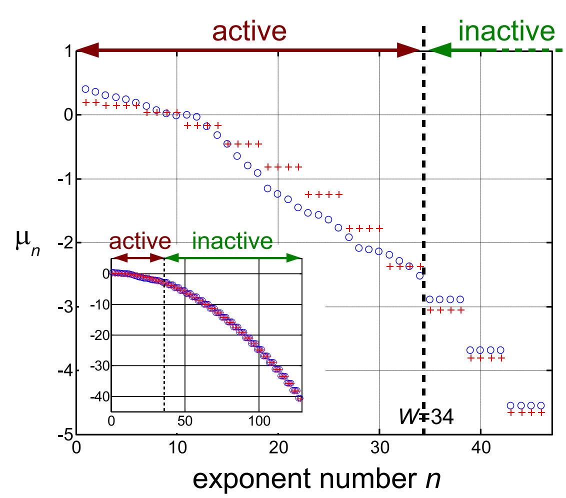

FIG. 2 (color online). Spectrum of Lyapunov exponents for the CGL with $L = 10\pi$, $c_1 = 4$, $c_2 = -4$. There are $N = 64$ modes and, thus, 128 exponents (all shown in the inset). The quadruplet structure of the lower exponents comes from the real and complex parts of corresponding positive and negative Fourier modes. Crosses are time averages of (5); circles are numerical values. There are $W = 34$ active exponents.

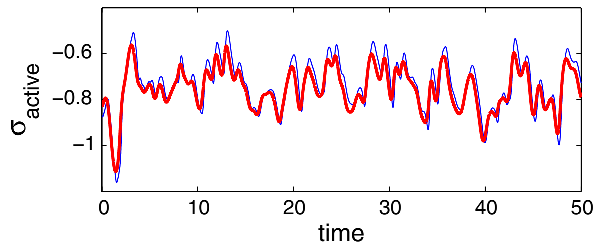

FIG. 3 (color online). Numerical test of Eq. (6). The time evolution of the sum of the active exponents (thick red line) is compared with the time evolution of $\varepsilon - 2\langle\varrho\rangle - [\pi^2(W^2 - 4)/12L^2]$ (thin blue line). The thin blue line has been shifted by -0.15.

Figure 1 shows the time dependence of the first 46 instantaneous Lyapunov exponents computed along a trajectory for a representative case of the CGL with $L = 10\pi$, $c_1 = 4$, $c_2 = -4$ [17] for a computation with 128 Fourier modes; both groups of exponents are clearly visible. There is a constant difference between theoretical prediction and the numerical value of the order of 0.15 for the first inactive exponents ($n = 9$ in this case), dropping to around 0.01 for exponents corresponding to $n = 25$.

Time averages of instantaneous Lyapunov exponents converge to the usual Lyapunov spectrum. They are shown in Fig. 2 for the same parameter values.

Theoretical predictions (5) are marked with crosses; circles mark numerical values. The staircase structure in the spectrum is well approximated by Eq. (5). To separate the changes of volumes on the inertial manifold from the trivial contraction in the orthogonal directions, we consider a contraction of W-dimensional volumes given by the sum of all the nontrivial instantaneous Lyapunov exponents. Since the sum of all the instantaneous Lyapunov exponents in the Galerkin representation is equal to the phase space contraction rate (3), and since the "inactive" exponents oscillate around the average field (5), the relevant value is

$$\tilde{\sigma}_{\text{active}} := \frac{1}{W}\sum_{i=1}^{W}\mu_i = \varepsilon - 2\langle\varrho\rangle - \frac{\pi^2(W^2-4)}{12L^2}. \quad (6)$$

Since $W \approx L$ and $\varepsilon = 1$, for large L the first and last terms are of order 1, which leads to $\tilde{\sigma}_{\text{active}} \approx -2\langle\varrho\rangle$. Figure 3 compares the evolution of $0.15 + \frac{1}{W}\sum_{i=1}^{W}\mu_i$ with $\varepsilon - 2\langle\varrho\rangle - [\pi^2(W^2 - 4)/12L^2]$.

To summarize, we have identified a natural division of the spectrum of instantaneous Lyapunov exponents in the complex Ginzburg-Landau equation into a nontrivial part corresponding to the dynamics on the inertial manifold and a part corresponding to the modes decaying towards it. The trivial exponents are approximately given by simple functions of the square of the field (5). With this result, we showed that the contraction rates of volumes restricted to inertial manifold, which is the sum of the nontrivial exponents, are given by a simple function of the spatial average of the squared modulus ϱ of the solution (6). This formula bridges the gap between the dynamical systems picture of the CGL (volumes contracting in the phase space and instantaneous Lyapunov exponents) and the macroscopic picture (spatiotemporal solution). The presented results are of relevance for physical systems described by the CGL [18]. We believe that such a division of the spectrum of instantaneous Lyapunov exponents is a generic phenomenon for a large class of systems described by nonlinear partial differential equations with inertial manifolds [8]. However, the connection between the phase space contraction rate and the field must be model-dependent. These issues are currently under study [12].

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*Electronic address: d.wojcik@nencki.gov.pl

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