

# Karhunen-Loève Decomposition of Extensive Chaos

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(October 1, 1996)

## Abstract

We show that the number of KLD (Karhunen-Loève decomposition) modes  $D_{\text{KLD}}(f)$  needed to capture a fraction  $f$  of the total variance of an extensively chaotic state scales extensively with subsystem volume  $V$ . This allows a correlation length  $\xi_{\text{KLD}}(f)$  to be defined that is easily calculated from spatially localized data. We show that  $\xi_{\text{KLD}}(f)$  has a parametric dependence similar to that of the dimension correlation length and demonstrate that this length can be used to characterize high-dimensional inhomogeneous spatiotemporal chaos.

47.27.Cn, 05.45.+b, 05.70.Ln, 82.40.Bj

arXiv:chao-dyn/9610007v1 2 Oct 1996

Spatiotemporal states that are nonperiodic both in space and time abound in nature and are often important technologically, e.g, for lasers, fibrillating hearts, and convective transport of heat [1]. Experiments and simulations of these dynamics raise questions that are presently poorly understood: Are there different kinds of spatiotemporal nonperiodic states? What kinds of bifurcations lead to such states? How do inhomogeneities and boundary conditions affect the dynamics? And how does the transport of energy and matter depend on the details of the spatiotemporal disorder? An essential first step towards answering these questions is to develop methods to quantify spatiotemporal dynamic states, so that one state can be distinguished from another and so that theory can be compared with experiment and with simulation. Data analysis and theoretical progress are presently limited by a scarcity of concepts and of computational tools for analyzing spatiotemporal disorder.

In the absence of a fundamental theory of sustained nonequilibrium systems that could indicate appropriate quantities to measure, researchers have used primarily two approaches for quantifying spatiotemporal disorder: two-point correlation functions and dynamical invariants such as Lyapunov exponents and fractal dimensions [2]. Temporal correlation functions have been effective for distinguishing periodic and quasiperiodic dynamical states from each other and from chaotic ones [3] while spatial correlation functions have played an important role in discovering and demonstrating the absence of long range spatial order [4]. Both correlation functions have been less useful for distinguishing one chaotic state from another or for comparing experimental with computational chaotic data. Dynamical invariants have been somewhat useful for ordering the chaotic states of low-dimensional dynamical systems but severe difficulties remain in calculating these quantities for higher-dimensional systems because of the demanding computational effort, the slow and often ambiguous convergence of time-series-based algorithms, and the need for large amounts of noise-free data [5].

In this Letter, we propose and analyze a new measure of spatiotemporal disorder, a correlation length  $\xi_{\text{KLD}}$  defined below, that seems promising especially for the analysis of large, high-dimensional, nontransient, driven-dissipative systems. This quantity has some of the flavor of correlation functions and also of dynamical invariants and is straightforward to

compute with moderate amounts of spatiotemporal data (unlike global dynamical invariants like the fractal dimension) since, as we show below, it is a *local* quantity that can be calculated from spatiotemporal data associated with a finite region of space. This last feature suggests that  $\xi_{\text{KLD}}$  will be useful for studying spatially inhomogeneous dynamics arising from slowly changing external parameters, from broken symmetries [6], or from the influence of boundaries [7]. As is the case for many measures of spatiotemporal chaos, the length  $\xi_{\text{KLD}}$  can not be evaluated analytically and so we investigate its properties numerically for two idealized mathematical models—the one-dimensional Kuramoto-Sivashinsky (KS) equation [1, 8] and the two-dimensional Miller-Huse model [9]—whose spatiotemporal chaotic solutions have been thoroughly studied and for which inhomogeneities can be introduced in a controlled manner. In later work, applications to experimental data will be reported.

Our motivation for defining and studying the correlation length  $\xi_{\text{KLD}}$  comes from three different ideas. First is the idea of extensive chaos, that a sufficiently big *homogeneous* spatiotemporal chaotic system has the property that its fractal dimension  $D$  is extensive, growing in proportion to the system volume  $V$  [1, 10–12]. This extensive scaling suggests that bounded *intensive* quantities, such as a dimension density  $\delta = \lim_{V \rightarrow \infty} D/V$  or the equivalent dimension correlation length  $\xi_\delta = \delta^{-1/d}$  [1, 12, 13] (where  $d$  is the number of asymptotically large spatial dimensions, e.g.,  $d = 2$  for a large-aspect-ratio convection experiment) are more appropriate for characterizing large nonequilibrium systems. It was shown recently that the length  $\xi_\delta$  varies independently of the two-point and mutual-information correlation lengths so that the average spatial disorder does not determine the fractal dimension  $D$  [13]. This suggests that certain measures of spatiotemporal dynamics should be sensitive to structure in phase space, not just to instantaneous [14] or time-averaged measures of spatial disorder in configuration space. The quantity  $\xi_{\text{KLD}}$  turns out to have this property.

The second idea is to extend the concept of local thermodynamic equilibrium [15, page 13] to slowly-varying inhomogeneous driven dissipative systems, with the implication that intensive dynamical quantities can be defined locally and will be slowly varying in space. As an illustration, assume that a large sustained nonequilibrium systems has a parameter  $p(x)$

that varies slowly with position  $x$  and consider a subsystem of size  $L$  centered at position  $x_0$ . Then over a certain time scale that decreases with decreasing subsystem size  $L$  (not necessarily diffusively), this subsystem will be approximately nontransient, even if the system containing the subsystem is not. Further, the values of intensive parameters associated with this approximately nontransient subsystem should correspond closely in value to those of an infinite homogeneous nontransient system with the parameter value  $p(x_0)$ . Unfortunately, there are no reliable algorithms that can estimate intensive quantities such as the dimension density  $\delta$  from information localized to some region of space (it is not even known whether such algorithms exist in principle). To date, calculations of intensive quantities such as the Lyapunov dimension density  $\delta$  have relied on the expensive calculation of global extensive quantities followed by taking the limit of some intensive ratio [13]. This is impractical for the analysis of experimental data or for the evaluation of local measures. As we show below, the measure  $\xi_{\text{KLD}}$  is able to indicate some of the behavior of the fractal dimension density using just local information.

The third idea is to make use of the Karhunen-Loève decomposition (KLD), which has been used by researchers over many years and in many disciplines to analyze spatiotemporal data [16], although not in the context of extensive chaos or of inhomogeneous systems. The KLD is a statistical method for compressing spatiotemporal data by finding the largest linear subspace that contains substantial statistical variations of the data. To illustrate the idea in the discrete case and also to introduce some notation, we consider a one-dimensional zero-mean field  $u(t, x)$  on a spatial interval  $[0, L]$  whose values are measured on a finite space-time mesh of  $T$  uniformly sampled time points  $t_i = i\Delta t$  and of  $S$  uniformly sampled spatial points  $x_j = j\Delta x$ . Then a  $T \times S$  rectangular data matrix  $A_{ij} = u(t_i, x_j)$  can be defined from which a  $S \times S$  symmetric positive semidefinite scatter matrix  $\mathbf{M} = \mathbf{A}^T \mathbf{A}$  can be calculated, where  $\mathbf{A}^T$  denotes the matrix transpose of  $\mathbf{A}$ . Using standard eigenvalue methods with complexity  $O(S^3)$  [17], the scatter matrix can be diagonalized to obtain its nonnegative eigenvalues  $\sigma_i^2$  which can be further ordered in decreasing size  $\sigma_1^2 \geq \sigma_2^2 \cdots \geq \sigma_S^2 \geq 0$ .

Since the ordered eigenvalues  $\sigma_i^2$  often decrease rapidly in magnitude with increasing

index  $i$ , researchers [18] have introduced a positive integer  $D_{\text{KLD}}(f)$ :

$$D_{\text{KLD}}(f) = \max \left\{ p : \sum_{i=1}^p \sigma_i^2 / \sum_{i=1}^S \sigma_i^2 \leq f \right\}, \quad (1)$$

which represents the number of KLD modes needed to capture some specified fraction  $f \leq 1$  of the total variance  $\sum_{i=1}^S \sigma_i^2$  of the data. Researchers have suggested using  $D_{\text{KLD}}(f)$  like a fractal dimension  $D$  to measure the complexity of spatiotemporal data [18] although care is needed when interpreting  $D_{\text{KLD}}(f)$ . The  $T$   $S$ -dimensional vectors defined by the rows of the data matrix  $\mathbf{A}$  constitute an embedding of the dynamics into a  $S$ -dimensional phase space. The quantity  $D_{\text{KLD}}(f)$  indicates the dimension of a linear subspace that includes most of the statistical variation of this embedding and is generally quite different from the attractor's fractal dimension  $D$ , e.g., a limit cycle with fractal dimension  $D = 1$  in a  $N$ -dimensional phase space could have a value of  $D_{\text{KLD}}(f)$  between 1 and  $N$  depending on how the limit cycle is folded in different orthogonal directions.

Although  $D_{\text{KLD}}(f)$  need have no particular relation to the data's fractal dimension  $D$ , we argue below that for *extensive* chaos, the rate of increase of  $D_{\text{KLD}}(f)$  with volume  $V$  will generally be similar to the rate of increase of fractal dimension  $D$  with  $V$  since the extensivity of the dimension arises from the appearance of new orthogonal directions, i.e., with increasing  $V$ , a larger linear space is needed to contain the increasing variance of the attractor. If true, we can then use the more readily calculated quantity  $D_{\text{KLD}}(f)$  to estimate intensive correlation lengths like the length  $\xi_\delta$  discussed above, and to study the dependence of such lengths on system parameters.

We now present some results that justify and illustrate these observations. When evaluated for spatiotemporal data of a large, approximately homogeneous, sustained nonequilibrium system of volume  $V$ , the KLD dimension  $D_{\text{KLD}}(f)$  of Eq. (1) grows extensively with  $V$  as shown in Fig. 1. Here we have used  $T \times S$  data matrices  $\mathbf{A}$  (with  $10^4 \leq T \leq 2 \times 10^4$  and  $100 \leq S \leq 800$ ) derived from the spatiotemporal field  $u(t, x)$  of the one-dimensional Kuramoto-Sivashinsky equation

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

with rigid boundary conditions  $u = \partial_x u = 0$  at  $x = 0$  and at  $x = L$ . Eq. (2) was integrated numerically with a semi-implicit finite-difference method that was first- and second-order accurate in time and space respectively. For  $L > 50$ , most initial conditions yield spatiotemporal chaotic states that were previously shown to be extensively chaotic [11]. Fig 1(a) shows that  $D_{\text{KLD}}(f)$  is extensive for  $L \geq 50$ , growing in proportion to the system volume  $L$  with a slope that depends on the fraction  $f$ . The dashed line indicates the extensive scaling of the Lyapunov dimension  $D$  [11] which corresponds to a fraction  $f = 0.81$ . Fig 1(b) shows further that  $D_{\text{KLD}}(f)$  is extensive for open subsystems centered on the middle of a system of size  $L = 400$ . The slope of a line in Fig 1(b) for a given fraction  $f$  is the *same* as the slope of the line of corresponding  $f$  in Fig 1(a). This implies the important point that the intensive density  $\lim_{V \rightarrow \infty} D_{\text{KLD}}(f)/V$  can be estimated from information localized to a certain region of space.

The extensivity of the KLD dimension, for both the entire system and for subsystems, suggests introducing an intensive KLD correlation length  $\xi_{\text{KLD}}(f)$ :

$$\xi_{\text{KLD}}(f) = \left( \lim_{V \rightarrow \infty} \frac{D_{\text{KLD}}(f)}{V} \right)^{-1/d}, \quad (3)$$

by analogy to the dimension correlation length  $\xi_\delta$  (where again  $d$  is the spatial dimensionality of the system). Based on the data in Fig. 1 for the KS equation, Fig. 2 shows how the length  $\xi_{\text{KLD}}(f)$  varies with the fraction  $f$ . The dependence is nonlinear, with the magnitude of  $\xi_{\text{KLD}}(f)$  changing by a factor of ten over the range  $0.3 \leq f \leq 1$ . Contrary to an earlier claim by Ciliberto and Nicolaenko [18], Fig. 2 shows that the fractal dimension of a high-dimensional system can not generally be estimated from a knowledge of  $\xi_{\text{KLD}}(f)$  since the fraction  $f$  corresponding to the dimension correlation length will not be known in advance and because  $\xi_{\text{KLD}}(f)$  can vary substantially with  $f$ . However, the onset of extensivity for  $D_{\text{KLD}}(f)$  does accurately predict the onset of extensivity for the Lyapunov dimension  $D$  with increasing volume  $V$ .

Fig. 3 shows how the length  $\xi_{\text{KLD}}(f)$  (for  $f = 0.95$ ) compares with the dimension correlation length  $\xi_\delta$  (derived from the extensive Lyapunov fractal dimension [13]) for a nonequi-

librium Ising-like phase-transition of a mathematical model invented by Miller and Huse [9]. The Miller-Huse (MH) model is a 2d coupled-map-lattice for which a 1d chaotic map of odd symmetry is placed at each node of a periodic  $L \times L$  square lattice. Each site is coupled diffusively to nearest neighbors with a strength  $g$  that acts as the bifurcation parameter for this system. Miller and Huse found that a quantity analogous to a lattice magnetization  $M$  bifurcated from a zero to non-zero value at a critical value  $g_c = 0.205$  at which point also a two-point correlation length  $\xi_2$  diverged to infinity. O'Hern et al [13] showed that the dimension correlation length  $\xi_\delta$  did not diverge near  $g_c$  but instead was a quantity of order one that smoothly reached a local maximum at a value  $g = 0.200$  distinctly less than the critical value  $g_c$ . Fig. 3 shows that the length  $\xi_{\text{KLD}}$  is somewhat larger than  $\xi_\delta$  and has a qualitatively similar dependence on  $g$  in that it increases to a local maximum at the *same*  $g$ -value. Unlike the dimension correlation length,  $\xi_{\text{KLD}}$  does not seem to vary smoothly near its maximum but we lack sufficient numerical resolution to determine unambiguously whether there is a finite jump in value, in analogy to the dependence of specific heat on temperature for a second-order equilibrium phase transition. The functional dependence of  $\xi_{\text{KLD}}(f)$  on parameter  $g$  depends only weakly on the fraction  $f$  which therefore is not an important parameter.

Finally, in Fig. 4 we demonstrate how the KLD correlation length  $\xi_{\text{KLD}}$  can be used to characterize inhomogeneous spatiotemporal chaos, a result that opens up interesting possibilities for the future analysis of experimental data. For this figure, we introduced a spatial inhomogeneity into a  $300 \times 30$  periodic MH lattice by allowing the coupling constant  $g = g(x)$  to vary periodically in the  $x$  lattice direction as shown in Fig. 4(b). At each of several  $x$ -coordinates  $i$ , we calculated the KLD dimension Eq. (1) for subsystems centered on  $i$  and of increasing width  $L$  with  $9 \leq L \leq 15$ . From these data, local extensive scaling was identified from which a length  $\xi_{\text{KLD}}(i)$  was calculated from Eq. (3). In Fig. 4(a), the lengths  $\xi_{\text{KLD}}(i)$  are given by the solid circles which can be compared with the dashed-curve representing the corresponding value of  $\xi_{\text{KLD}}$  that would be obtained from Fig. 3 for an infinite homogeneous system with constant value  $g = g(i)$ . The agreement is good to about 4% throughout, which

is sufficient to determine the spatial dependence of the inhomogeneity.

In conclusion, the correlation length Eq. (3) obtained by studying the extensive scaling of the Karhunen-Loève decomposition with increasing subsystem volume provides an easily calculated and novel way to characterize the spatiotemporal disorder of an extensively chaotic system, including the case of slowly varying spatial inhomogeneities. We believe that the ideas on which our analysis is based—namely extensivity, local stationarity, and the Karhunen-Loève decomposition—will be important ingredients in the future analysis of large nonequilibrium systems.

This work was supported by a DOE Computational Science Fellowship, by NSF grants NSF-DMS-93-07893 and NSF-CDA-92123483-04, and by DOE grant DOE-DE-FG05-94ER25214.



## REFERENCES

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- [1] M. C. Cross and P. C. Hohenberg, *Rev. Mod. Phys.* **65**, 851 (1993).
- [2] E. Ott, *Chaos in Dynamical Systems* (Cambridge U. Press, New York, 1993).
- [3] G. Ahlers and R. P. Behringer, *Prog. Theor. Phys. Suppl.* **64**, 186 (1978).
- [4] J. P. Gollub and R. Ramshankar, in *New Perspectives in Turbulence*, edited by S. Orszag and L. Sirovich (Springer-Verlag, Berlin, 1990), pp. 165–194; M. C. Cross, D. Meiron, and Y. Tu, *Chaos* **4**, 607 (1994).
- [5] H. D. Abarbanel, R. Brown, and L. S. Tsimring, *Rev. Mod. Phys.* **65**, 1331 (1993).
- [6] S. Sasa, *Chaos* **6**, 238 (1996).
- [7] B. J. Gluckman, C. B. Arnold, and J. P. Gollub, *Phys. Rev. E* **51**, 1128 (1995).
- [8] P. Manneville, in *Propagation in Systems Far From Equilibrium*, Vol. 41 of *Springer Series in Synergetics*, edited by J. E. W. et al (Springer-Verlag, New York, 1988), pp. 265–280.
- [9] J. Miller and D. A. Huse, *Phys. Rev. E* **48**, 2528 (1993).
- [10] D. Ruelle, *Commun. Math. Phys.* **87**, 287 (1982).
- [11] P. Manneville, in *Macroscopic modeling of turbulent flows*, Vol. 230 of *Lecture Notes in Physics*, edited by O. Pironneau (Springer-Verlag, New York, 1985), pp. 319–326.
- [12] D. A. Egolf and H. S. Greenside, *Phys. Rev. Lett.* **74**, 1751 (1995).
- [13] C. O’Hern, D. Egolf, and H. Greenside, *Phys. Rev. E* **53**, 3374 (1996).
- [14] G. H. Gunaratne, R. E. Jones, Q. Ouyang, and H. L. Swinney, *Phys. Rev. Lett.* **75**,

3281 (1995).

- [15] L. Landau and E. Lifshitz, *Statistical Physics*, Third ed. (Pergamon, New York, 1980), Vol. 5, Part 1.
- [16] R. W. Preisendorfer, *Principal Component Analysis in Meteorology and Oceanography*, Vol. 17 of *Developments in Atmospheric Science* (Elsevier, Amsterdam, 1988); K. Fukunaga, *Introduction to Statistical Pattern Recognition*, 2nd ed. (Academic Press, Boston, 1990); G. Berkooz, P. Holmes, and J. L. Lumley, *Ann. Rev. Fluid Mech.* **25**, 539 (1993).
- [17] E. Anderson *et al.*, *LAPACK User's Guide*, 2nd ed. (SIAM, Philadelphia, USA, 1992).
- [18] S. Ciliberto and B. Nicolaenko, *Europhys. Lett.* **14**, 303 (1991); L. Sirovich and A. E. Deane, *J. Fluid Mech.* **222**, 251 (1991); R. Vautard and M. Ghil, *Physica D* **35**, 395 (1989).

## FIGURES

FIG. 1. (a) KLD dimension  $D_{\text{KLD}}(f)$  Eq. (1) versus system size  $L$  for Eq. (2) with rigid boundary conditions, for system sizes  $50 \leq L \leq 400$ . The percentage labels indicate the value of the fraction  $f$  for each curve. After integrating  $10^6$  time steps to allow transients to decay,  $T = 2 \times 10^4$  time-samples with step  $\Delta t = 2$  time units were used to construct the scatter matrix  $\mathbf{M}$ . The dashed line shows the extensive Lyapunov dimension from Ref. [11] which corresponds to a fraction  $f = 0.81$ . (b) For the same numerical parameters and for a fixed system size of 400, a plot of  $D_{\text{KLD}}(f)$  versus subsystem size  $L$  of the 1d KS equation. The subsystems were centered at  $x = 200$ . In both (a) and (b), the slopes of the lines corresponding to the same  $f$  values are the same.

FIG. 2. KLD correlation length  $\xi_{\text{KLD}}(f)$  versus fraction  $f$  for the data of Fig. 1, showing a nonlinear dependence over an order of magnitude in  $\xi_{\text{KLD}}(f)$ .

FIG. 3. (a) Comparison of the KLD and Lyapunov dimension correlation lengths (squares and circles respectively) for the non-equilibrium transition of the 2d Miller-Huse model, for which the two-point correlation length  $\xi_2$  diverges at  $g = 0.205$  [9]. The values for  $\xi_\delta$  were taken from Ref. [13] while the values for  $\xi_{\text{KLD}}(f)$  were calculated for the fraction  $f = 0.95$  using spatiotemporal data of the Miller-Huse model on a 2D square lattice of size  $L = 30$  with periodic boundary conditions. After a transient time of  $2 \times 10^6$  iterations,  $T = 10^4$  time-samples of  $S = L^2$  lattice sites in the range  $12^2 \leq S \leq 20^2$  were used to define the data matrix  $\mathbf{A}$ . The double-headed arrow indicates the range in parameter  $g$  used to study weakly inhomogeneous dynamics in Fig. 4.

FIG. 4. (a) KLD correlation length  $\xi_{\text{KLD}}(f)$  with  $f = 0.95$  (solid circles) versus spatial coordinate  $i$  for a weakly inhomogeneous 2D Miller-Huse model on a square lattice with periodic boundary conditions, with rectangular geometry  $L_x = 300$  and  $L_y = 30$ . The solid circles were obtained by studying the extensive scaling of  $D_{\text{KLD}}(f)$  for subsystems of size  $L_x = 9, 11, 13,$  and  $15$  centered on the particular coordinate  $i$ . The dashed curve in (a) represents the value of  $\xi_{\text{KLD}}(f)$  interpolated from Fig. 3, corresponding to an infinite nontransient homogeneous system with constant value  $g(i)$  corresponding to that particular location in space. The scatter matrix was calculated from  $T = 10^4$  time-samples after waiting  $2 \times 10^6$  time units for transients to decay. (b) The coupling constant  $g(i)$  varied spatially in the  $x$ -direction according to the equation  $g = 0.17 + 0.02 \sin(2\pi i/300)$ .

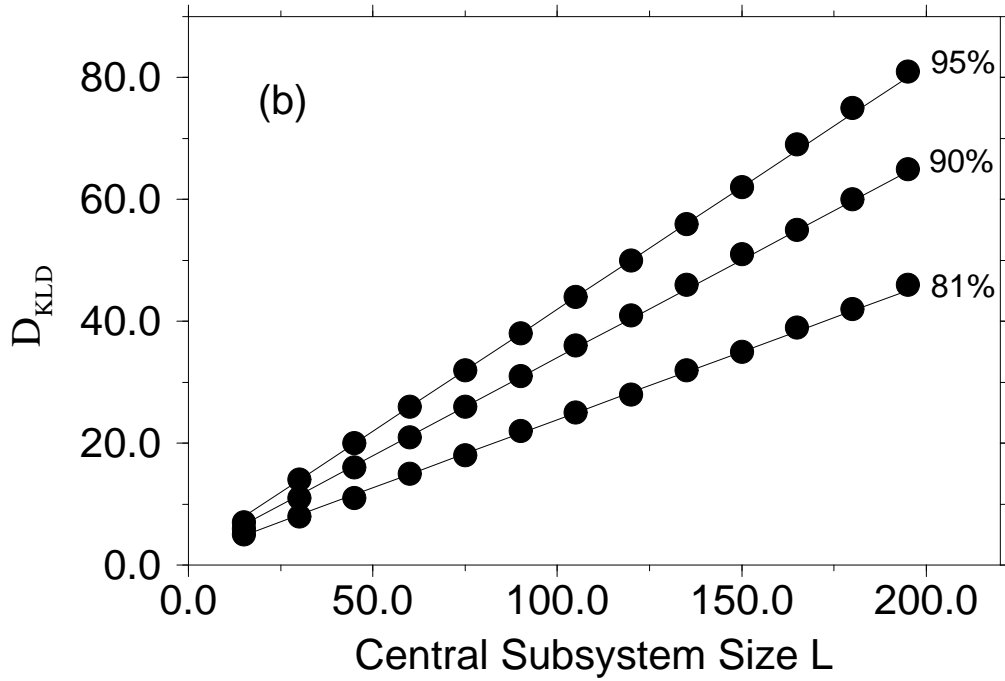
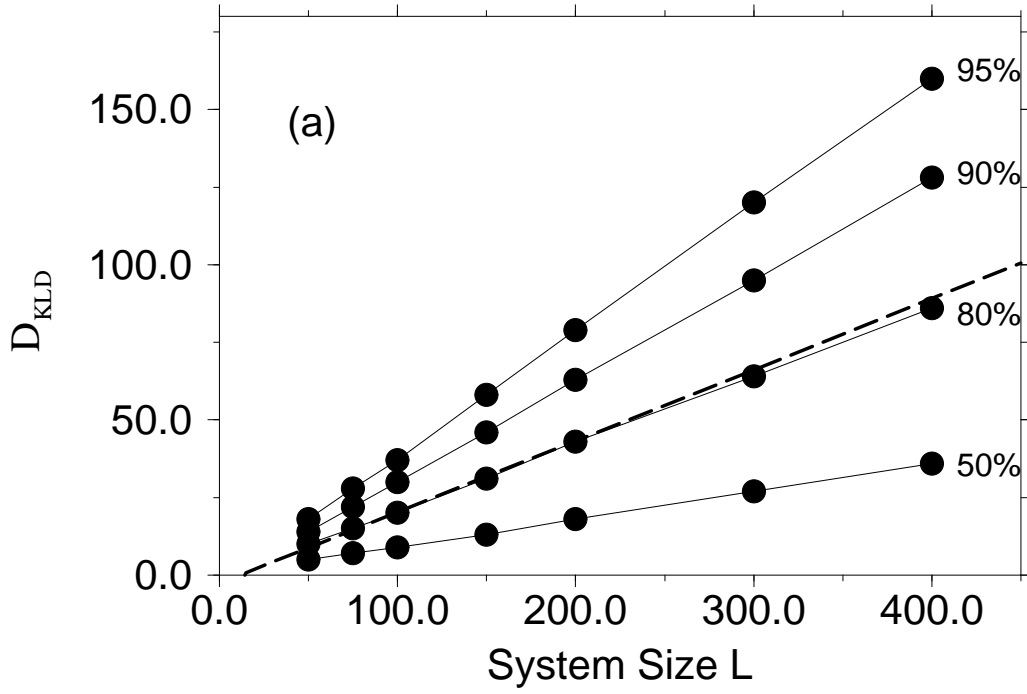


Fig 1 of Zoldi and Greenside

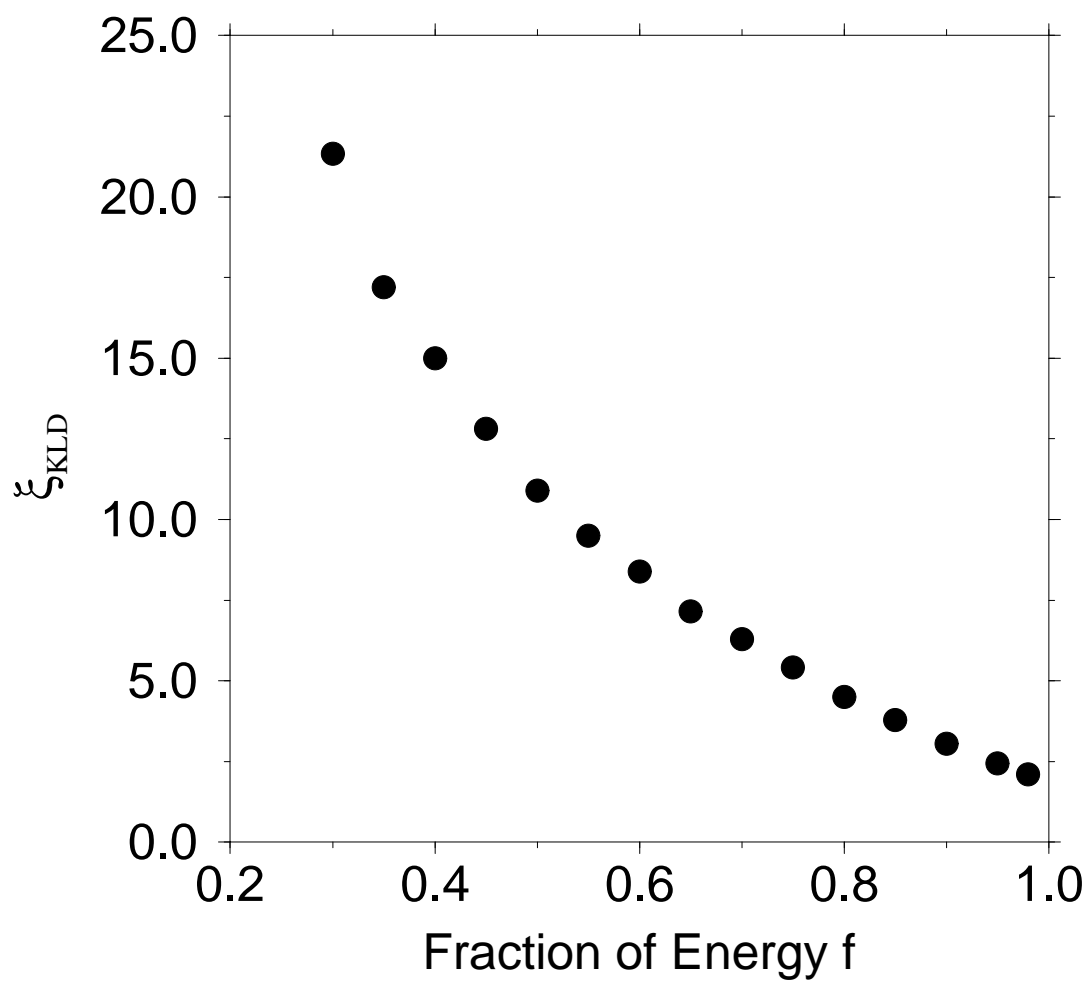


Fig 2 of Zoldi and Greenside

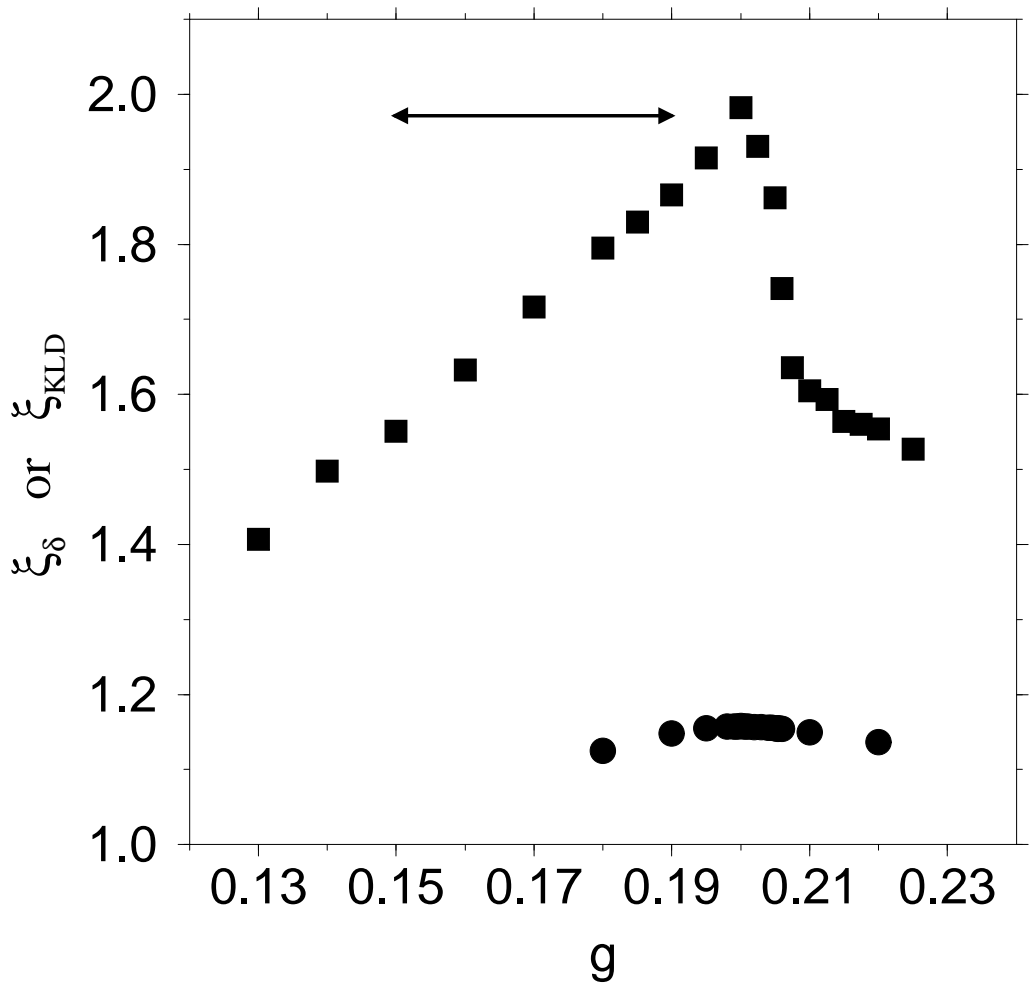


Fig 3 of Zoldi and Greenside

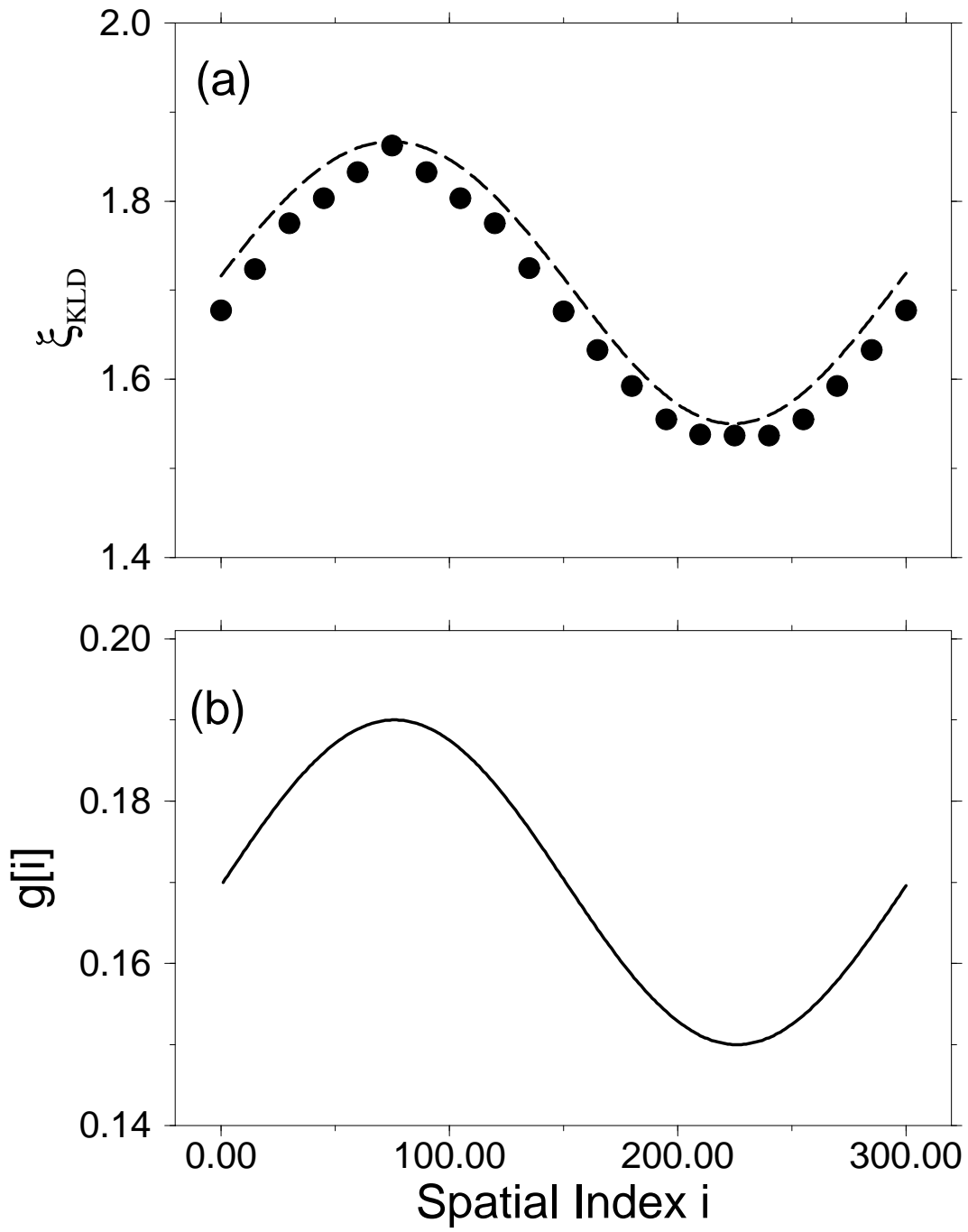


Fig 4 of Zoldi and Greenside