

Numerical approaches for investigating the chaotic behavior of multidimensional Hamiltonian systems

Haris Skokos

**Department of Mathematics and Applied Mathematics
University of Cape Town
Cape Town, South Africa**

E-mail: haris.skokos@uct.ac.za
URL: http://math_research.uct.ac.za/~hskokos/

OttoChaos: From the nonlinear dynamical systems theory to observational chaos
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Outline

- The one-dimensional quartic disordered Klein-Gordon (1D DKG) model: Different dynamical regimes
- Maximum Lyapunov Exponent (MLE): strength of chaos
- Deviation Vector Distributions (DVDs): mechanisms of chaotic spreading
- Frequency Map Analysis (FMA): characteristics of spatiotemporal evolution of chaos
- Generalized Alignment Index (GALI): localized vs. spreading chaos
- Summary

The one-dimensional disordered Klein Gordon model (1D DKG)

$$H = \sum_{l=1}^N \frac{p_l^2}{2} + \frac{\tilde{\varepsilon}_l}{2} u_l^2 + \frac{1}{4} u_l^4 + \frac{1}{2W} (u_{l+1} - u_l)^2$$

with **fixed boundary conditions** $u_0 = p_0 = u_{N+1} = p_{N+1} = 0$. Typically $N=1000$.

Parameters: **W** and the **total energy H**. $\tilde{\varepsilon}_l$ chosen uniformly from $\left[\frac{1}{2}, \frac{3}{2}\right]$.

Linear case (neglecting the term $u_l^4/4$)

Ansatz: $u_l = A_l \exp(i\omega t)$. **Normal modes (NMs)** $A_{v,l}$ - **Eigenvalue problem:**

$$\lambda A_l = \varepsilon_l A_l - (A_{l+1} + A_{l-1}) \text{ with } \lambda = W\omega^2 - W - 2, \quad \varepsilon_l = W(\tilde{\varepsilon}_l - 1)$$

Anderson localization [Anderson, Phys. Rev. (1958)]. Experiments on BEC [Billy et al., Nature (2008)]

What happens in the presence of nonlinearity?

Will nonlinearity destroy localization?

Characteristics of energy distributions

We consider normalized **energy distributions** $\xi_l = \frac{H_l}{\sum_m H_m}$

with $H_l = \frac{p_l^2}{2} + \frac{\tilde{\varepsilon}_l}{2} u_l^2 + \frac{1}{4} u_l^4 + \frac{1}{4W} (u_{l+1} - u_l)^2$

Second moment: $m_2 = \sum_{l=1}^N (l - \bar{l})^2 \xi_l$ with $\bar{l} = \sum_{l=1}^N l \xi_l$

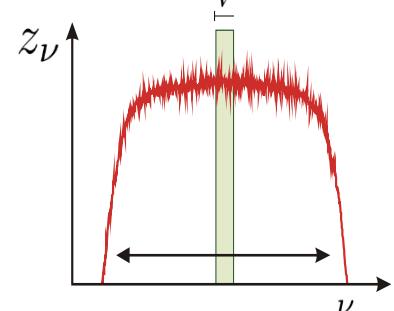
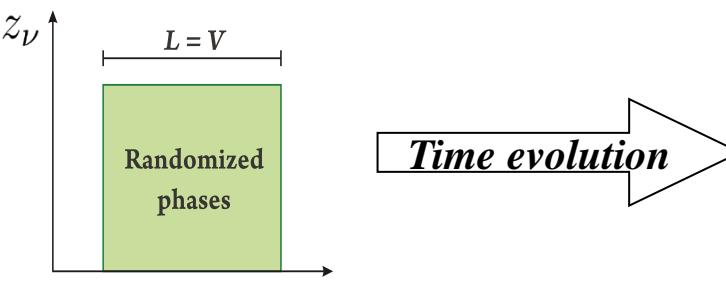
Participation number: $P = \frac{1}{\sum_{l=1}^N \xi_l^2}$

measures the number of stronger excited sites in ξ_l .

Single site $P=1$. Equipartition of energy $P=N$.

Strong and weak chaos regimes (1D DKG)

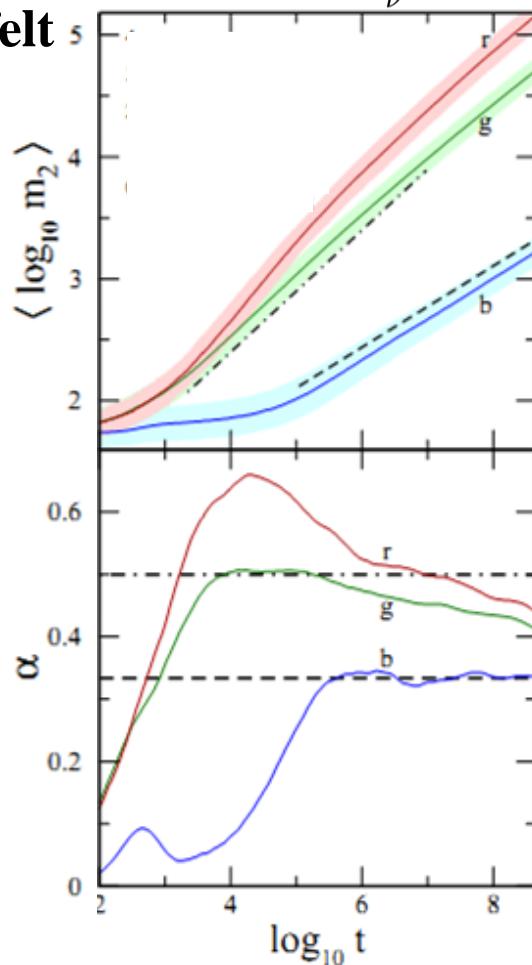
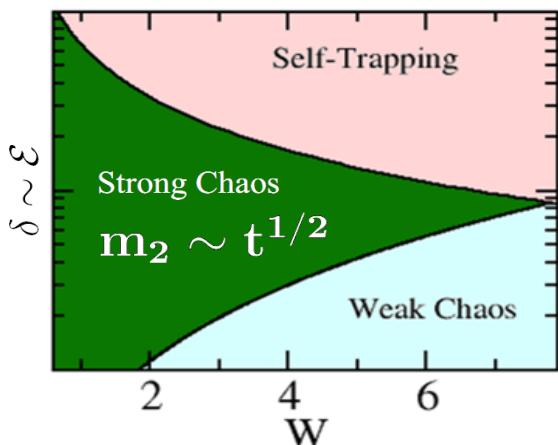
We consider **compact initial wave packets of width L**
 [Flach et al. PRL (2009) – S.
 et al PRE (2009) – Laptyeva
 et al., EPL (2010) – Bodyfelt
 et al., PRE (2011)]



$H = 0.01, 0.2, 0.75$

$W=4$

Average over 1000 realizations!



$$\alpha = 1/2$$

$$\alpha = 1/3$$

$$\alpha(\log t) = \frac{d \langle \log m_2 \rangle}{d \log t}$$

Maximum Lyapunov Exponent (MLE)

Chaos: sensitive dependence on initial conditions.

Roughly speaking, the MLE of a given orbit characterizes the **mean exponential rate of divergence** of trajectories surrounding it.

Consider an orbit in the $2N$ -dimensional phase space with **initial condition $x(0)$** and **an initial deviation vector (small perturbation) from it $v(0)$** .

Then the mean exponential rate of divergence is:

$$\text{MLE} = \lambda_1 = \lim_{t \rightarrow \infty} \Lambda(t) = \lim_{t \rightarrow \infty} \frac{1}{t} \ln \frac{\|v(t)\|}{\|v(0)\|}$$

$\lambda_1 = 0 \rightarrow \text{Regular motion } (\Lambda \propto t^{-1})$

$\lambda_1 > 0 \rightarrow \text{Chaotic motion}$

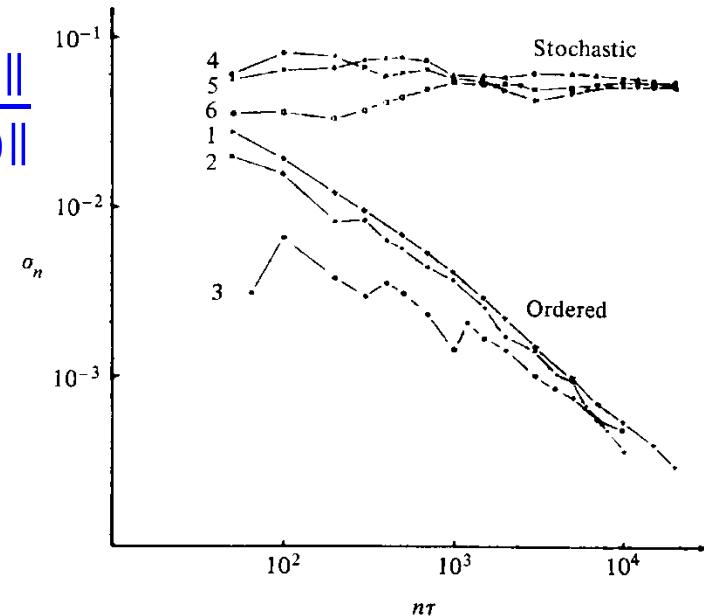
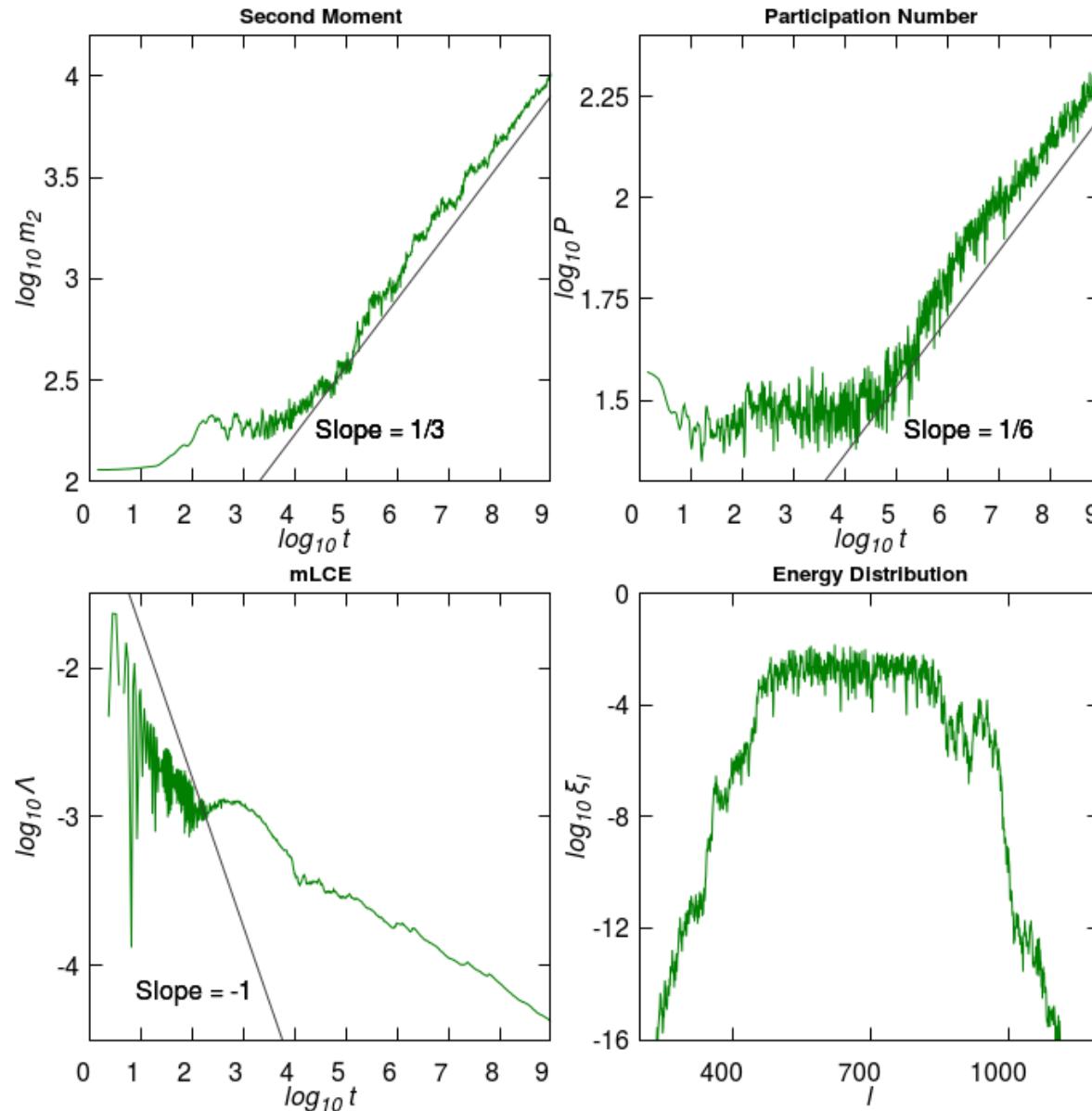


Figure 5.7. Behavior of σ_n at the intermediate energy $E = 0.125$ for initial points taken in the ordered (curves 1–3) or stochastic (curves 4–6) regions (after Benettin *et al.*, 1976).

A weak chaos case

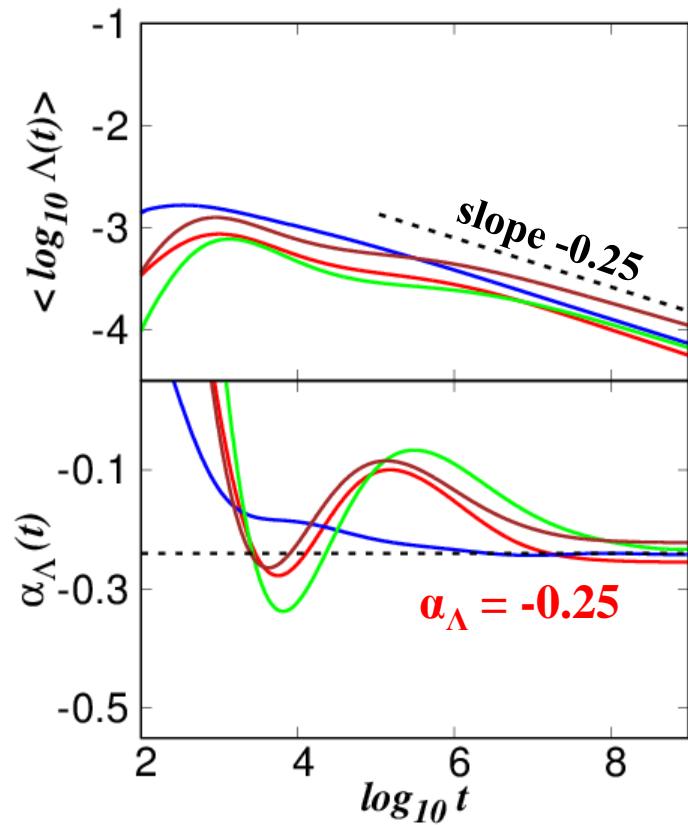
Block excitation
L=37 sites,
H=0.37, W=3.

**One disorder
realization**

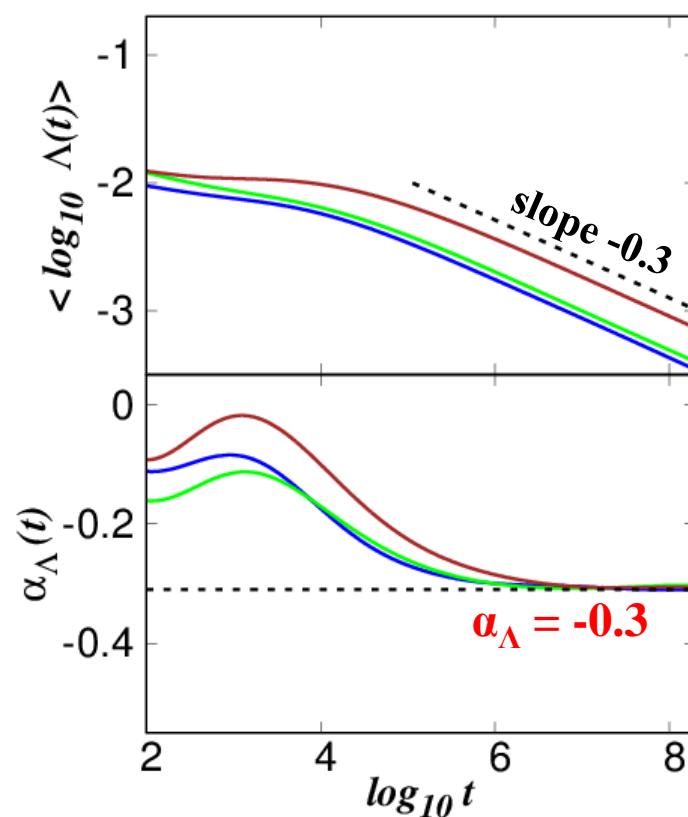


Time evolution of the MLE: $\Lambda \propto t^{\alpha_\Lambda}$

Weak
chaos



Strong
chaos



Average over 100 realizations [Senyange et al., PRE (2018)]

Block excitation (L=37 sites) H=0.37, W=3

Single site excitation H=0.4, W=4

Block excitation (L=21 sites) H=0.21, W=4

Block excitation (L=13 sites) H=0.26, W=5

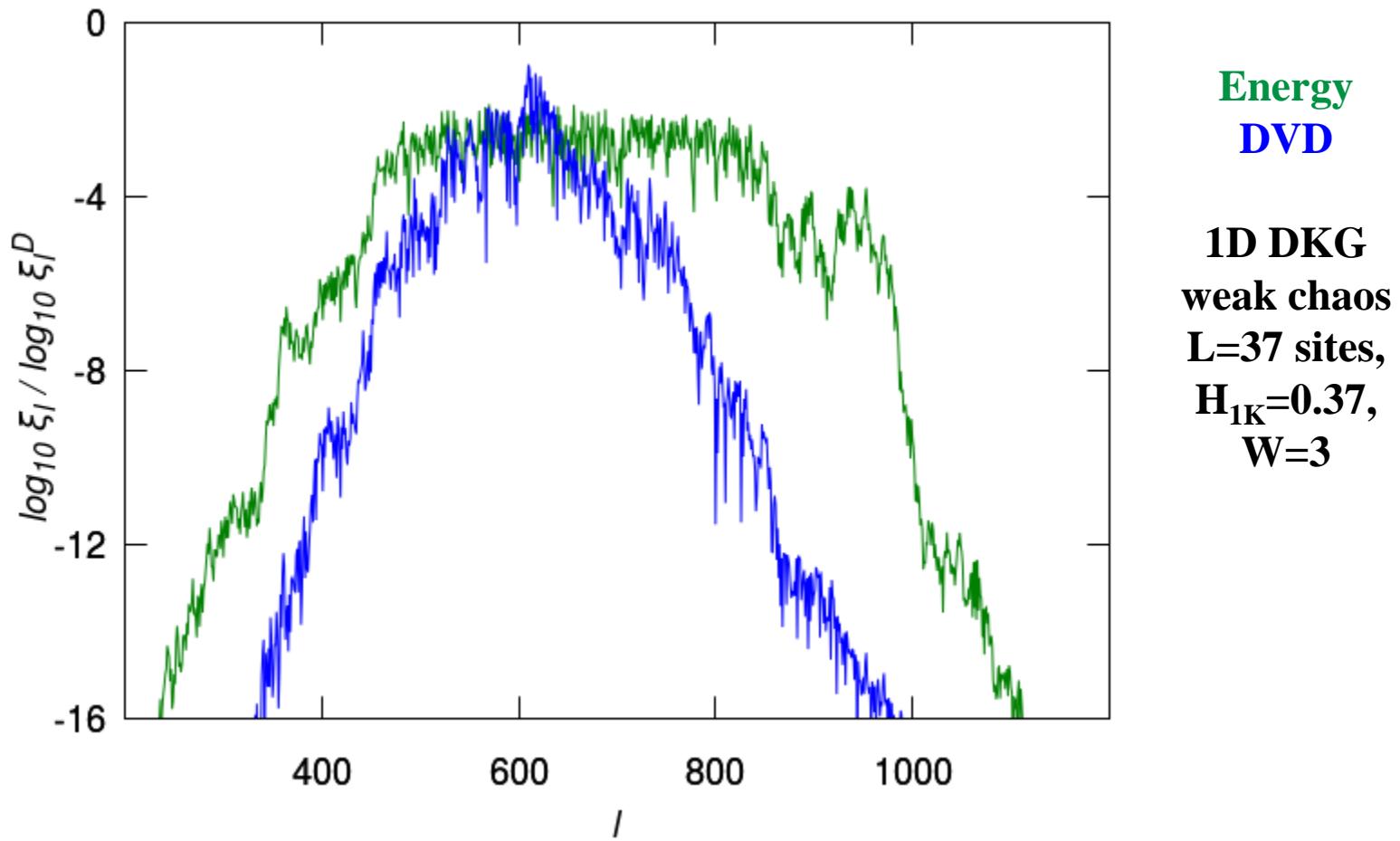
Block excitation (L=83 sites) H=0.83, W=2

Block excitation (L=37 sites) H=0.37, W=3

Block excitation (L=83 sites) H=0.83, W=3

The weak chaos case was also studied in S. et al., PRL (2013)

Deviation Vector Distributions (DVDs)



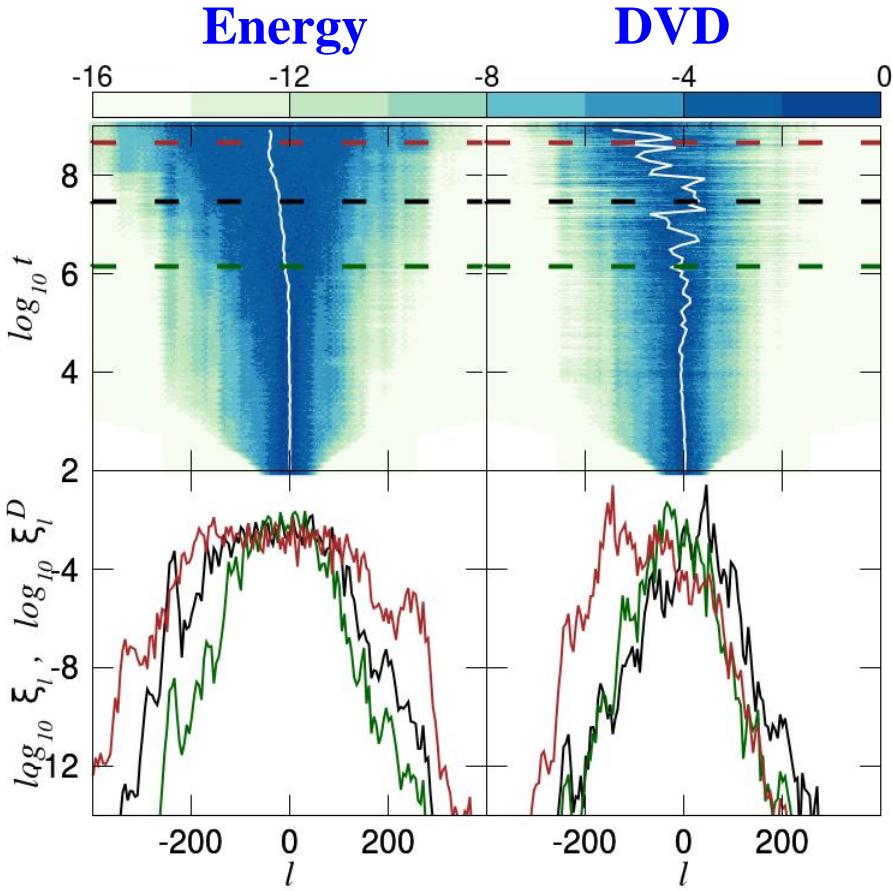
Deviation vector:

$$\mathbf{v}(t) = (\delta u_1(t), \delta u_2(t), \dots, \delta u_N(t), \delta p_1(t), \delta p_2(t), \dots, \delta p_N(t))$$

$$\text{DVD: } \xi_l^D = \frac{\delta u_l^2 + \delta p_l^2}{\sum_l (\delta u_l^2 + \delta p_l^2)}$$

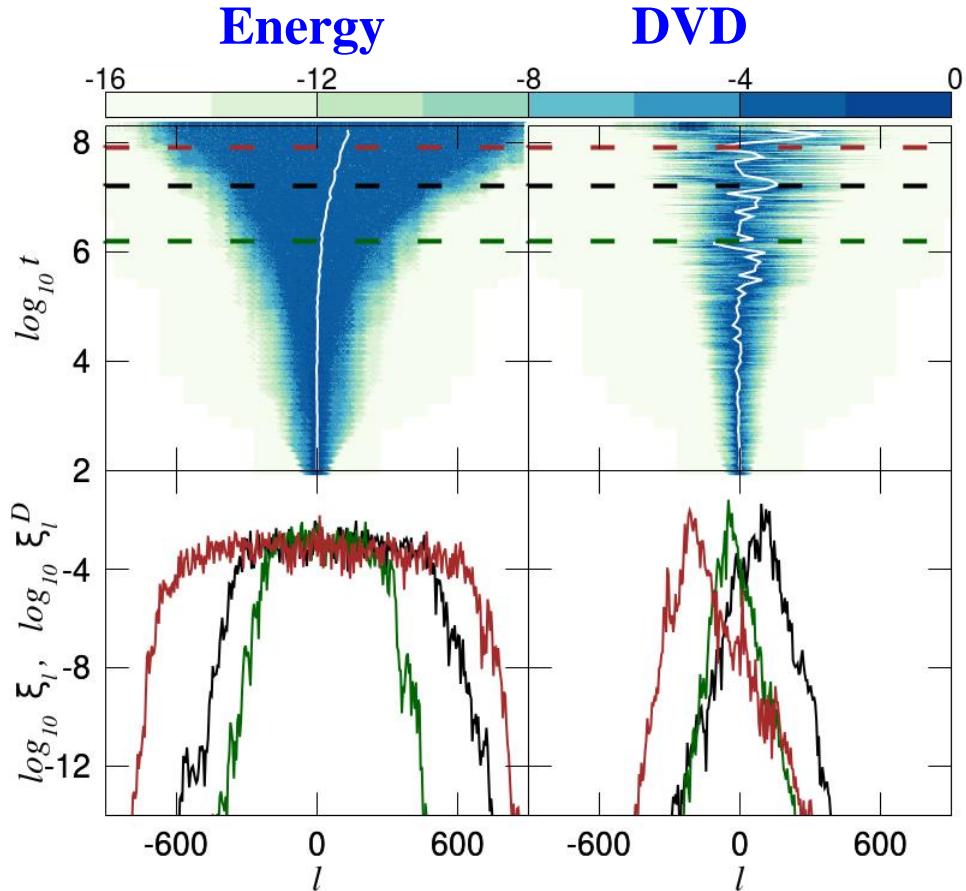
DVDs: Weak and Strong Chaos

Weak chaos (1D DKG)



$W=3, L=37, H=0.37$

Strong chaos (1D DKG)



$W=3, L=83, H=8.3$

Chaotic hot spots meander through the system, supporting the homogeneity of chaos inside the wave packet.

Frequency Map Analysis (FMA)

Compute the **fundamental frequencies**, f_1 and f_2 , of an observable related to the evolution of an orbit in **two successive time windows** of the same length, and check **whether or not these frequencies change in time** [Laskar, Icarus (1990) – Laskar et al., Physica D (1992) – Laskar, Physica D (1993) – Robutel & Laskar, Icarus (2000)].

Regular motion: The computed frequencies do not vary in time

Chaotic motion: The computed frequencies vary in time

For every lattice site l we compute the fundamental frequencies f_{1l} and f_{2l} for time windows of length $T = 6 \cdot 10^5$ time units and evaluate the **relative change of these two frequencies**:

$$D_l = \left| \frac{f_{2l} - f_{1l}}{f_{1l}} \right|$$

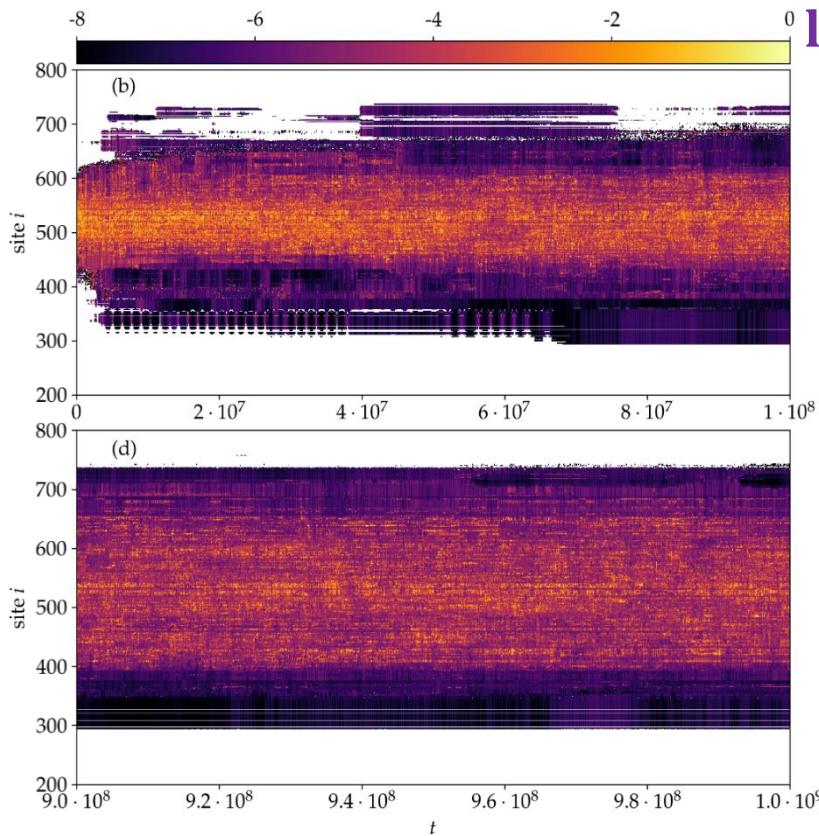
Regular motion: small D_l values

Chaotic motion: large D_l values

FMA: Weak and Strong Chaos

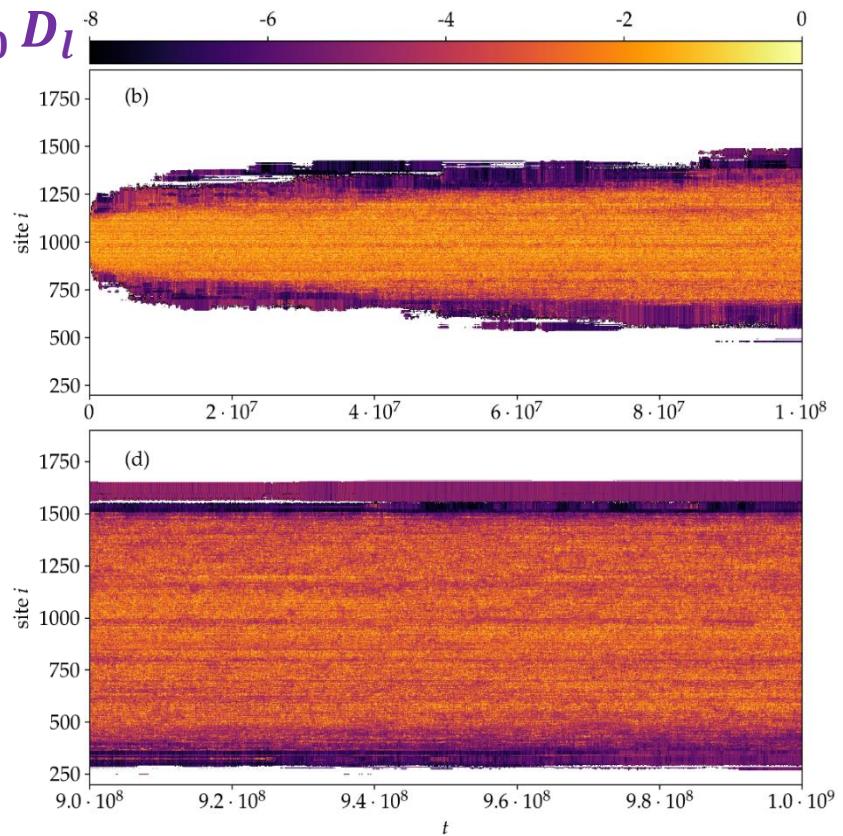
Weak chaos

$L=1, H=0.4, W=4, N=999$



Strong chaos

$L=21, H=4.2, W=4, N=3499$



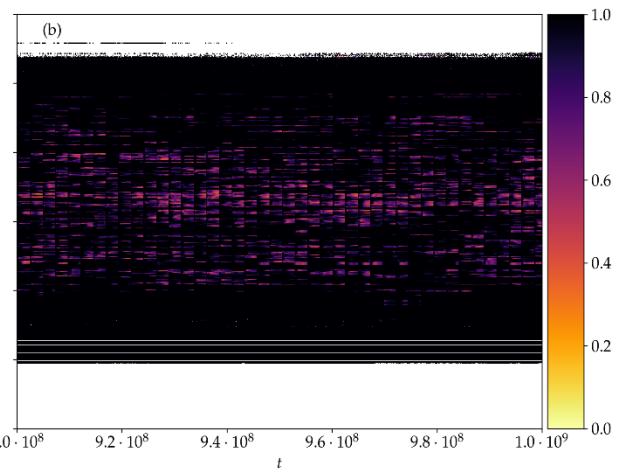
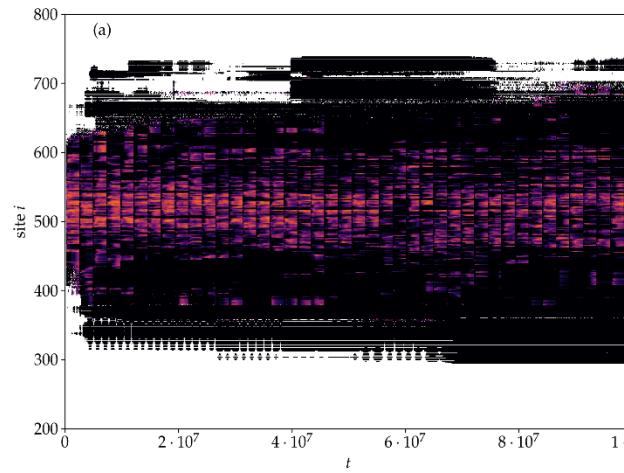
Chaotic behavior appears at the central regions of the wave packet, where the energy density is relatively large. The chaotic component of the wave packet is more extended in the strong chaos case [S. et al., IJBC (2022)]

Frequency Locking (FL)

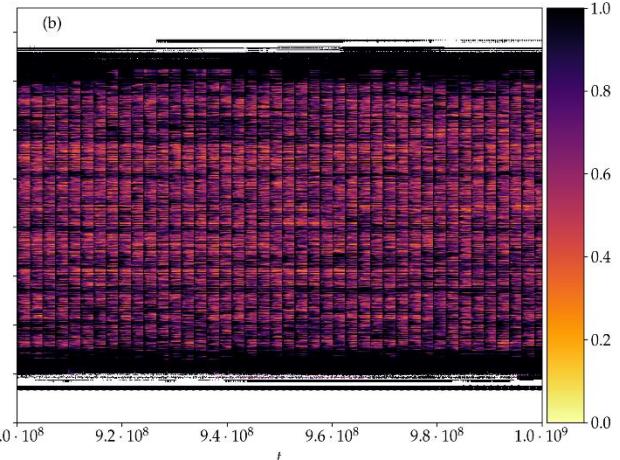
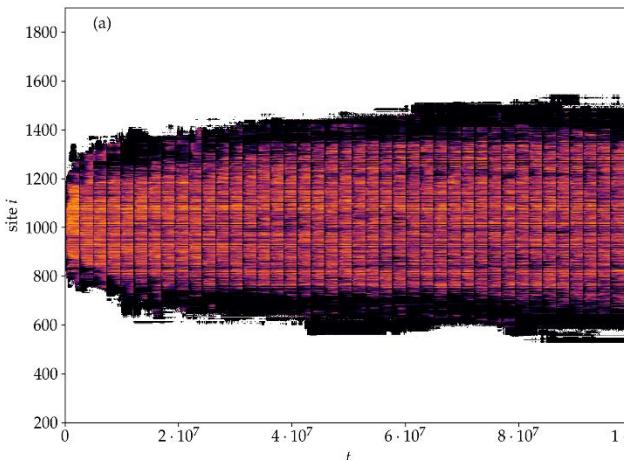
Frequency bins of width 10^{-4} . For each lattice site and a duration of $t = 2.4 \cdot 10^7$ we compute the fundamental frequencies in 200 time windows and register the related bins.

FL_l : the fraction of the most visited bin ($0 \leq FL_l \leq 1$). Measures the degree of practical frequency constancy (denoting nonchaotic behavior) of each oscillator.

Weak chaos



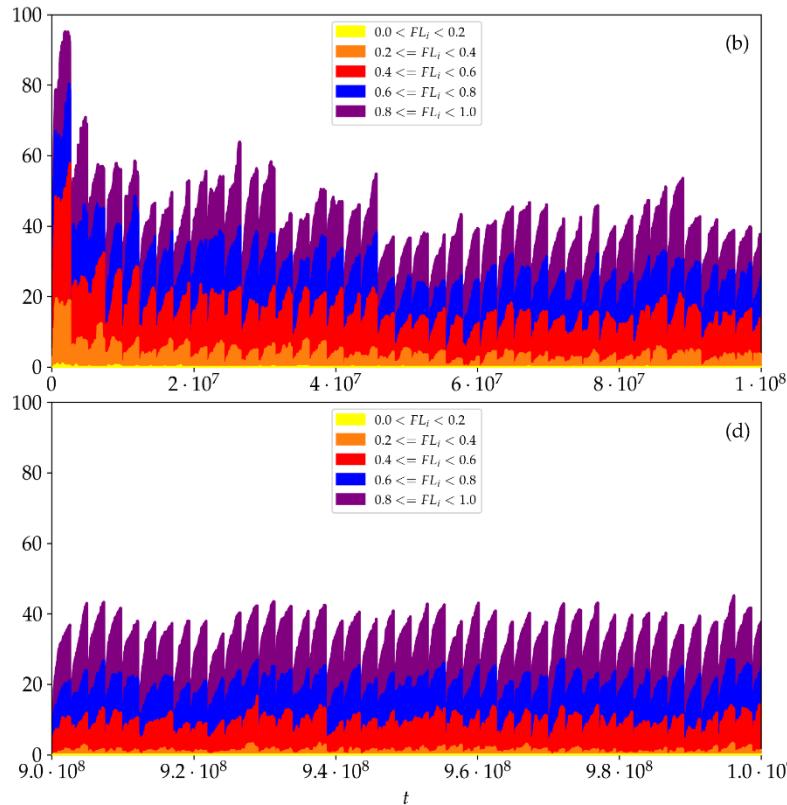
Strong chaos



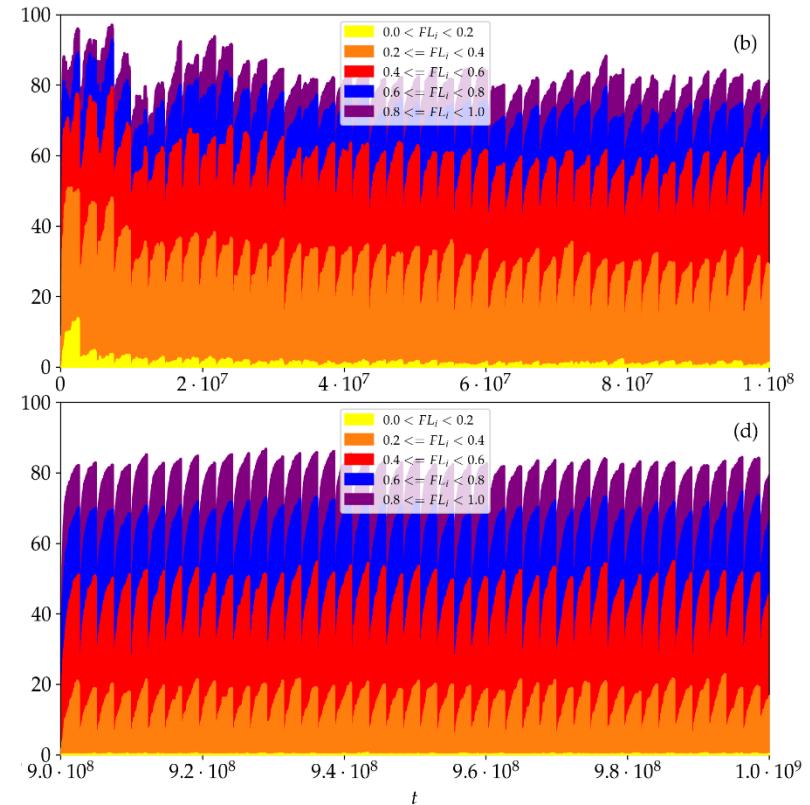
Frequency Locking (FL)

Accumulated percentages P_{FL} of sites with values in a particular FL range

Weak chaos



Strong chaos



The fraction of sites behaving chaotically is much larger in the strong chaos regime.

The percentage of strongly chaotic sites (having $FL_l < 0.4$) is about 5 times larger for strong chaos.

For both spreading regimes, the fraction of highly chaotic oscillators ($FL_l < 0.4$) decreases in time, although the percentage of chaotic sites remains practically constant.

The Generalized Alignment Index (GALI)

In the case of an N degree of freedom Hamiltonian system we follow the evolution of k deviation vectors with $2 \leq k \leq 2N$, and define [S. et al., Physica D, (2007)] the Generalized Alignment Index (GALI) of order k :

$$GALI_k(t) = \|\hat{v}_1(t) \wedge \hat{v}_2(t) \wedge \dots \wedge \hat{v}_k(t)\|$$

where $\hat{v}_1(t) = \frac{v_1(t)}{\|v_1(t)\|}$.

Chaotic motion: $GALI_k(t) \propto e^{-[(\lambda_1 - \lambda_2) + (\lambda_1 - \lambda_3) + \dots + (\lambda_1 - \lambda_k)]t}$
with $\lambda_1, \lambda_2, \dots, \lambda_k$ being the first k largest Lyapunov exponents.

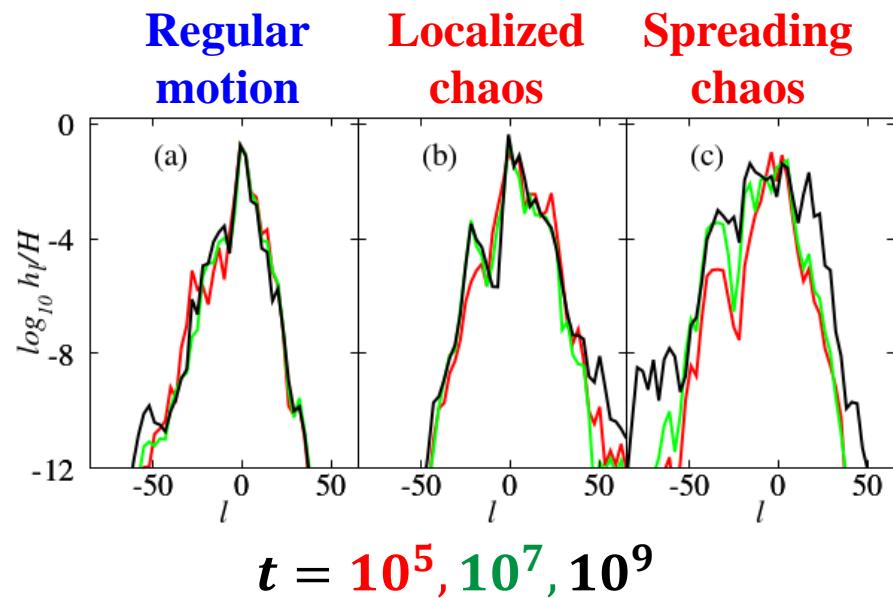
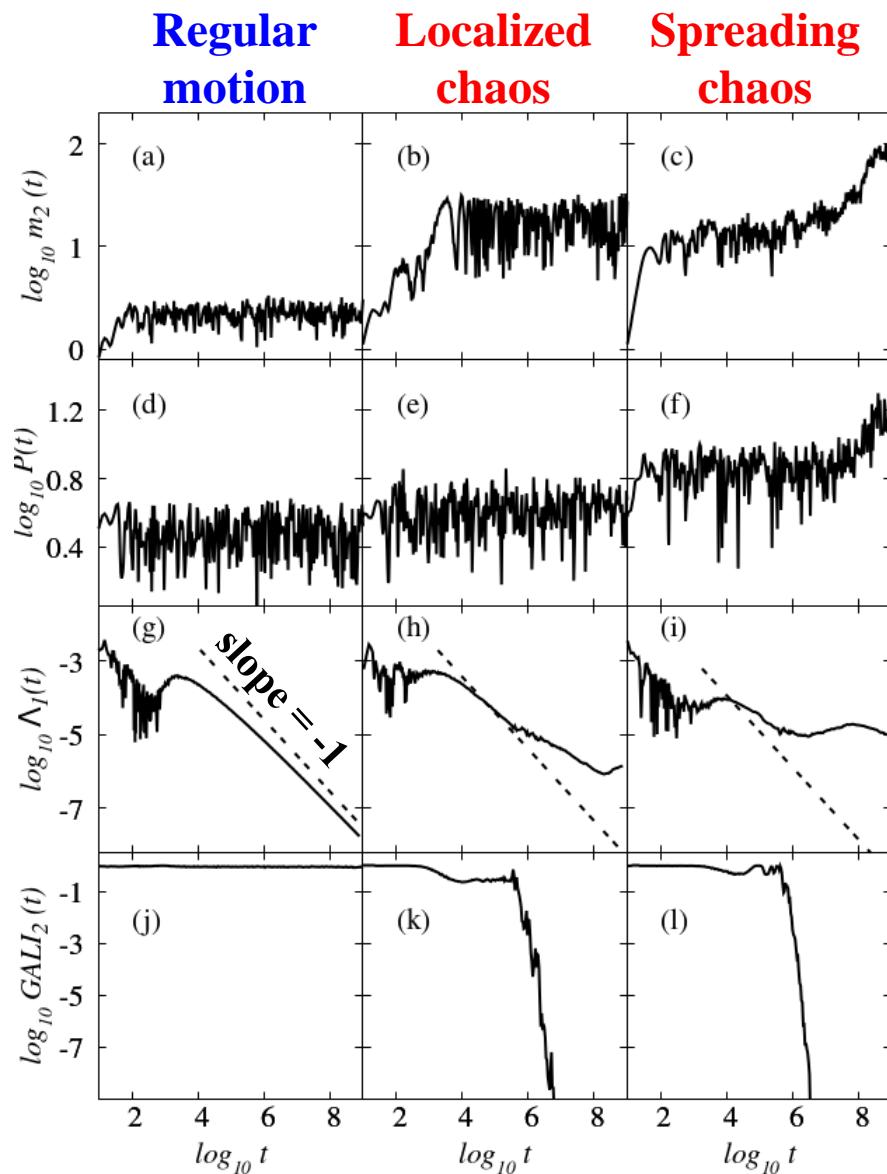
Regular motion: When the motion occurs on an N -dimensional torus [S. et al., Eur. Phys. J. Sp. Top. (2008)]:

$$GALI_k(t) \propto \text{constant, if } 2 \leq k \leq N$$

Here we consider **GALI₂** ($k=2$) which is equivalent to the **Smaller Alignment Index (SALI)** [S, J. Phys A (2001)].

Regular vs. chaotic (localized or spreading) motion

Different disorder realizations can exhibit different behaviors.

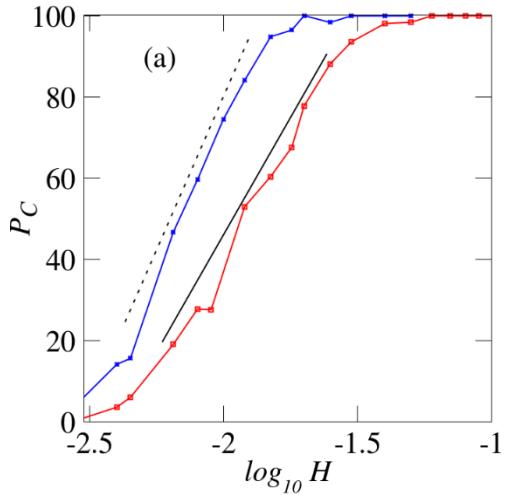


$t = 10^5, 10^7, 10^9$
Single site excitations, $L=1$, for
 $W=6, H=0.02$ [Senyange & S.,
Physica D (2022)].

The GALI_2 can identify chaos
much more clearly than the MLE.

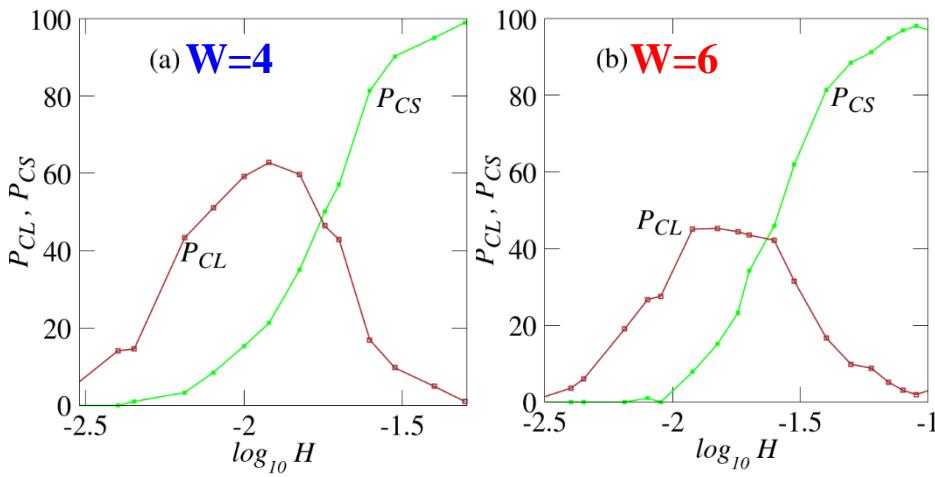
Decreasing nonlinearity

Single site excitations

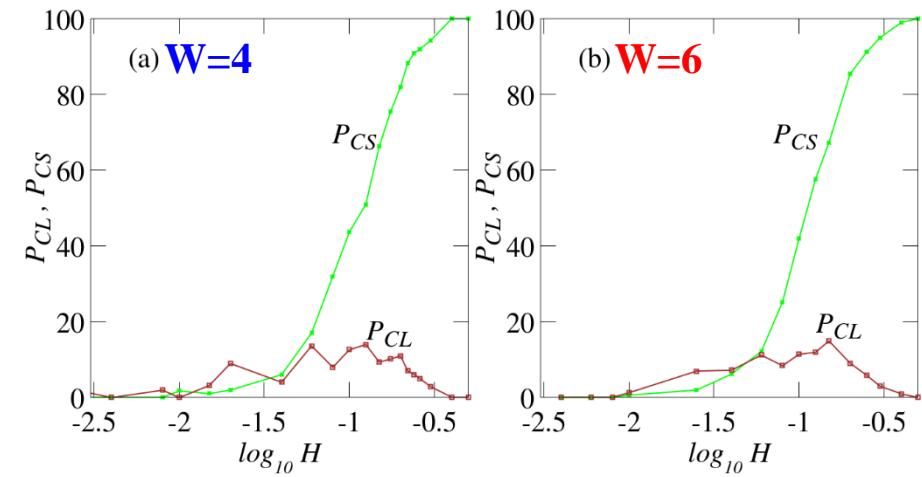
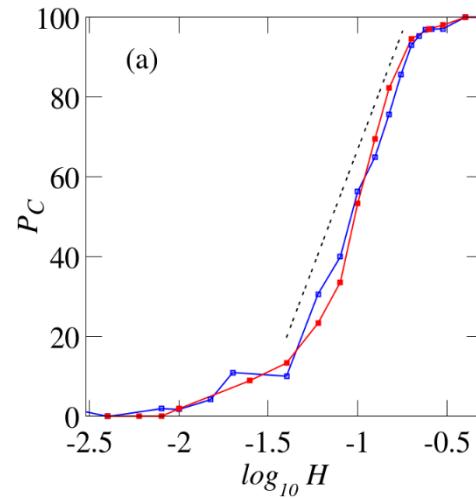


P_C : % of chaotic orbits
 $W=4, W=6$

P_{CL} : % of localized chaos P_{CS} : % of spreading chaos



Single mode excitations



Energy thresholds for transition to regular motion and to spreading chaos are lower for single site excitations which permit mode interactions [Senyange & S., Physica D (2022)].

Summary

We investigated in depth the spatiotemporal chaotic behavior of the DKG multidimensional Hamiltonian system.

- Identification of 2 different dynamical spreading regimes: **weak and strong chaos**
- The MLE reveals the decrease of the system's chaoticity in time
Weak chaos: $\Lambda \propto t^{-0.25}$ - Strong chaos: $\Lambda \propto t^{-0.30}$
- The DVDs provide information about the propagation of chaos
Wandering of localized **chaotic hot spots** in the lattice's excited part homogenize chaos.
- FMA computations uncover the characteristics of chaos evolution
Chaotic behavior appears at the central regions of the wave packet, being more pronounced in the strong chaos case.
- The GALI method allows the detailed study of the system's behavior when it approaches its linear limit
Clear identification of chaos.
Efficient distinction between **localized and spreading chaos**.
Identification of **energy thresholds** leading to global chaotic spreading and to the total absence of chaos.

Main references

- S. (2001) J. Phys. A, 34, 10029
- S., Bountis, Antonopoulos (2007) Physica D, 231, 30
- S., Bountis, Antonopoulos (2008) Eur. Phys. J. Sp. Top., 165, 5
- Flach, Krimer, S. (2009) PRL, 102, 024101
- S., Flach (2010) PRE, 82, 016208
- Laptyeva, Bodyfelt, Krimer, S., Flach (2010) EPL, 91, 30001
- Bodyfelt, Laptyeva, S., Krimer, Flach (2011) PRE, 84, 016205
- S., Gkolias, Flach (2013) PRL, 111, 064101
- Senyange, Many Manda, S. (2018) PRE, 98, 052229
- Senyange, S. (2022) Physica D, 432, 133154
- S., Gerlach, Flach (2022) Int. J. Bifurc. Chaos, 32, 2250074