

Chaotic behavior of disordered nonlinear systems

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**Work in collaboration with
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Outline

- **Disordered 1D lattices:**
 - ✓ **The quartic Klein-Gordon (KG) model**
 - ✓ **The disordered nonlinear Schrödinger equation (DNLS)**
 - ✓ **Different dynamical behaviors**
- **Chaotic behavior of the KG model**
 - ✓ **Lyapunov exponents**
 - ✓ **Deviation Vector Distributions**
 - ✓ **Integration techniques (Symplectic integrators and Tangent Map method)**
- **Summary**

The Klein – Gordon (KG) model

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

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

Parameters: W and the total energy E . $\tilde{\varepsilon}_l$ 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:

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

The discrete nonlinear Schrödinger (DNLS) equation

We also consider the system:

$$H_D = \sum_{l=1}^N \varepsilon_l |\psi_l|^2 + \frac{\beta}{2} |\psi_l|^4 - (\psi_{l+1} \psi_l^* + \psi_{l+1}^* \psi_l)$$

where ε_l chosen uniformly from $\left[-\frac{W}{2}, \frac{W}{2} \right]$ and β is the nonlinear parameter.

Conserved quantities: The energy and the norm $S = \sum_l |\psi_l|^2$ of the wave packet.

Distribution characterization

We consider normalized **energy distributions** in normal mode (NM) space

$$z_\nu \equiv \frac{E_\nu}{\sum_m E_m} \quad \text{with} \quad E_\nu = \frac{1}{2} \left(\dot{A}_\nu^2 + \omega_\nu^2 A_\nu^2 \right), \quad \text{where } A_\nu \text{ is the amplitude}$$

of the ν th NM (KG) or **norm distributions** (DNLS).

Second moment:
$$m_2 = \sum_{\nu=1}^N (\nu - \bar{\nu})^2 z_\nu \quad \text{with} \quad \bar{\nu} = \sum_{\nu=1}^N \nu z_\nu$$

Participation number:
$$P = \frac{1}{\sum_{\nu=1}^N z_\nu^2}$$

measures the number of stronger excited modes in z_ν .

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

Scales

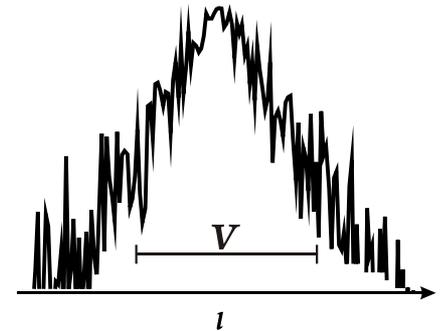
Linear case: $\omega_v^2 \in \left[\frac{1}{2}, \frac{3}{2} + \frac{4}{W} \right]$, width of the squared frequency spectrum:

$$\Delta_K = 1 + \frac{4}{W}$$

$$(\Delta_D = W + 4)$$

Localization
volume of an
eigenstate:

$$V \sim \frac{1}{\sum_{l=1}^N A_{v,l}^4}$$



Average spacing of squared eigenfrequencies of NMs within the range of a localization volume: $d_K \approx \frac{\Delta_K}{V}$

Nonlinearity induced squared frequency shift of a single site oscillator

$$\delta_l = \frac{3E_l}{2\tilde{\epsilon}_l} \propto E \quad (\delta_l = \beta |\psi_l|^2)$$

The relation of the two scales $d_K \leq \Delta_K$ with the nonlinear frequency shift δ_l determines the packet evolution.

Different Dynamical Regimes

Three expected evolution regimes [Flach, Chem. Phys (2010) - S. & Flach, PRE (2010) - Lapyteva et al., EPL (2010) - Bodyfelt et al., PRE (2011)]

Δ : width of the frequency spectrum, d : average spacing of interacting modes, δ : nonlinear frequency shift.

Weak Chaos Regime: $\delta < d$, $m_2 \sim t^{1/3}$

Frequency shift is less than the average spacing of interacting modes. NMs are weakly interacting with each other. [Molina, PRB (1998) – Pikovsky, & Shepelyansky, PRL (2008)].

Intermediate Strong Chaos Regime: $d < \delta < \Delta$, $m_2 \sim t^{1/2} \rightarrow m_2 \sim t^{1/3}$

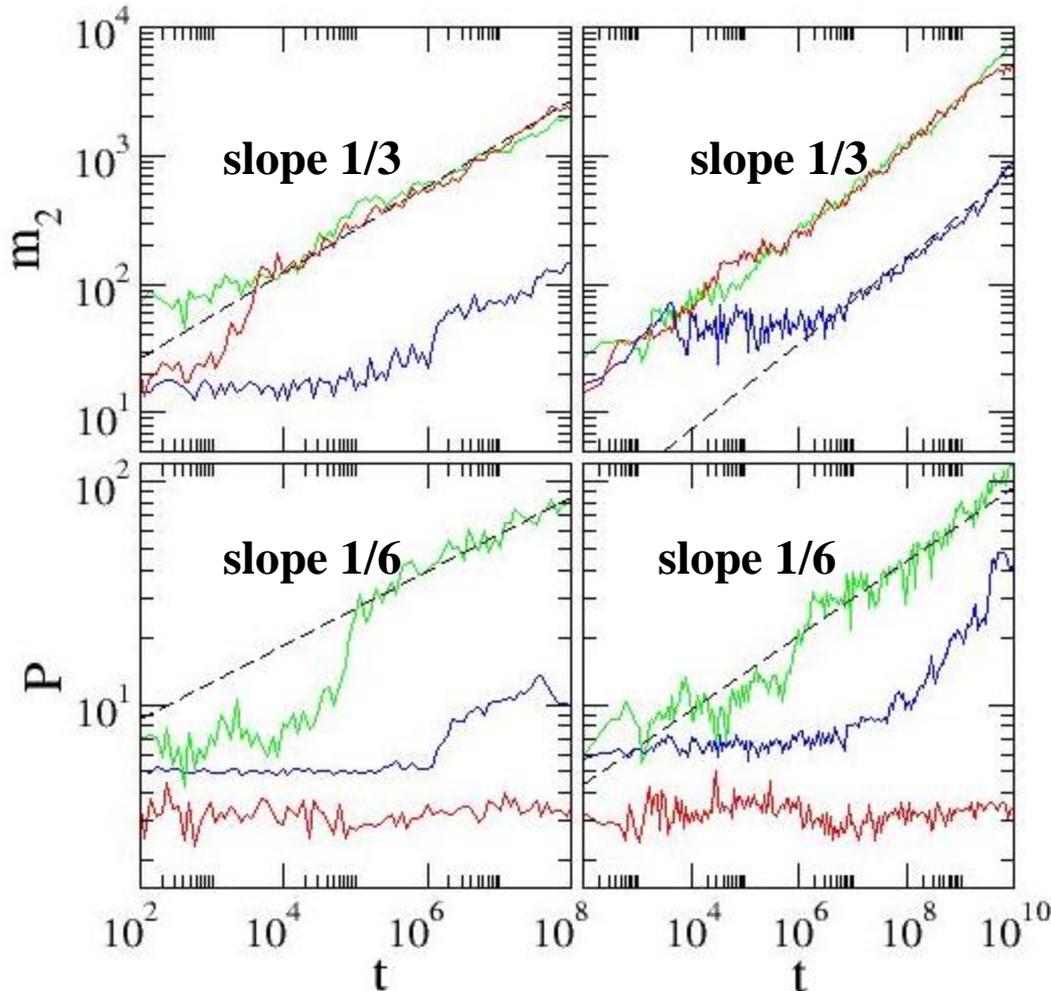
Almost all NMs in the packet are resonantly interacting. Wave packets initially spread faster and eventually enter the weak chaos regime.

Selftrapping Regime: $\delta > \Delta$

Frequency shift exceeds the spectrum width. Frequencies of excited NMs are tuned out of resonances with the nonexcited ones, leading to selftrapping, while a small part of the wave packet subdiffuses [Kopidakis et al., PRL (2008)].

Single site excitations

DNLS $W=4$, $\beta= 0.1, 1, 4.5$ **KG** $W = 4$, $E = 0.05, 0.4, 1.5$



No strong chaos regime

In weak chaos regime we averaged the measured exponent α ($m_2 \sim t^\alpha$) over 20 realizations:

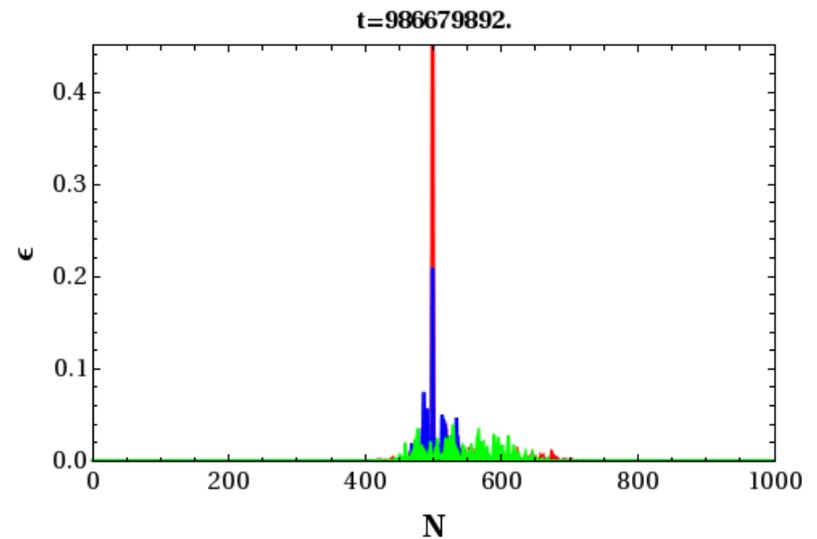
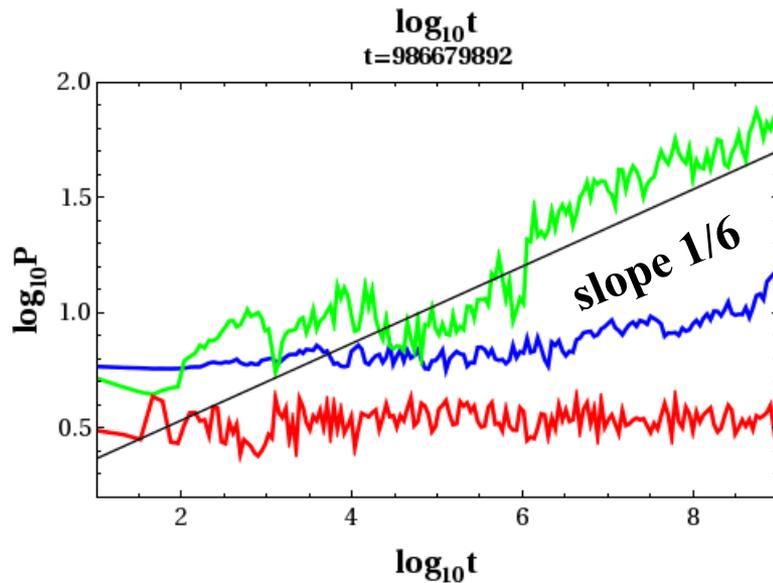
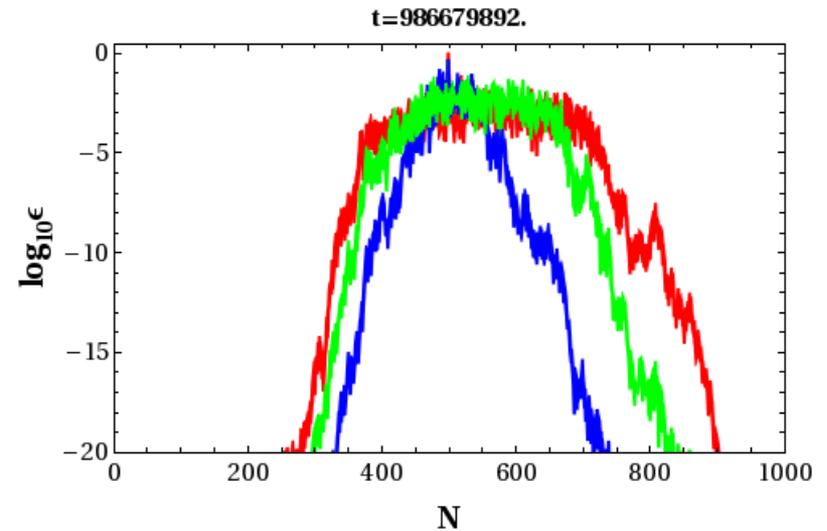
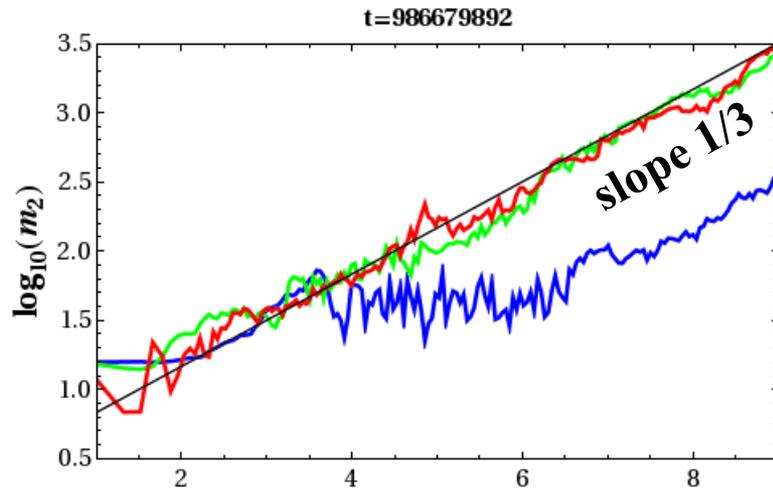
$$\alpha = 0.33 \pm 0.05 \text{ (KG)}$$

$$\alpha = 0.33 \pm 0.02 \text{ (DLNS)}$$

Flach et al., PRL (2009)

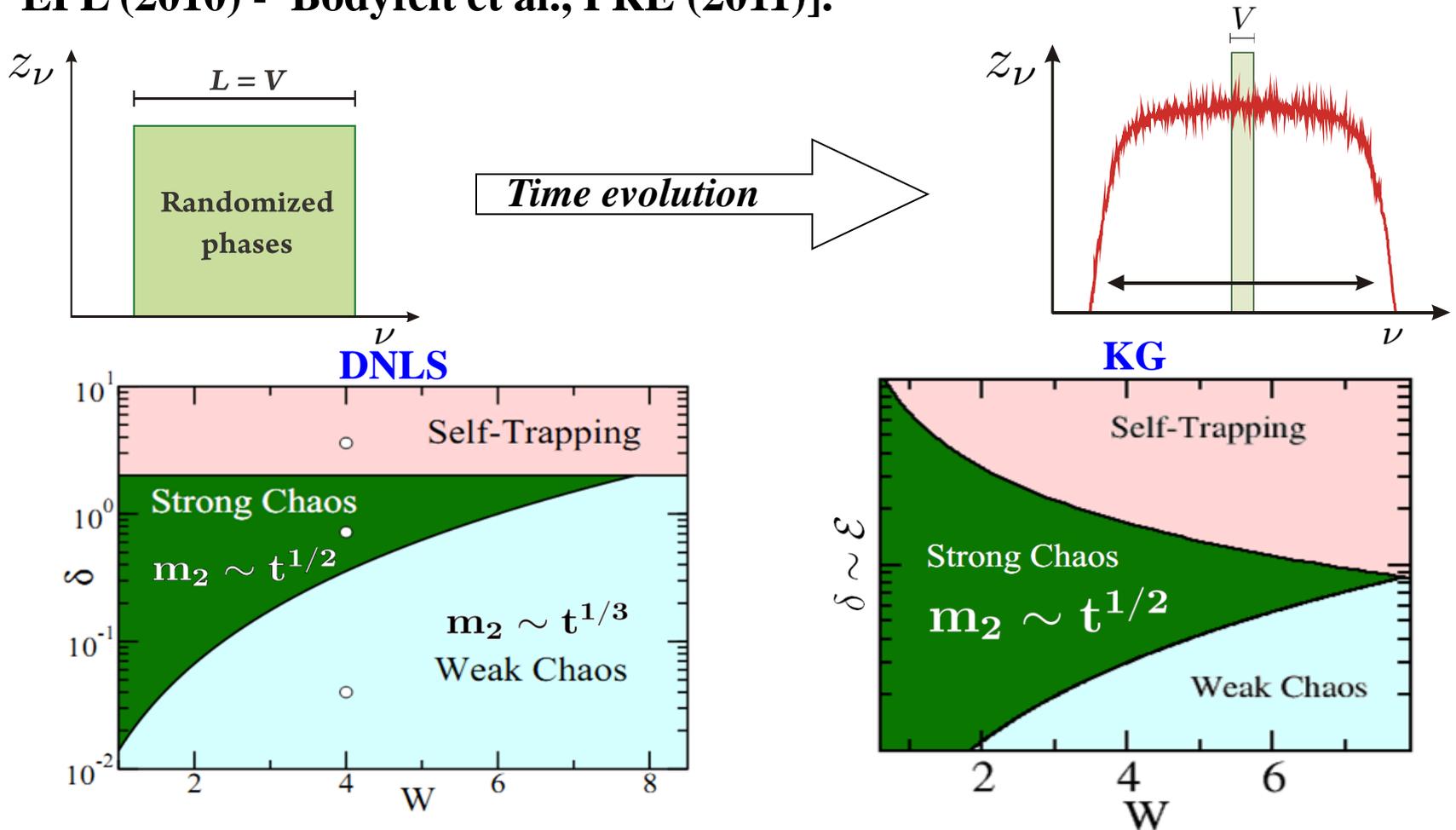
S. et al., PRE (2009)

KG: Different spreading regimes



Crossover from strong to weak chaos

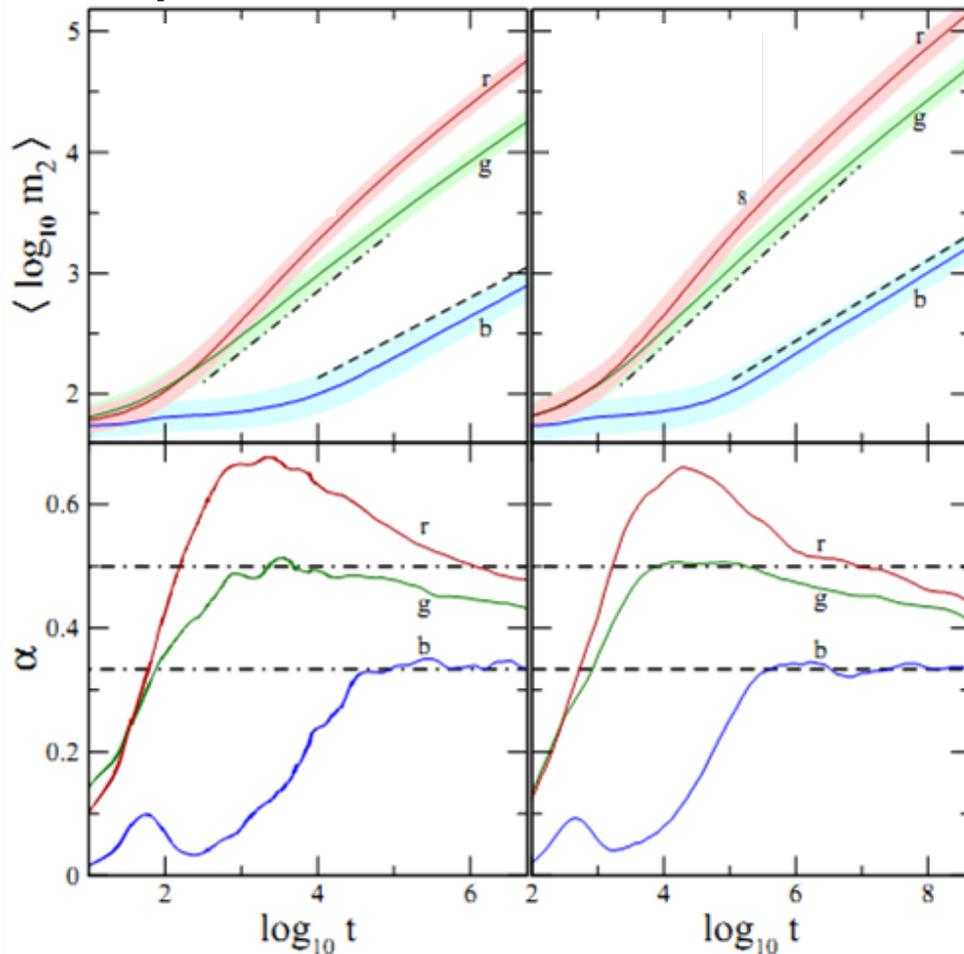
We consider **compact initial wave packets of width $L=V$** [Laptyeva et al., EPL (2010) - Bodyfelt et al., PRE (2011)].



Crossover from strong to weak chaos (block excitations)

DNLS $\beta = 0.04, 0.72, 3.6$ KG $E = 0.01, 0.2, 0.75$

W=4



Average over 1000 realizations!

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

$\alpha = 1/2$

$\alpha = 1/3$

Laptyeva et al., EPL (2010)

Bodyfelt et al., PRE (2011)

Lyapunov Exponents (LEs)

Roughly speaking, the Lyapunov exponents of a given orbit characterize the **mean exponential rate of divergence** of trajectories surrounding it.

Consider an orbit in the $2N$ -dimensional phase space with **initial condition $\mathbf{x}(0)$** and an **initial deviation vector from it $\mathbf{v}(0)$** . Then the mean exponential rate of divergence is:

$$\text{m L C E} = \lambda_1 = \lim_{t \rightarrow \infty} \frac{1}{t} \ln \frac{\|\vec{\mathbf{v}}(t)\|}{\|\vec{\mathbf{v}}(0)\|}$$

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

$\lambda_1 \neq 0 \rightarrow$ Chaotic motion

Autonomous Hamiltonian systems

Let us consider an **N degree of freedom** autonomous Hamiltonian systems of the form:

$$H(\vec{q}, \vec{p}) = \frac{1}{2} \sum_{i=1}^N p_i^2 + V(\vec{q})$$

As an example, we consider the Hénon-Heiles system:

$$H_2 = \frac{1}{2}(p_x^2 + p_y^2) + \frac{1}{2}(x^2 + y^2) + x^2y - \frac{1}{3}y^3$$

Hamilton equations of motion:

$$\left\{ \begin{array}{l} \dot{x} = p_x \\ \dot{y} = p_y \\ \dot{p}_x = -x - 2xy \\ \dot{p}_y = y^2 - x^2 - y \end{array} \right.$$

Variational equations:

$$\left\{ \begin{array}{l} \dot{\delta x} = \delta p_x \\ \dot{\delta y} = \delta p_y \\ \dot{\delta p}_x = -(1 + 2y)\delta x - 2x\delta y \\ \dot{\delta p}_y = -2x\delta x + (-1 + 2y)\delta y \end{array} \right.$$

Symplectic Integrators (SIs)

Formally the solution of the Hamilton equations of motion can be written as:

$$\frac{d\vec{X}}{dt} = \{H, \vec{X}\} = L_H \vec{X} \Rightarrow \vec{X}(t) = \sum_{n \geq 0} \frac{t^n}{n!} L_H^n \vec{X} = e^{tL_H} \vec{X}$$

where \vec{X} is the full coordinate vector and L_H the Poisson operator:

$$L_H f = \sum_{j=1}^N \left\{ \frac{\partial H}{\partial p_j} \frac{\partial f}{\partial q_j} - \frac{\partial H}{\partial q_j} \frac{\partial f}{\partial p_j} \right\}$$

If the Hamiltonian H can be split into two integrable parts as $H=A+B$, a symplectic scheme for integrating the equations of motion from time t to time $t+\tau$ consists of approximating the operator $e^{\tau L_H}$ by

$$e^{\tau L_H} = e^{\tau(L_A + L_B)} = \prod_{i=1}^j e^{c_i \tau L_A} e^{d_i \tau L_B} + O(\tau^{n+1})$$

for appropriate values of constants c_i, d_i . This is an integrator of order n .

So the dynamics over an integration time step τ is described by a series of successive acts of Hamiltonians A and B .

Symplectic Integrator SABA₂C

The operator $e^{\tau L_H}$ can be approximated by the symplectic integrator [Laskar & Robutel, Cel. Mech. Dyn. Astr. (2001)]:

$$S A B A_2 = e^{c_1 \tau L_A} e^{d_1 \tau L_B} e^{c_2 \tau L_A} e^{d_1 \tau L_B} e^{c_1 \tau L_A}$$

with $c_1 = \frac{1}{2} - \frac{\sqrt{3}}{6}$, $c_2 = \frac{\sqrt{3}}{3}$, $d_1 = \frac{1}{2}$.

The integrator has only **small positive steps** and its **error is of order 2**.

In the case where **A is quadratic in the momenta and B depends only on the positions** the method can be improved by introducing a corrector C, having a small negative step:

$$C = e^{-\tau^3 \frac{c}{2} L_{\{\{A,B\},B\}}}$$

with $c = \frac{2 - \sqrt{3}}{24}$.

Thus the full integrator scheme becomes: **SABAC₂ = C (SABA₂) C** and its **error is of order 4**.

Tangent Map (TM) Method

Use symplectic integration schemes for the whole set of equations (S. & Gerlach, PRE (2010))

We apply the **SABAC₂** integrator scheme to the Hénon-Heiles system by using **the splitting**:

$$A = \frac{1}{2}(p_x^2 + p_y^2), \quad B = \frac{1}{2}(x^2 + y^2) + x^2y - \frac{1}{3}y^3,$$

with a **corrector term** which corresponds to the Hamiltonian function:

$$C = \{\{A, B\}, B\} = (x + 2xy)^2 + (x^2 - y^2 + y)^2$$

We approximate the dynamics by **the act of Hamiltonians A, B and C**, which correspond to the symplectic maps:

$$e^{\tau L_A} : \begin{cases} x' = x + p_x \tau \\ y' = y + p_y \tau \\ p'_x = p_x \\ p'_y = p_y \end{cases}, \quad e^{\tau L_C} : \begin{cases} x' = x \\ y' = y \\ p'_x = p_x - 2x(1 + 2x^2 + 6y + 2y^2)\tau \\ p'_y = p_y - 2(y - 3y^2 + 2y^3 + 3x^2 + 2x^2y)\tau \end{cases}$$
$$e^{\tau L_B} : \begin{cases} x' = x \\ y' = y \\ p'_x = p_x - x(1 + 2y)\tau \\ p'_y = p_y + (y^2 - x^2 - y)\tau \end{cases},$$

Tangent Map (TM) Method

Let $\vec{u} = (x, y, p_x, p_y, \delta x, \delta y, \delta p_x, \delta p_y)$

The system of the Hamilton's equations of motion and the variational equations is split into two integrable systems which correspond to Hamiltonians A and B.

$$\begin{array}{l}
 \dot{x} = p_x \\
 \dot{y} = p_y \\
 \dot{p}_x = -x - 2xy \\
 \dot{p}_y = y^2 - x^2 - y \\
 \\
 \dot{\delta x} = \delta p_x \\
 \dot{\delta y} = \delta p_y \\
 \dot{\delta p}_x = -(1 + 2y)\delta x - 2x\delta y \\
 \dot{\delta p}_y = -2x\delta x + (-1 + 2y)\delta y
 \end{array}
 \xrightarrow{A(\vec{p})}
 \left. \begin{array}{l}
 \dot{x} = p_x \\
 \dot{y} = p_y \\
 \dot{p}_x = 0 \\
 \dot{p}_y = 0 \\
 \dot{\delta x} = \delta p_x \\
 \dot{\delta y} = \delta p_y \\
 \dot{\delta p}_x = 0 \\
 \dot{\delta p}_y = 0
 \end{array} \right\}
 \Rightarrow \frac{d\vec{u}}{dt} = L_{AV}\vec{u} \Rightarrow e^{\tau L_{AV}} : \left\{ \begin{array}{l}
 x' = x + p_x\tau \\
 y' = y + p_y\tau \\
 px' = p_x \\
 py' = p_y \\
 \delta x' = \delta x + \delta p_x\tau \\
 \delta y' = \delta y + \delta p_y\tau \\
 \delta p'_x = \delta p_x \\
 \delta p'_y = \delta p_y
 \end{array} \right.$$

$$\left. \begin{array}{l}
 \dot{x} = 0 \\
 \dot{y} = 0 \\
 \dot{p}_x = -x - 2xy \\
 \dot{p}_y = y^2 - x^2 - y \\
 \dot{\delta x} = 0 \\
 \dot{\delta y} = 0 \\
 \dot{\delta p}_x = -(1 + 2y)\delta x - 2x\delta y \\
 \dot{\delta p}_y = -2x\delta x + (-1 + 2y)\delta y
 \end{array} \right\}
 \xrightarrow{B(\vec{q})}
 \frac{d\vec{u}}{dt} = L_{BV}\vec{u} \Rightarrow e^{\tau L_{BV}} : \left\{ \begin{array}{l}
 x' = x \\
 y' = y \\
 p'_x = p_x - x(1 + 2y)\tau \\
 p'_y = p_y + (y^2 - x^2 - y)\tau \\
 \delta x' = \delta x \\
 \delta y' = \delta y \\
 \delta p'_x = \delta p_x - [(1 + 2y)\delta x + 2x\delta y]\tau \\
 \delta p'_y = \delta p_y + [-2x\delta x + (-1 + 2y)\delta y]\tau
 \end{array} \right.$$

Tangent Map (TM) Method

Any symplectic integration scheme used for solving the Hamilton equations of motion, which involves the act of Hamiltonians A and B, can be extended in order to integrate simultaneously the variational equations [S. & Gerlach, PRE (2010) – Gerlach & S., Discr. Cont. Dyn. Sys. (2011) – Gerlach et al., IJBC (2012)].

$$\begin{array}{ccc}
 e^{\tau L_A} : \begin{cases} x' = x + p_x \tau \\ y' = y + p_y \tau \\ p'_x = p_x \\ p'_y = p_y \end{cases} & \xrightarrow{\quad} & e^{\tau L_{AV}} : \begin{cases} x' = x + p_x \tau \\ y' = y + p_y \tau \\ px' = p_x \\ py' = p_y \\ \delta x' = \delta x + \delta p_x \tau \\ \delta y' = \delta y + \delta p_y \tau \\ \delta p'_x = \delta p_x \\ \delta p'_y = \delta p_y \end{cases} \\
 \\
 e^{\tau L_B} : \begin{cases} x' = x \\ y' = y \\ p'_x = p_x - x(1 + 2y)\tau \\ p'_y = p_y + (y^2 - x^2 - y)\tau \end{cases} & \xrightarrow{\quad} & e^{\tau L_{BV}} : \begin{cases} x' = x \\ y' = y \\ p'_x = p_x - x(1 + 2y)\tau \\ p'_y = p_y + (y^2 - x^2 - y)\tau \\ \delta x' = \delta x \\ \delta y' = \delta y \\ \delta p'_x = \delta p_x - [(1 + 2y)\delta x + 2x\delta y]\tau \\ \delta p'_y = \delta p_y + [-2x\delta x + (-1 + 2y)\delta y]\tau \end{cases} \\
 \\
 e^{\tau L_C} : \begin{cases} x' = x \\ y' = y \\ p'_x = p_x - 2x(1 + 2x^2 + 6y + 2y^2)\tau \\ p'_y = p_y - 2(y - 3y^2 + 2y^3 + 3x^2 + 2x^2y)\tau \end{cases} & \xrightarrow{\quad} & e^{\tau L_{CV}} : \begin{cases} x' = x \\ y' = y \\ p'_x = p_x - 2x(1 + 2x^2 + 6y + 2y^2)\tau \\ p'_y = p_y - 2(y - 3y^2 + 2y^3 + 3x^2 + 2x^2y)\tau \\ \delta x' = \delta x \\ \delta y' = \delta y \\ \delta p'_x = \delta p_x - 2[(1 + 6x^2 + 2y^2 + 6y)\delta x + 2x(3 + 2y)\delta y]\tau \\ \delta p'_y = \delta p_y - 2[2x(3 + 2y)\delta x + (1 + 2x^2 + 6y^2 - 6y)\delta y]\tau \end{cases}
 \end{array}$$

The KG model

We apply the **SABAC₂** integrator scheme to the KG Hamiltonian by using the **splitting**:

$$H_K = \sum_{l=1}^N \left(\underbrace{\frac{p_l^2}{2}}_A + \underbrace{\frac{\tilde{\varepsilon}_l}{2} u_l^2 + \frac{1}{4} u_l^4 + \frac{1}{2W} (u_{l+1} - u_l)^2}_B \right)$$

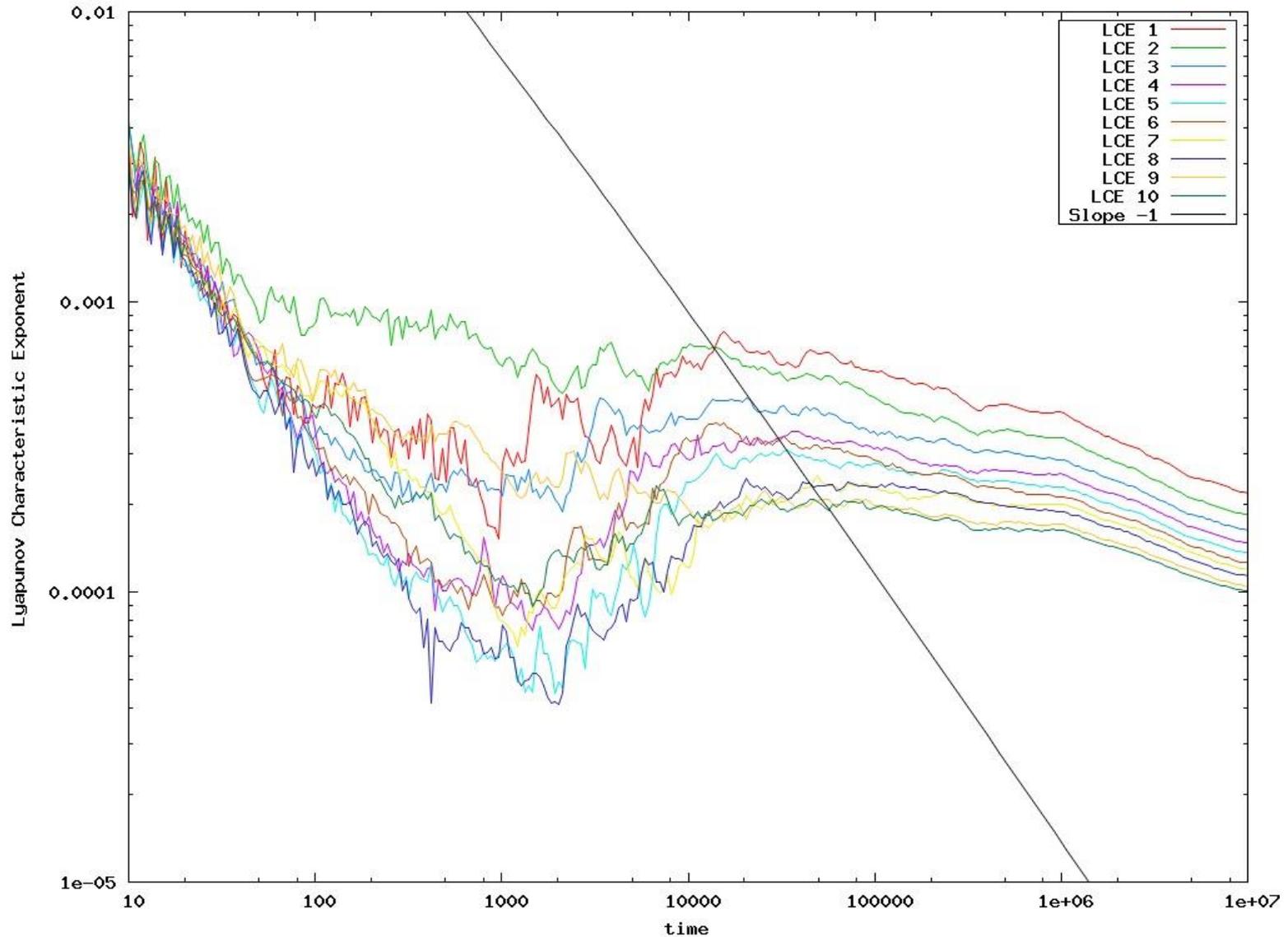
$$e^{\tau L_A}: \begin{cases} u'_l = p_l \tau + u_l \\ p'_l = p_l, \end{cases}$$

$$e^{\tau L_B}: \begin{cases} u'_l = u_l \\ p'_l = \left[-u_l(\tilde{\varepsilon}_l + u_l^2) + \frac{1}{W}(u_{l-1} + u_{l+1} - 2u_l) \right] \tau + p_l, \end{cases}$$

with a **corrector term** which corresponds to the Hamiltonian function:

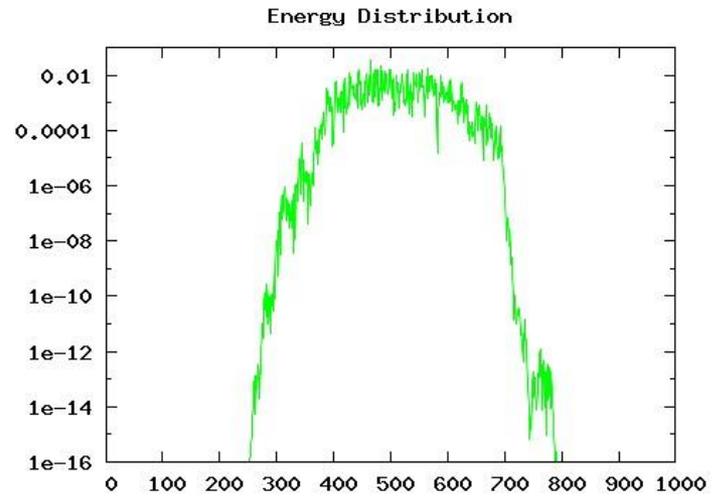
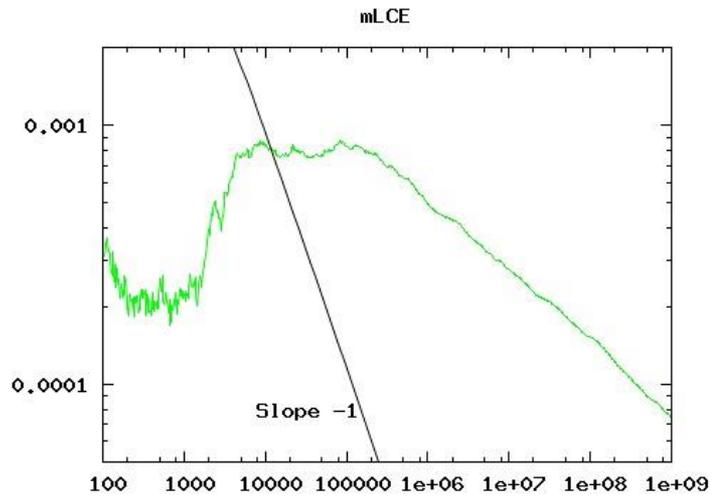
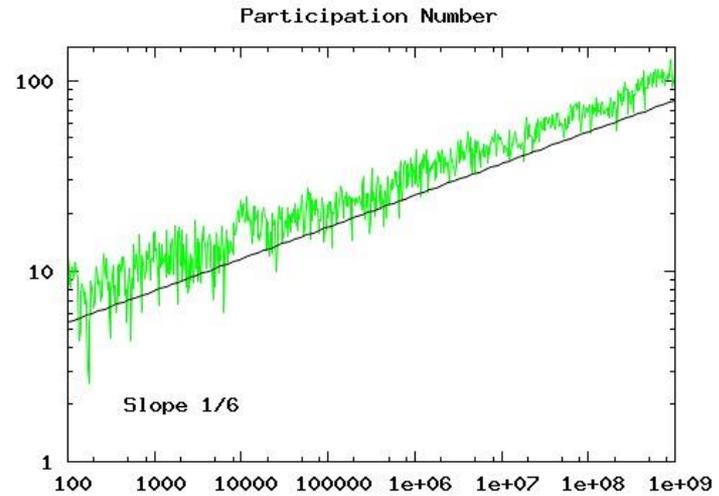
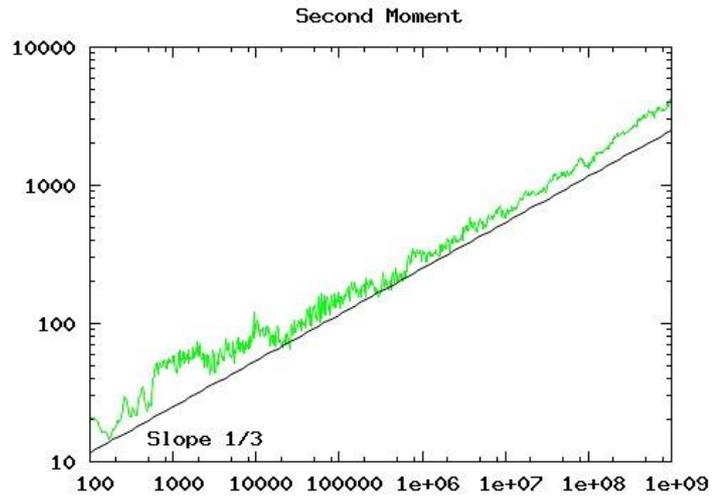
$$C = \{ \{A, B\}, B \} = \sum_{l=1}^N \left[u_l (\tilde{\varepsilon}_l + u_l^2) - \frac{1}{W} (u_{l-1} + u_{l+1} - 2u_l) \right]^2.$$

KG: LEs for single site excitations ($E=0.4$)



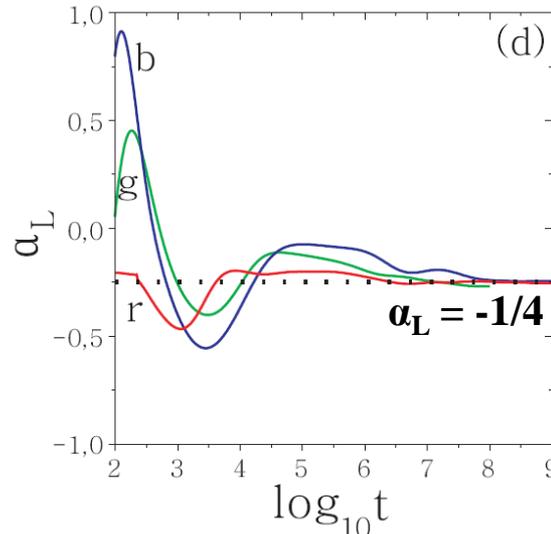
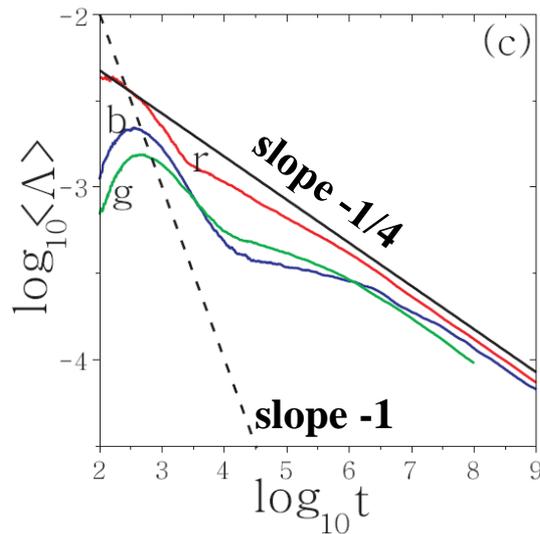
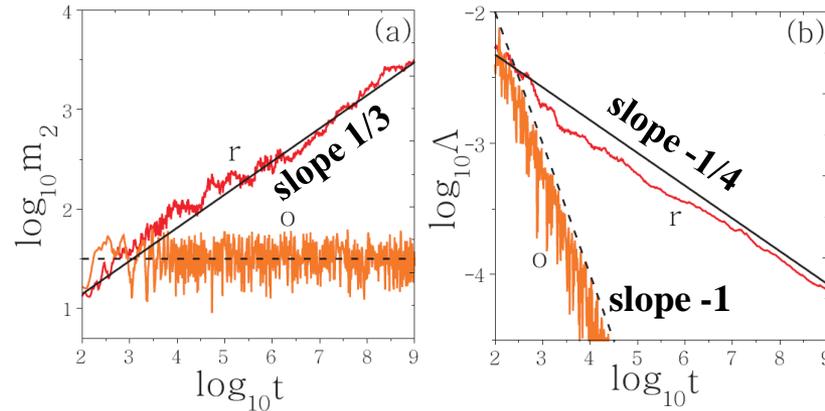
KG: Weak Chaos ($E=0.4$)

$t = 1000000000.00$



KG: Weak Chaos

Individual runs
Linear case
E=0.4, W=4



$$\alpha_L = \frac{d(\log \langle \Lambda \rangle)}{d \log t}$$

Average over 50 realizations

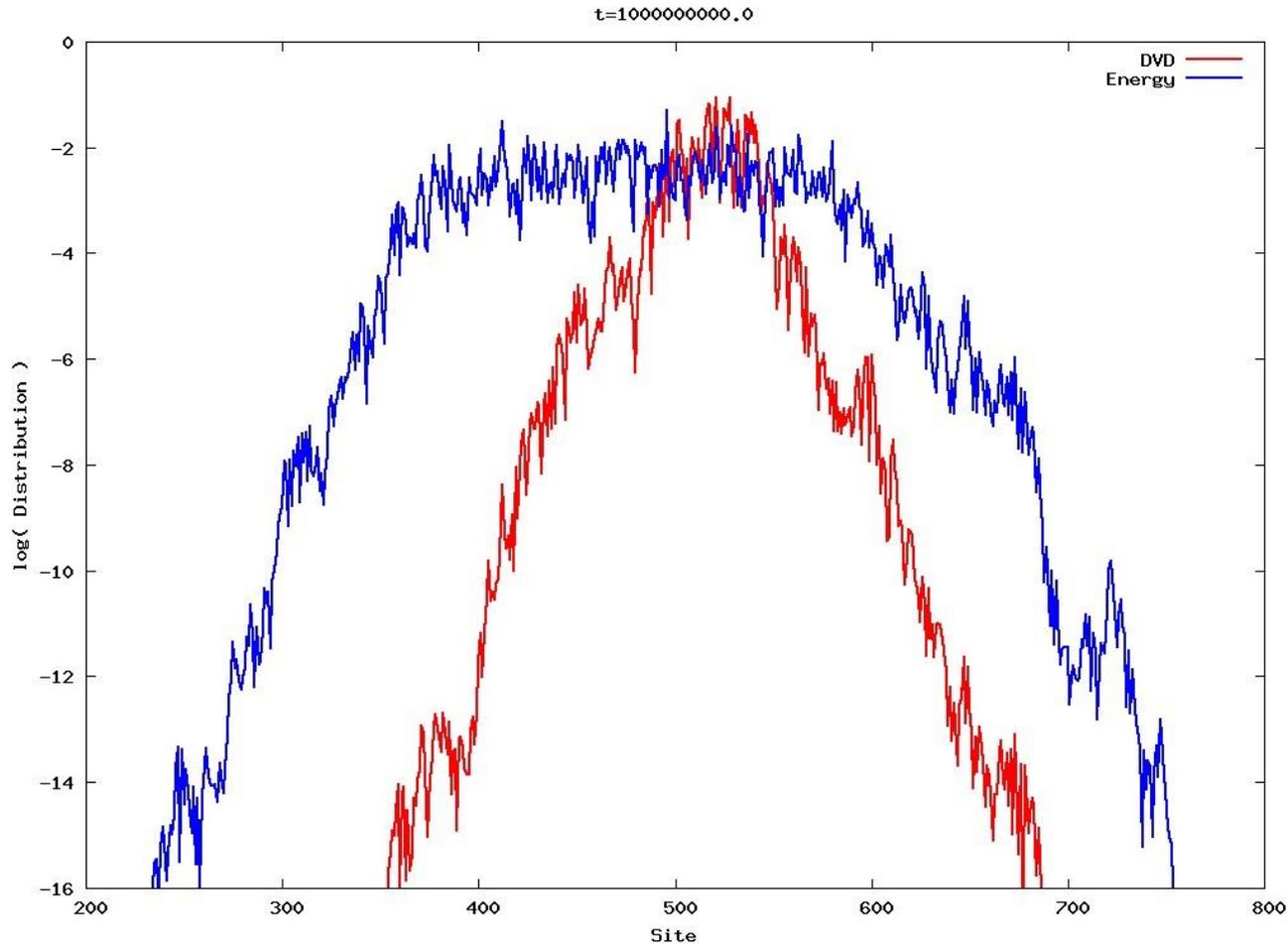
Single site excitation E=0.4, W=4

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

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

S. et al., PRL (2013)

Deviation Vector Distributions (DVDs)

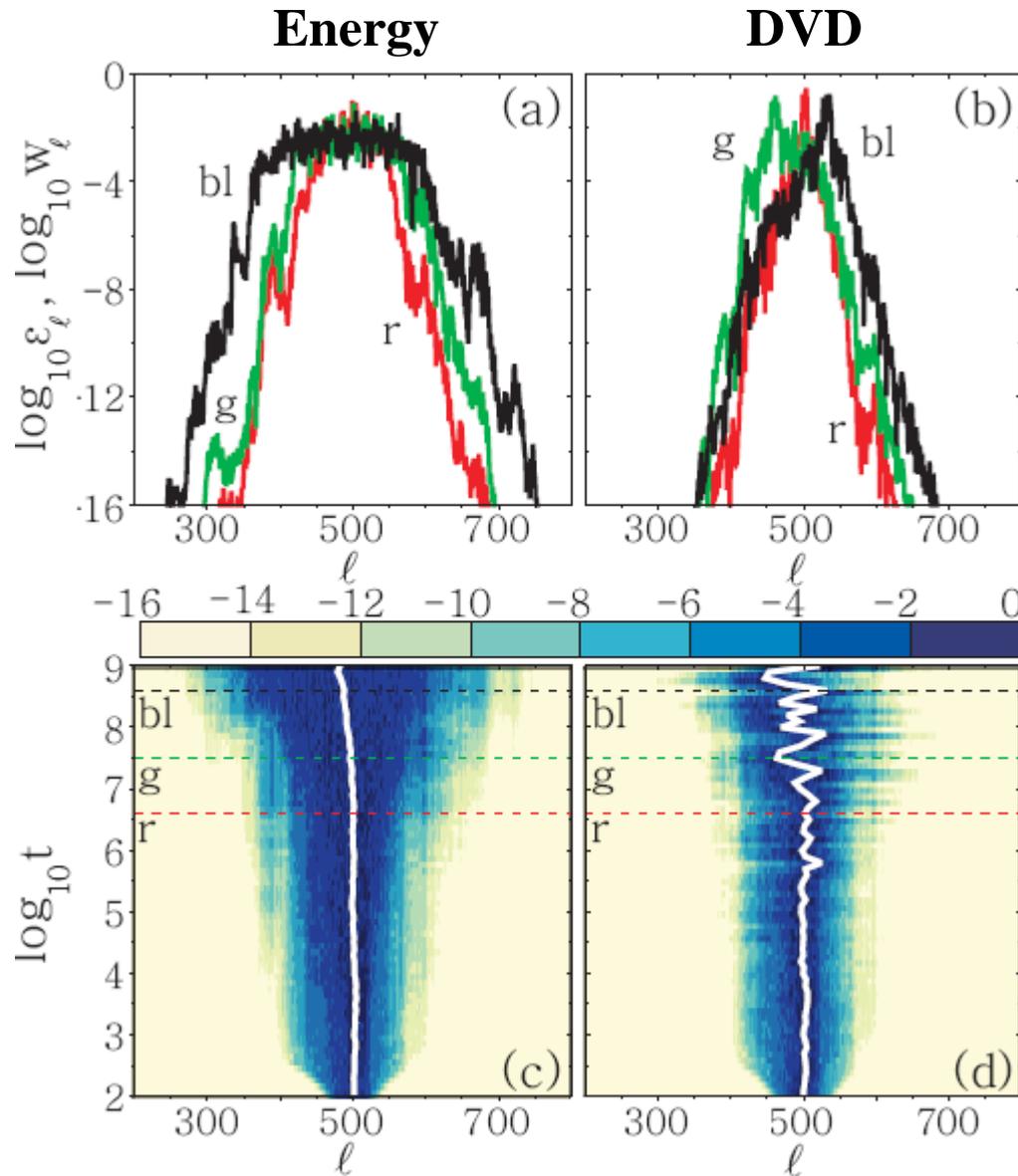


Deviation vector:

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

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

Deviation Vector Distributions (DVDs)



Individual run
 $E=0.4$, $W=4$

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

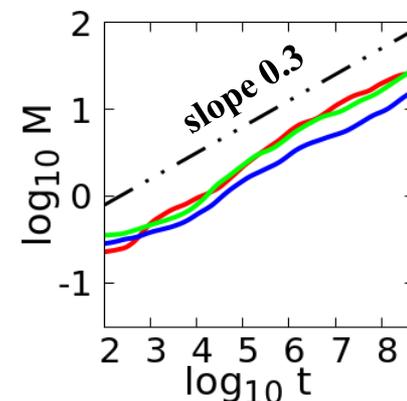
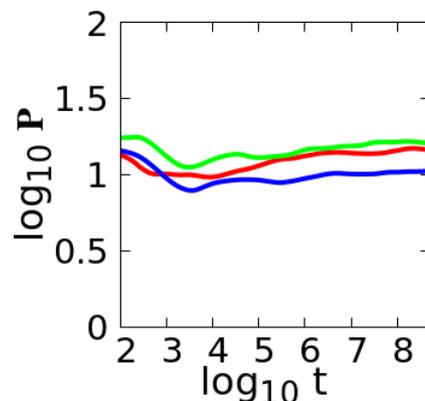
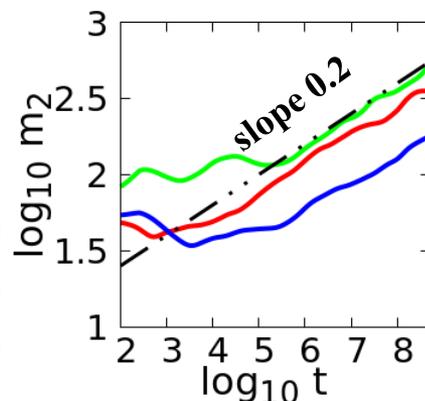
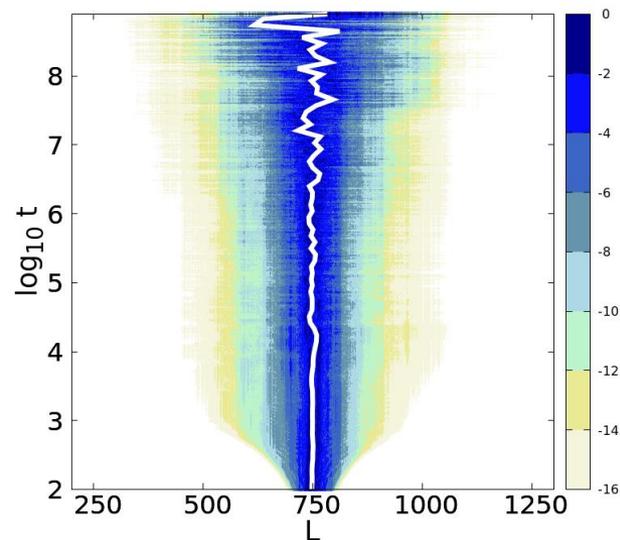
DVDs – Weak chaos

Individual run, $L=37$,
 $E=0.37$, $W=3$

Single site excitation $E=0.4$, $W=4$

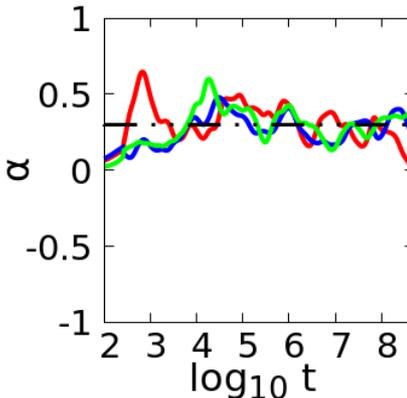
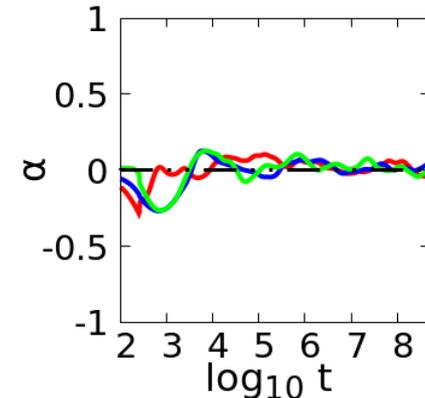
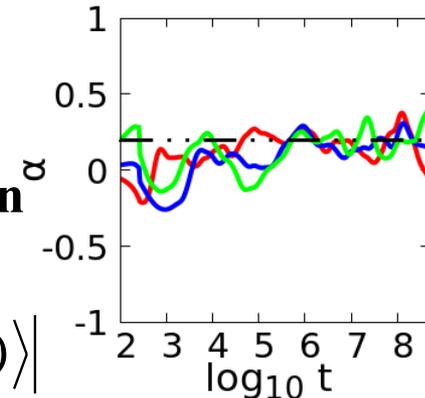
Block excitation (21 sites) $E=0.21$, $W=4$

Block excitation (37 sites) $E=0.37$, $W=3$

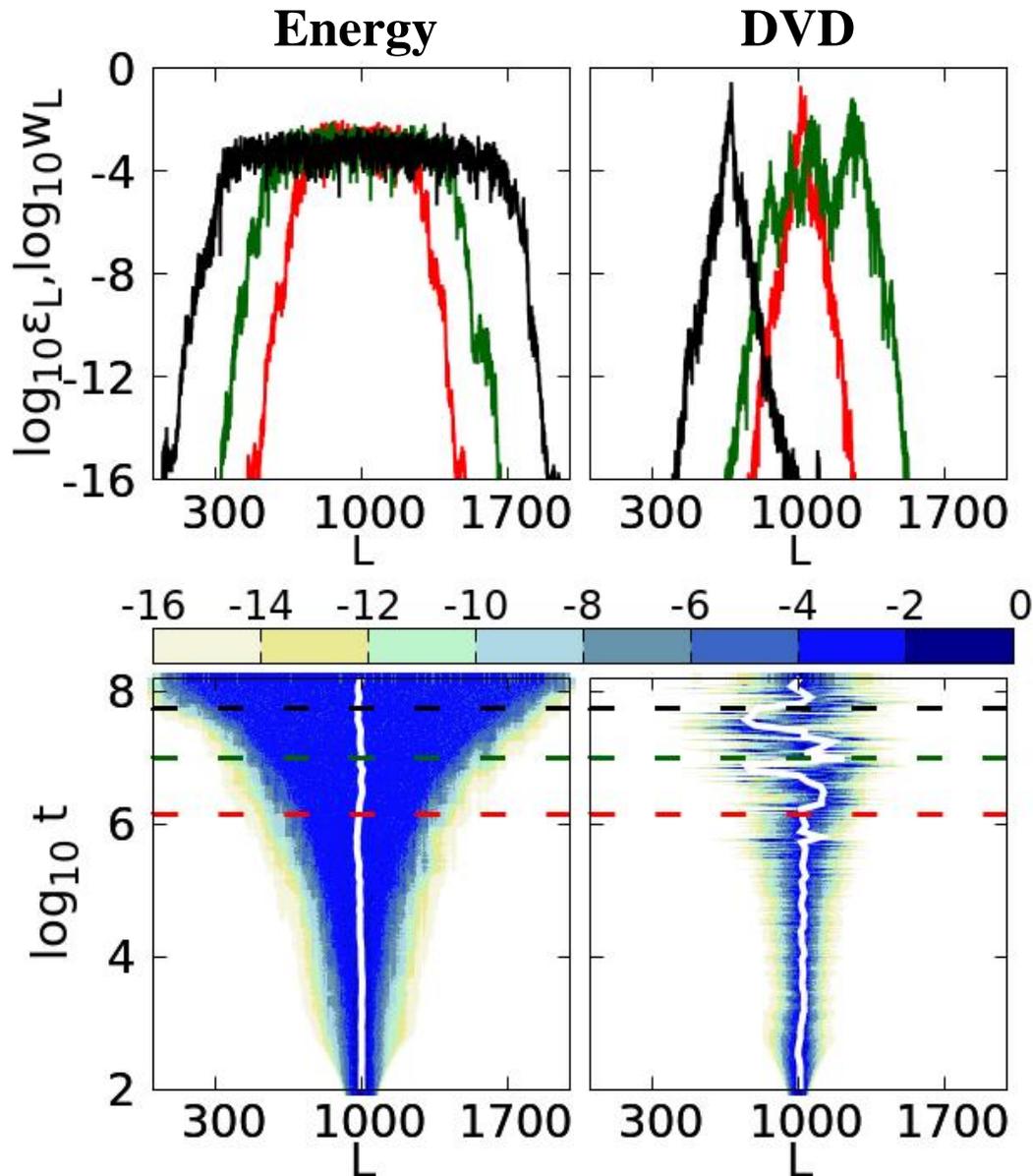


Maximum absolute
 deviation of DVD's mean
 position

$$M(t) = \max_{[t, t+\Delta t]} \left| \bar{w}(t) - \langle \bar{w}(t) \rangle \right|$$



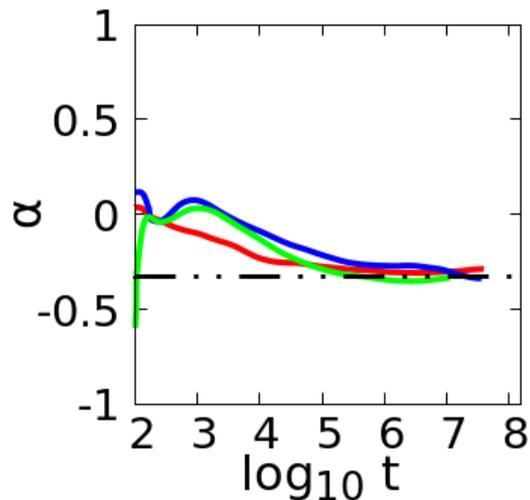
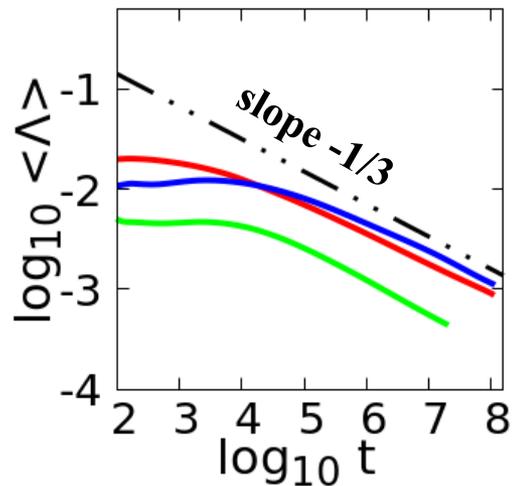
KG: Strong chaos



Individual run
 $L=83, E=8.3, W=3$

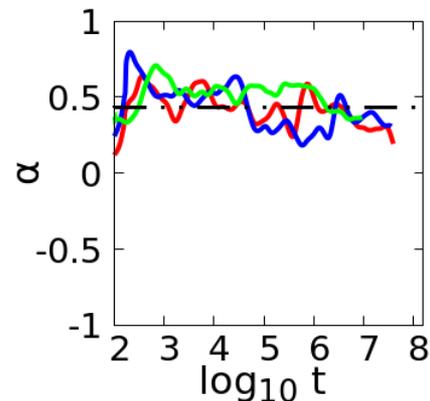
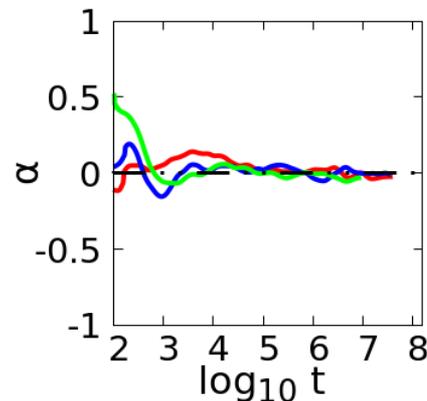
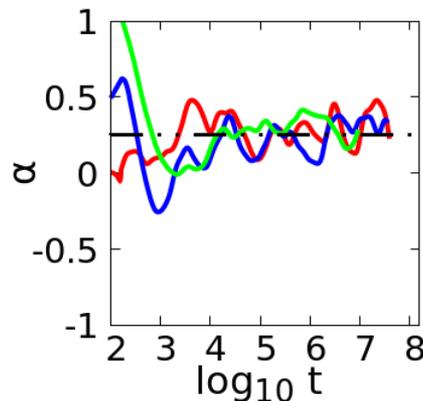
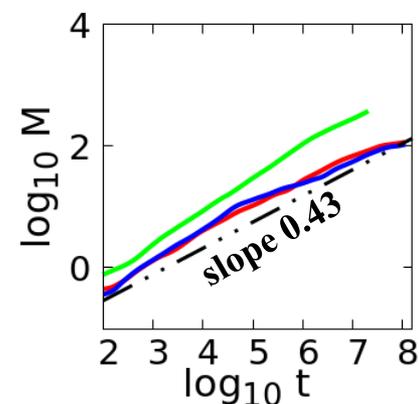
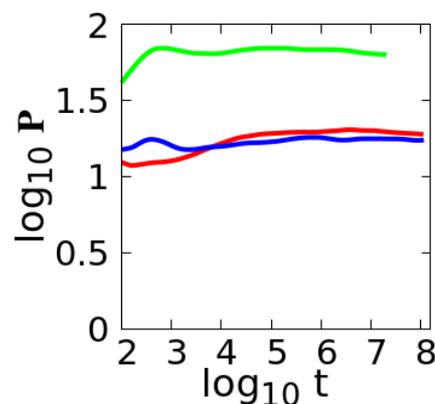
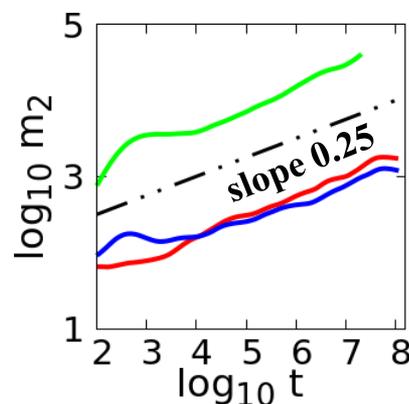
KG: Strong chaos

Lyapunov exponent



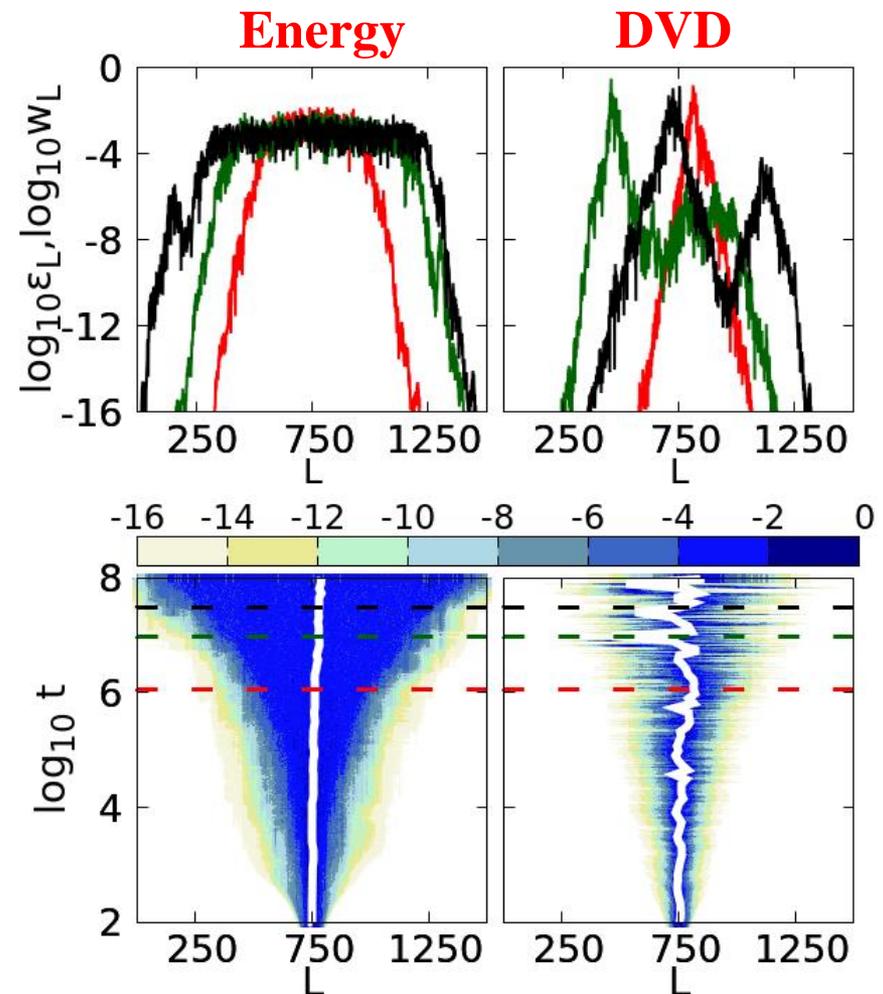
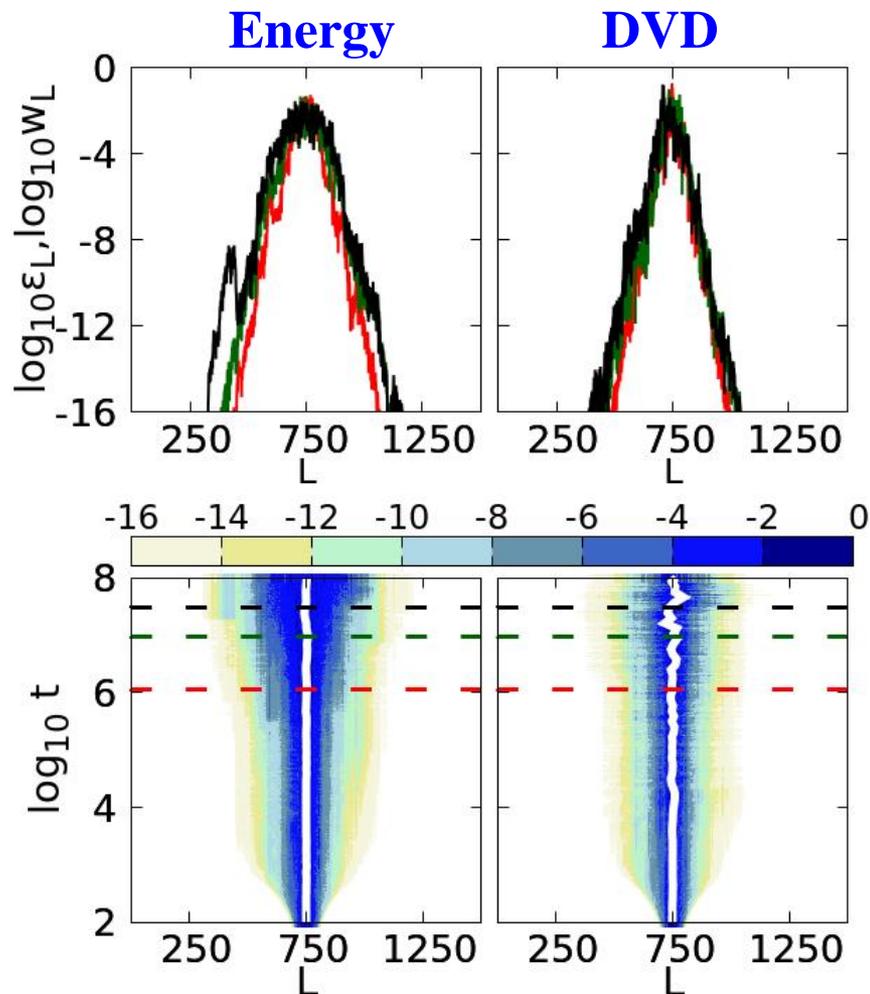
Block excitation (37 sites) $E=7.4, W=3$
Block excitation (83 sites) $E=8.3, W=3$
Block excitation (330 sites) $E=33.0, W=1$

Characteristics of DVD

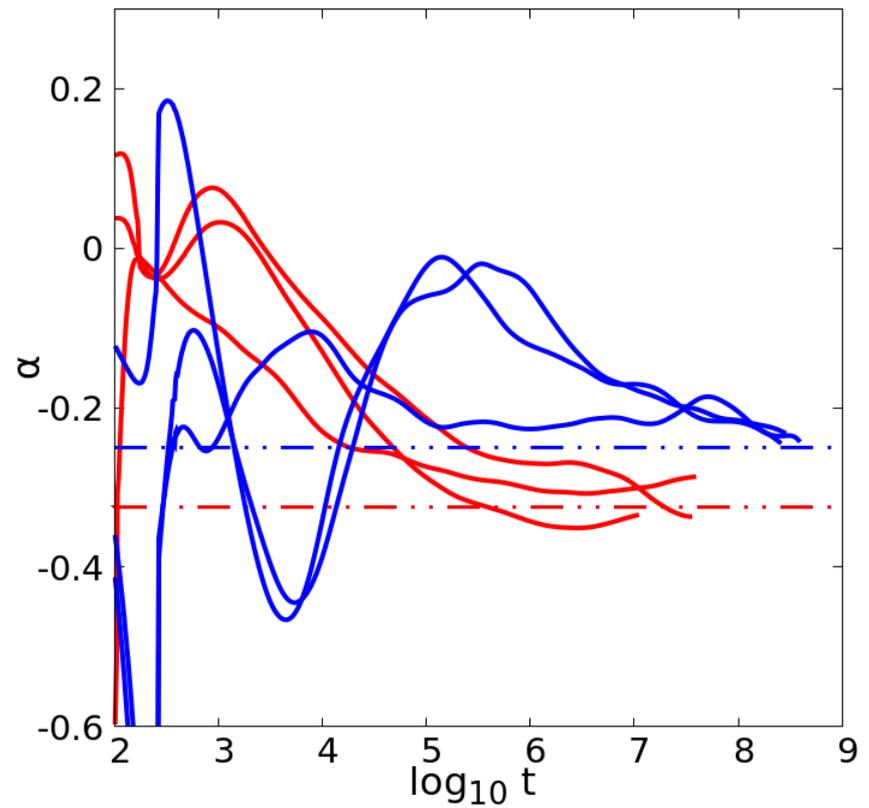
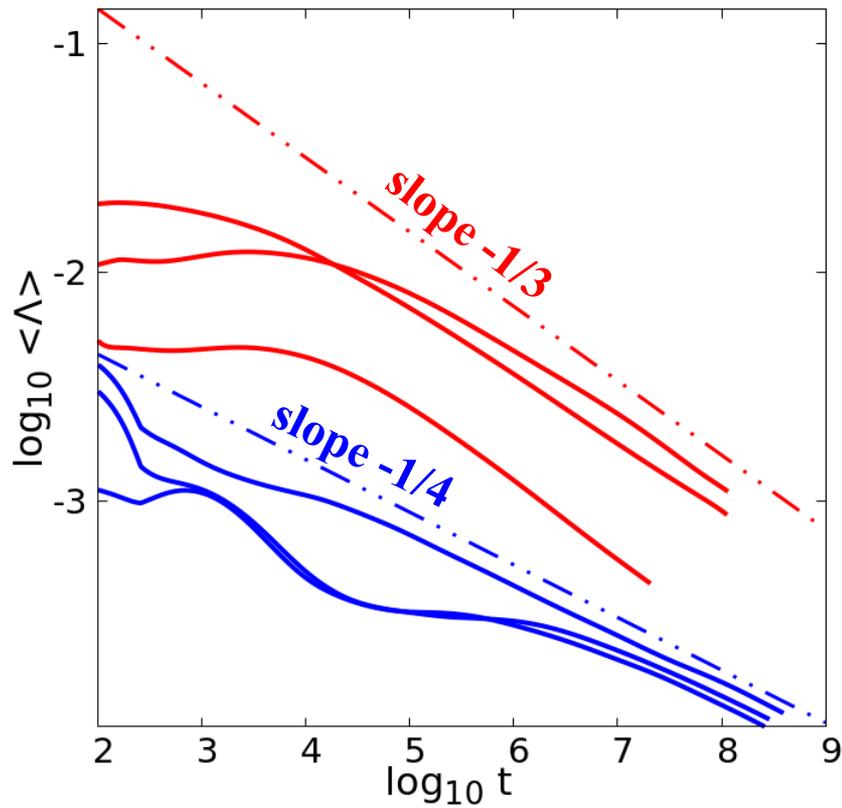


Weak and Strong chaos

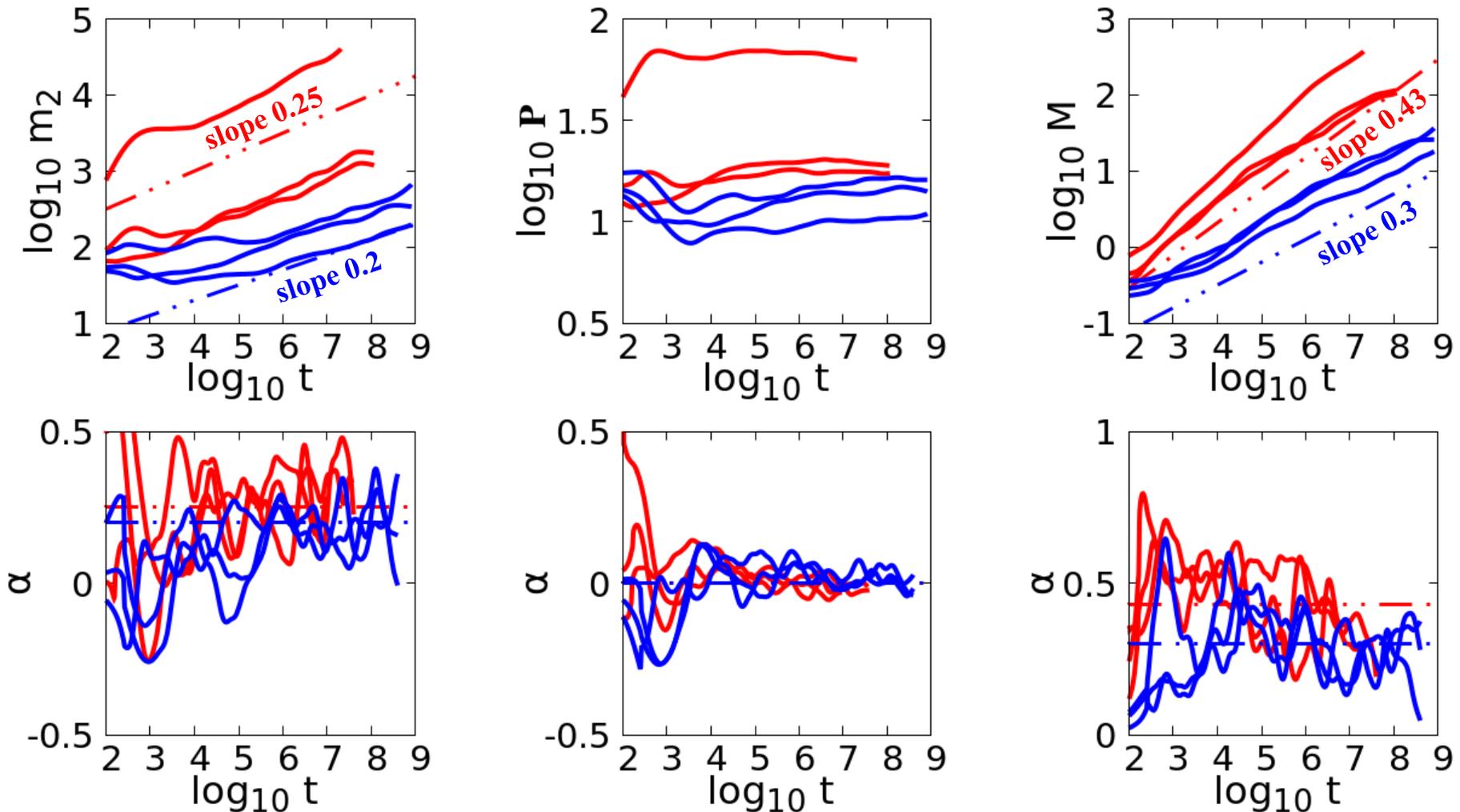
Same disordered realization, $L=37$, $W=3$, $E=0.37$ and $E=7.4$



Weak and Strong chaos: LEs



Weak and Strong chaos: DVDs



For both cases the DVD's participation number remains practically constant.

Summary

- We presented **three different dynamical behaviors** for wave packet spreading in 1d nonlinear disordered lattices (KG and DNLS models):
 - ✓ **Weak Chaos Regime:** $\delta < d$, $m_2 \sim t^{1/3}$
 - ✓ **Intermediate Strong Chaos Regime:** $d < \delta < \Delta$, $m_2 \sim t^{1/2} \rightarrow m_2 \sim t^{1/3}$
 - ✓ **Selftrapping Regime:** $\delta > \Delta$
- **KG model**
 - ✓ **Lyapunov exponent computations show that:**
 - Chaos not only exists, but also persists.
 - Slowing down of chaos does not cross over to regular dynamics.
 - ✓ **mLEs and DVDs show different behaviors for the weak and the strong chaos regimes.**
 - ✓ **Chaotic hot spots meander through the system, supporting a homogeneity of chaos inside the wave packet.**
- **The behavior of DVDs can provide important information about the chaotic behavior of a dynamical system.**

A ...shameless promotion

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