Chaos in disordered nonlinear lattices

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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 and DNLS models**
  - ✓ **Lyapunov exponents**
  - ✓ **Deviation Vector Distributions**
- **Summary**

The Klein – Gordon (KG) model

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

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) $A_{\nu,l}$ - 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:

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

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 $S = \sum_l \left|\psi_l\right|^2$ of the wave packet.

Distribution characterization

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

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

, where A_ν is the amplitude

of the νth NM (KG) or norm distributions (DNLS).

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

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 $P=N$.

Different Dynamical Regimes

Three expected evolution regimes [Flach, Chem. Phys (2010) - S. & Flach, PRE (2010) - Laptyeva 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: $d < \delta < \Delta$, $m_2 \sim t^{1/2} \longrightarrow m_2 \sim t^{1/3}$

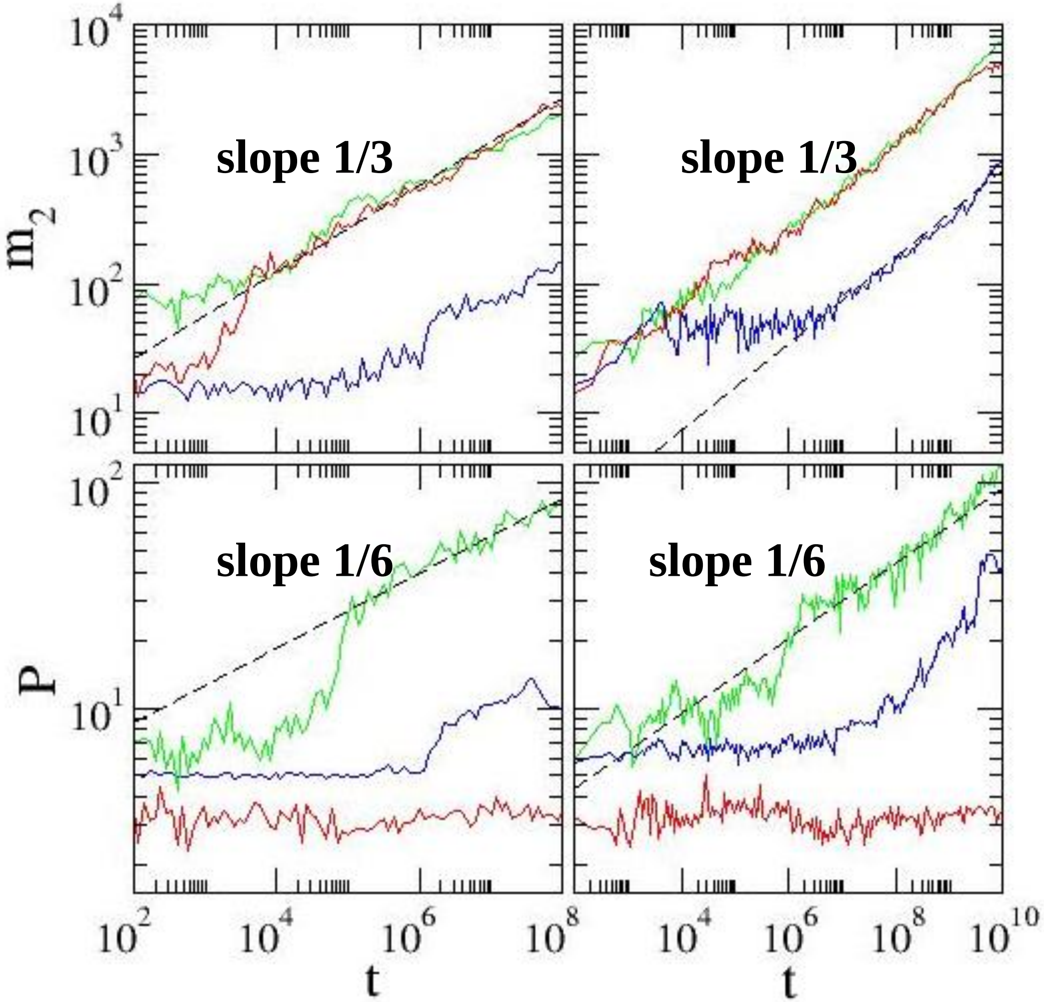
Almost all NMs in the packet are resonantly interacting. Wave packets initially spread faster and eventually enter the weak chaos regime.

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, β= 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:

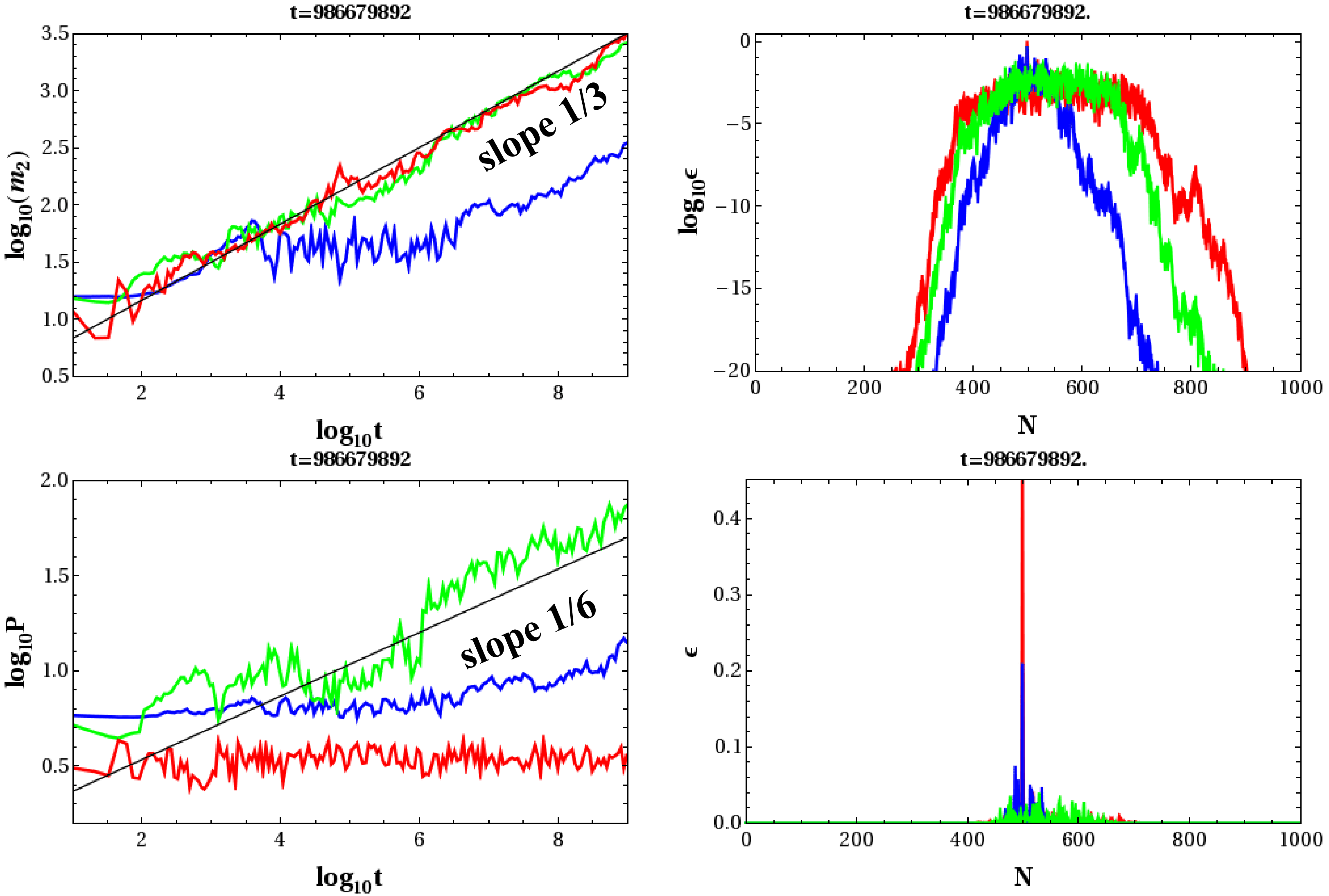
α=0.33±0.05 (KG)

α=0.33±0.02 (DLNS)

Flach et al., PRL (2009)

S. et al., PRE (2009)

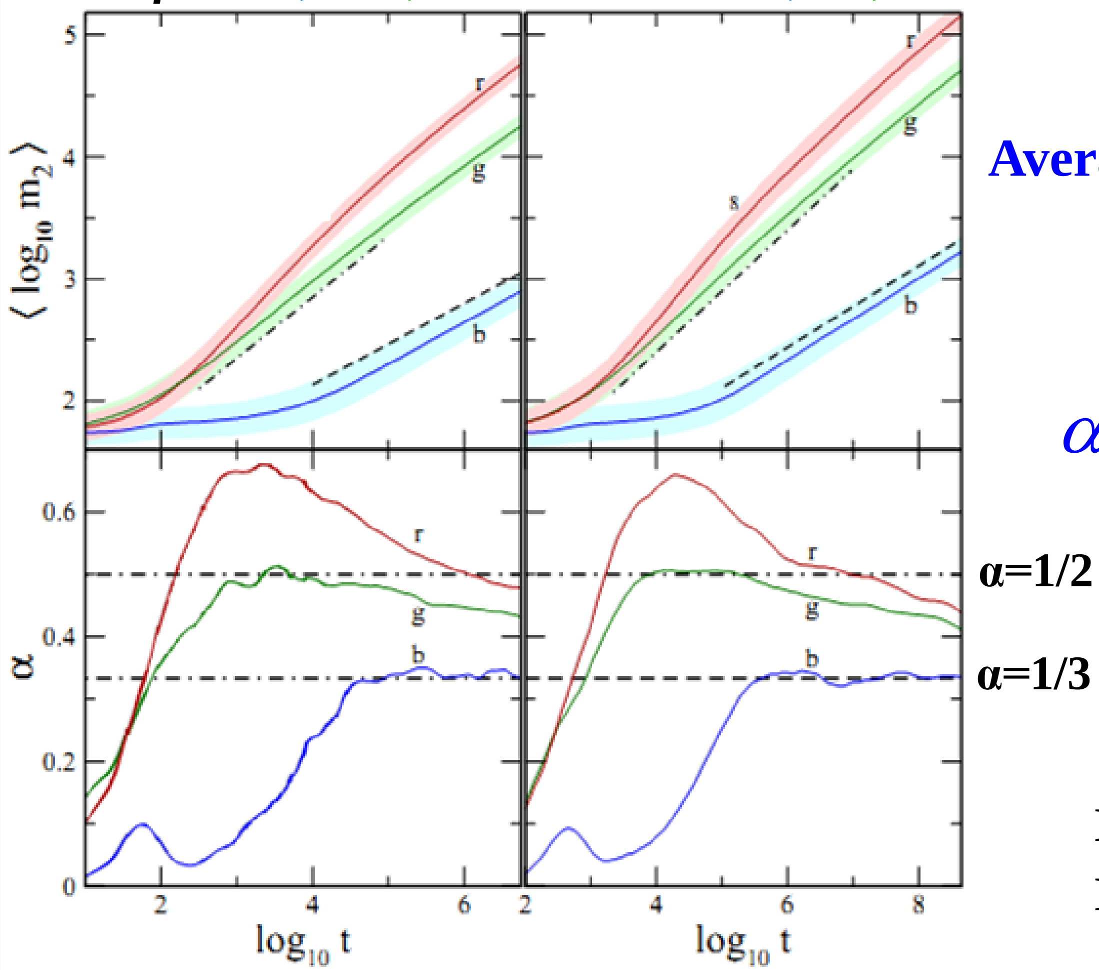
KG: Different spreading regimes



Crossover from strong to weak chaos (block excitations)

DNLS β= 0.04, 0.72, 3.6 KG E= 0.01, 0.2, 0.75

W=4



Average over 1000 realizations!

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

Laptyeva et al., EPL (2010)

Bodyfelt et al., PRE (2011)

Symplectic integration

We apply the 2-part splitting integrator ABA864 [Blanes et al., Appl. Num. Math. (2013) – Senyange & S., EPJ ST (2018)] to the KG model:

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

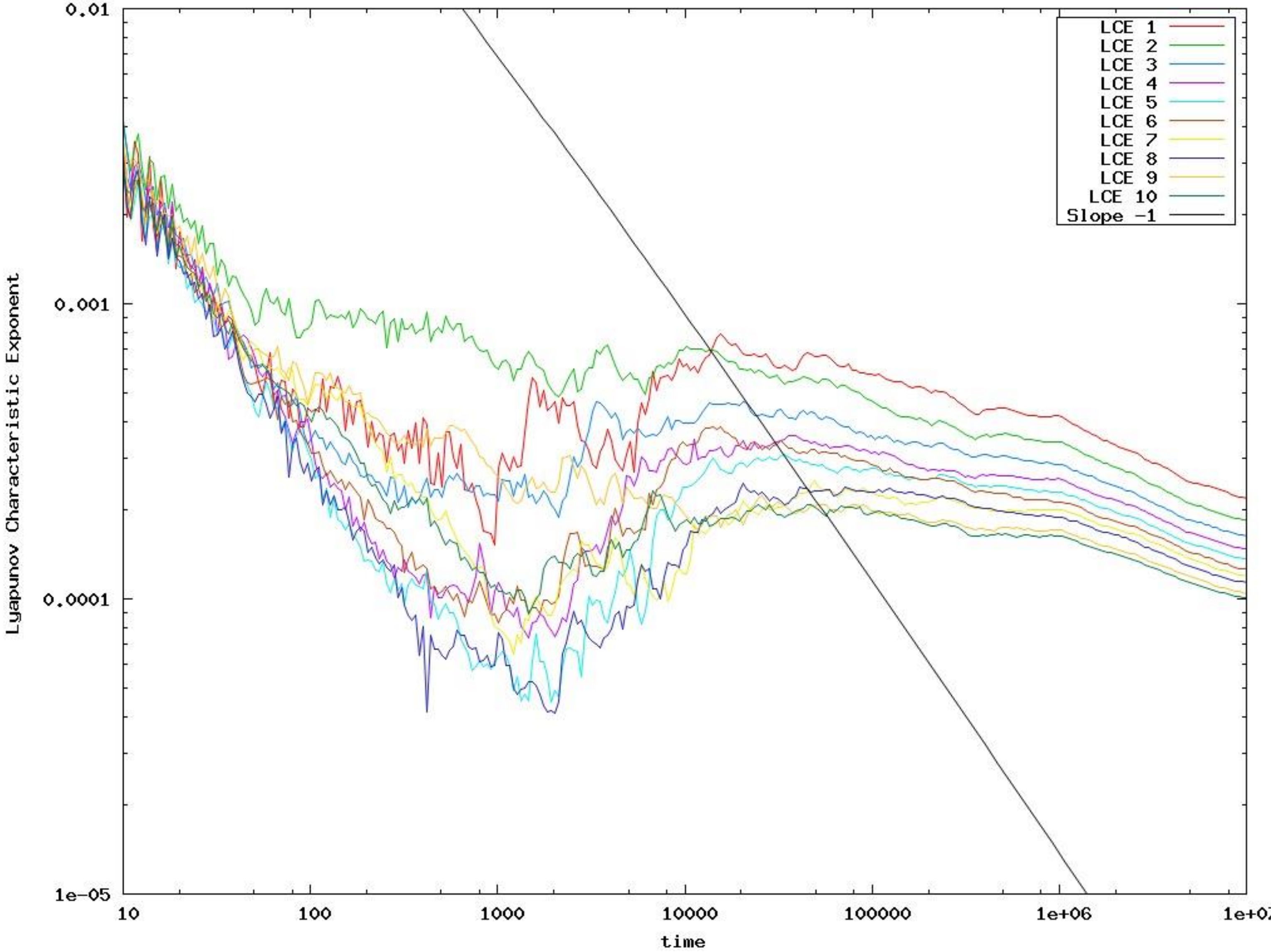
and the 3-part splitting integrator $ABC^6_{[SS]}$ [S. et al., Phys. Let. A (2014) – Gerlach et al., EPJ ST (2016)] to the DNLS system:

$$H_D = \sum_l \varepsilon_l \left|\psi_l\right|^2 + \frac{\beta}{2} \left|\psi_l\right|^4 - \left(\psi_{l+1} \psi_l^* + \psi_{l+1}^* \psi_l \right), \qquad \psi_l = \frac{1}{\sqrt{2}} \left(q_l + i p_l \right)$$

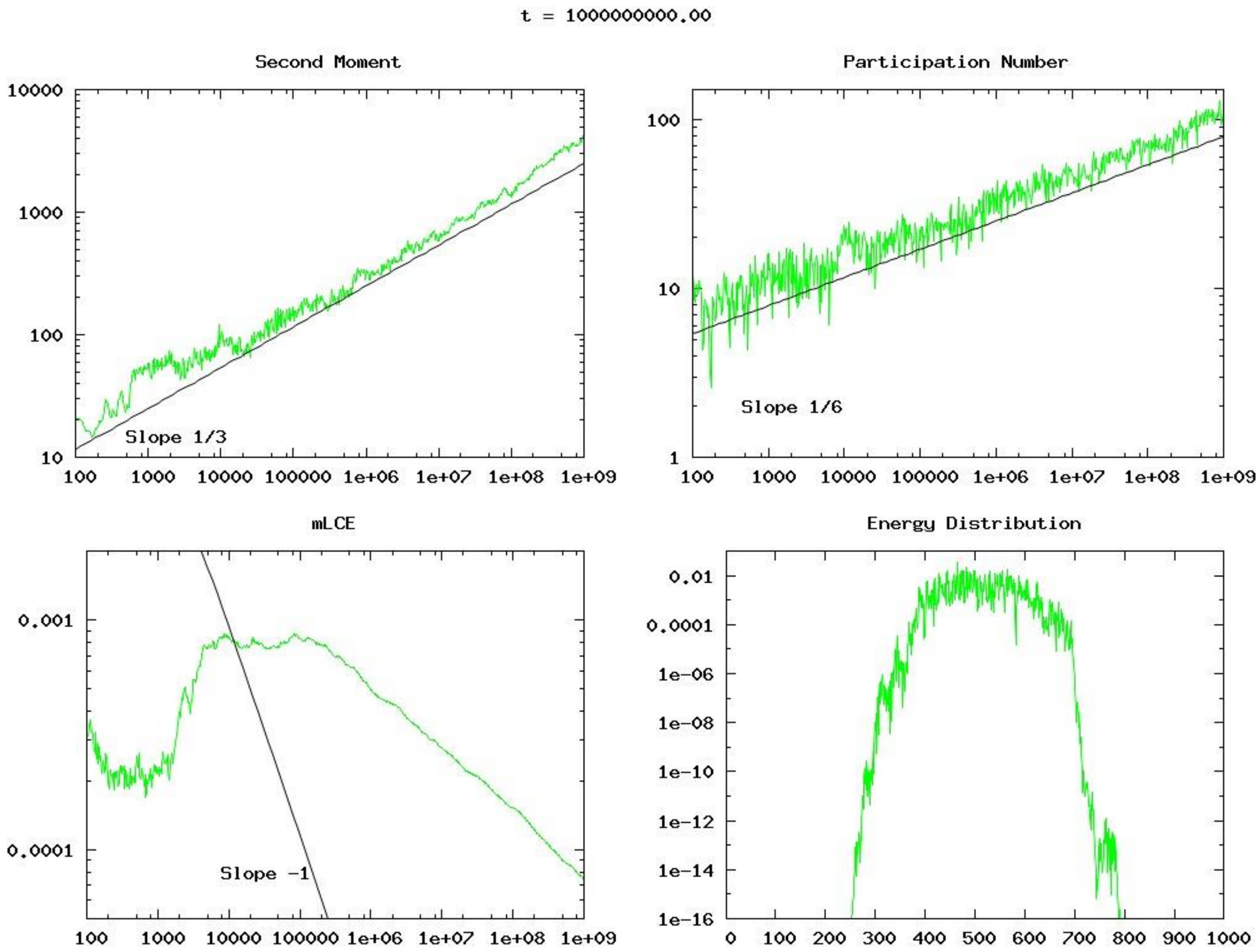
$$H_D = \sum_l \left(\frac{\varepsilon_l}{2} \left(q_l^2 + p_l^2 \right) + \frac{\beta}{8} \left(q_l^2 + p_l^2 \right)^2 - q_n q_{n+1} - p_n p_{n+1} \right)$$

By using the so-called Tangent Map method we extend these symplectic integration schemes in order to integrate simultaneously the variational equations [S. & Gerlach, PRE (2010) – Gerlach & S., Discr. Cont. Dyn. Sys. (2011) – Gerlach et al., IJBC (2012)].

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



KG: Weak Chaos (E=0.4)

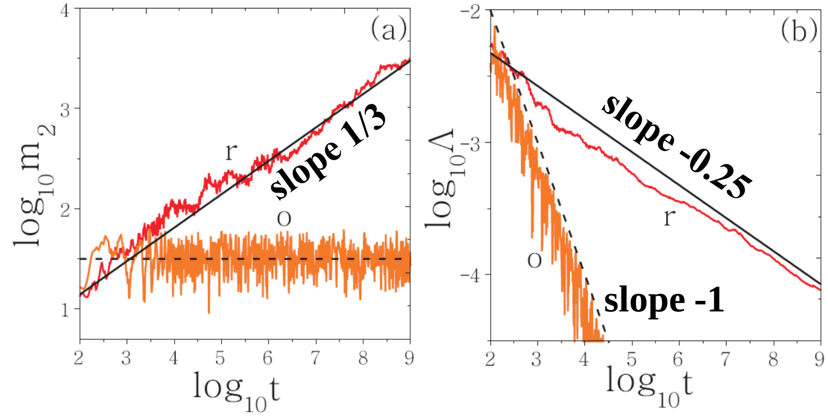


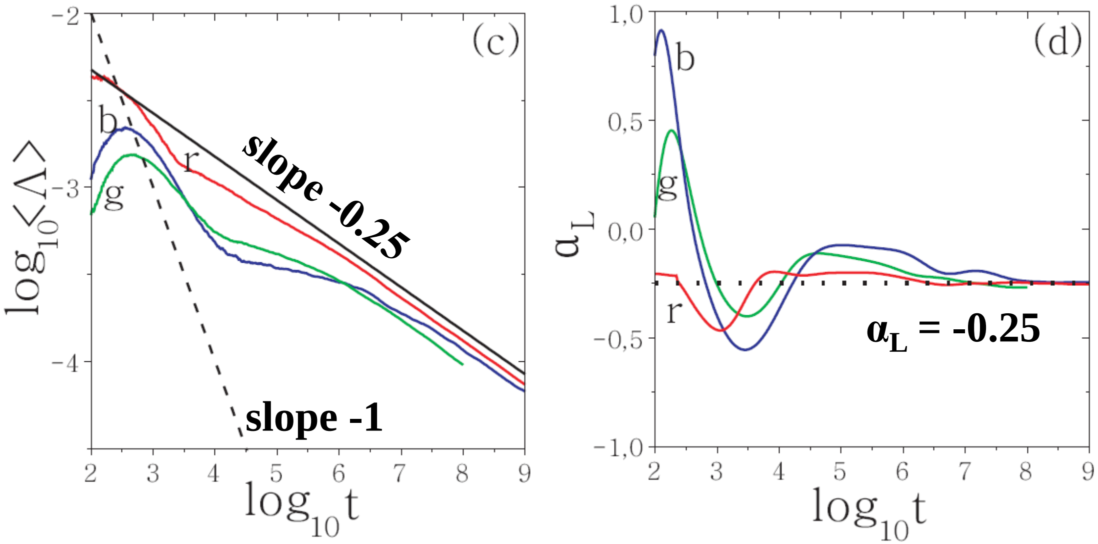
KG: Weak Chaos

Individual runs

Linear case

E=0.4, W=4





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

Average over 50 realizations

Single site excitation E=0.4, W=4

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

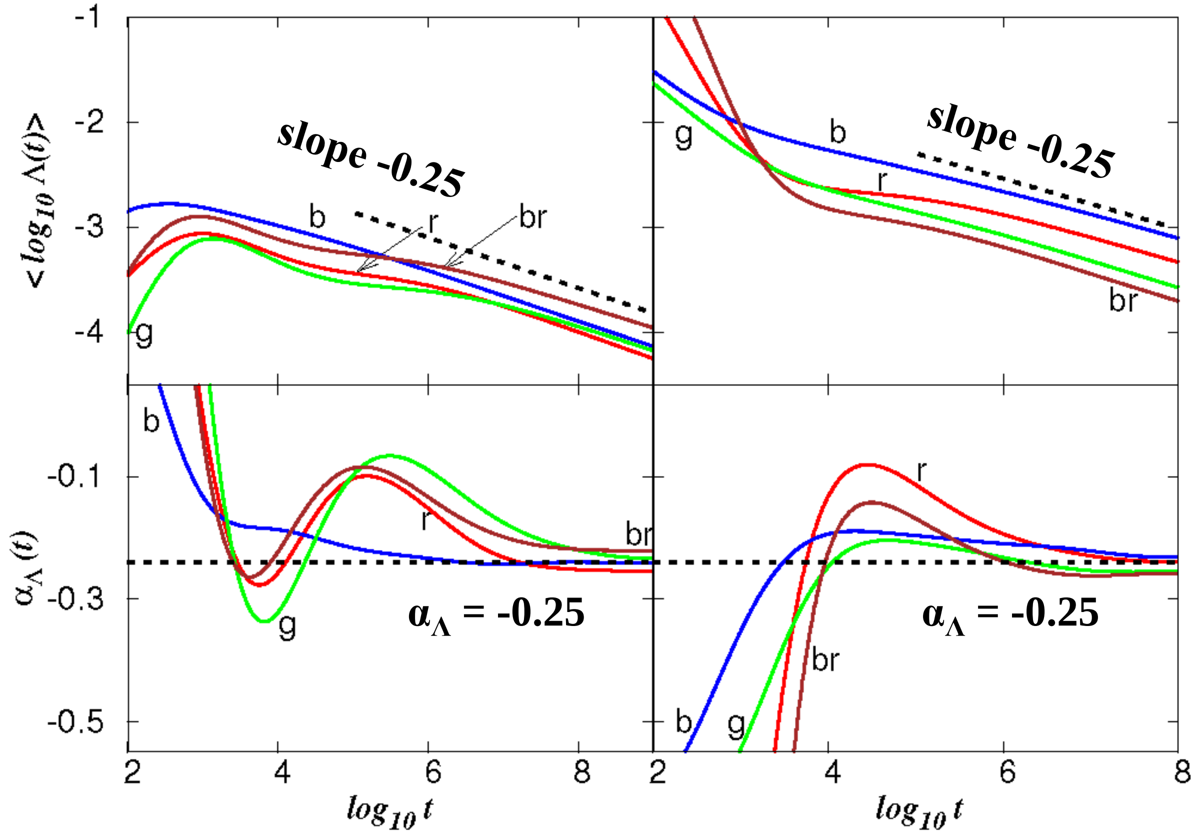
Block excitation (L=37 sites) E=0.37, W=3

S. et al., PRL (2013)

Weak Chaos: KG and DNLS

KG

DNLS



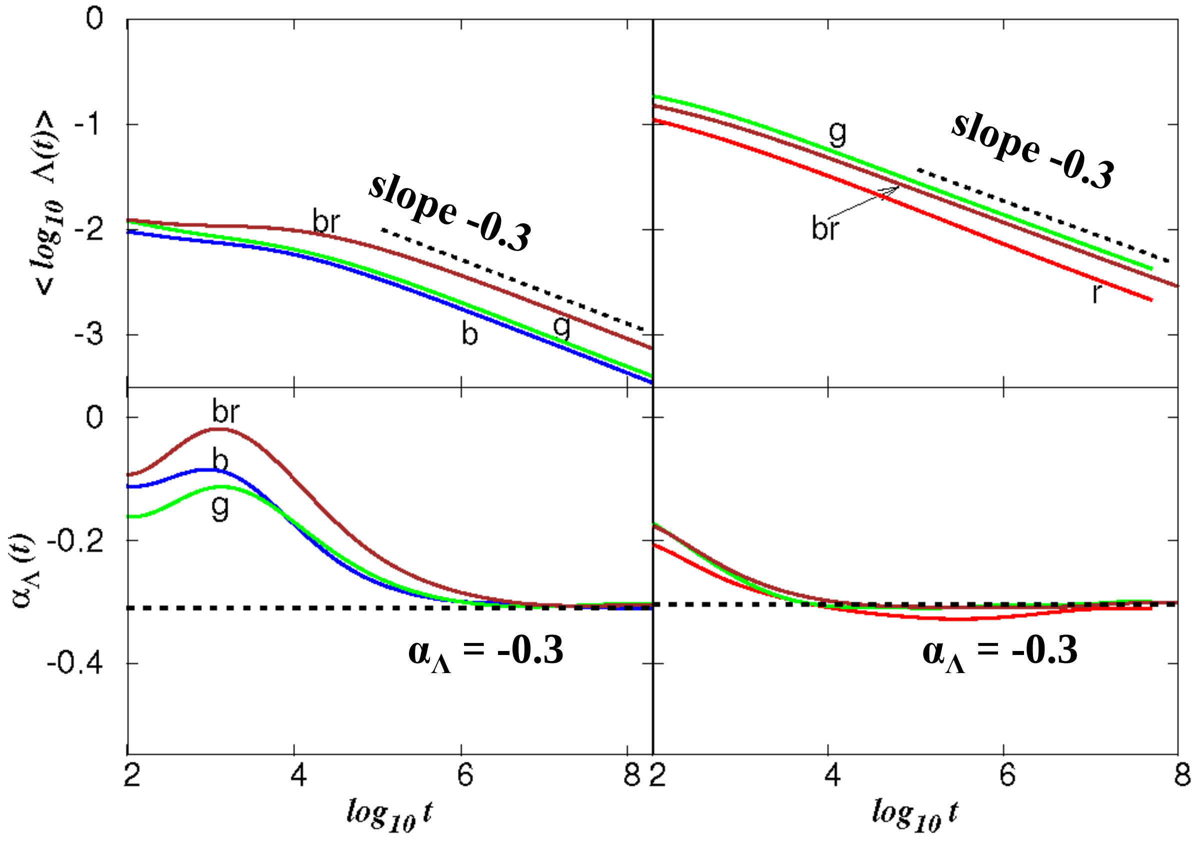
Average over 100 realizations

Block excitation (L=83 sites) E=0.415, W=2	**Block excitation (L=21 sites) β=0.04, W=4**
Block excitation (L=37 sites) E=0.37, W=3	**Single site excitation β=1, W=4**
Single site excitation E=0.4, W=4	**Single site excitation β=0.6, W=3**
Block excitation (L=21 sites) E=0.21, W=4	**Block excitation (L=21 sites) β=0.03, W=3**

Strong Chaos: KG and DNLS

KG

DNLS



Average over 100 realizations

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

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

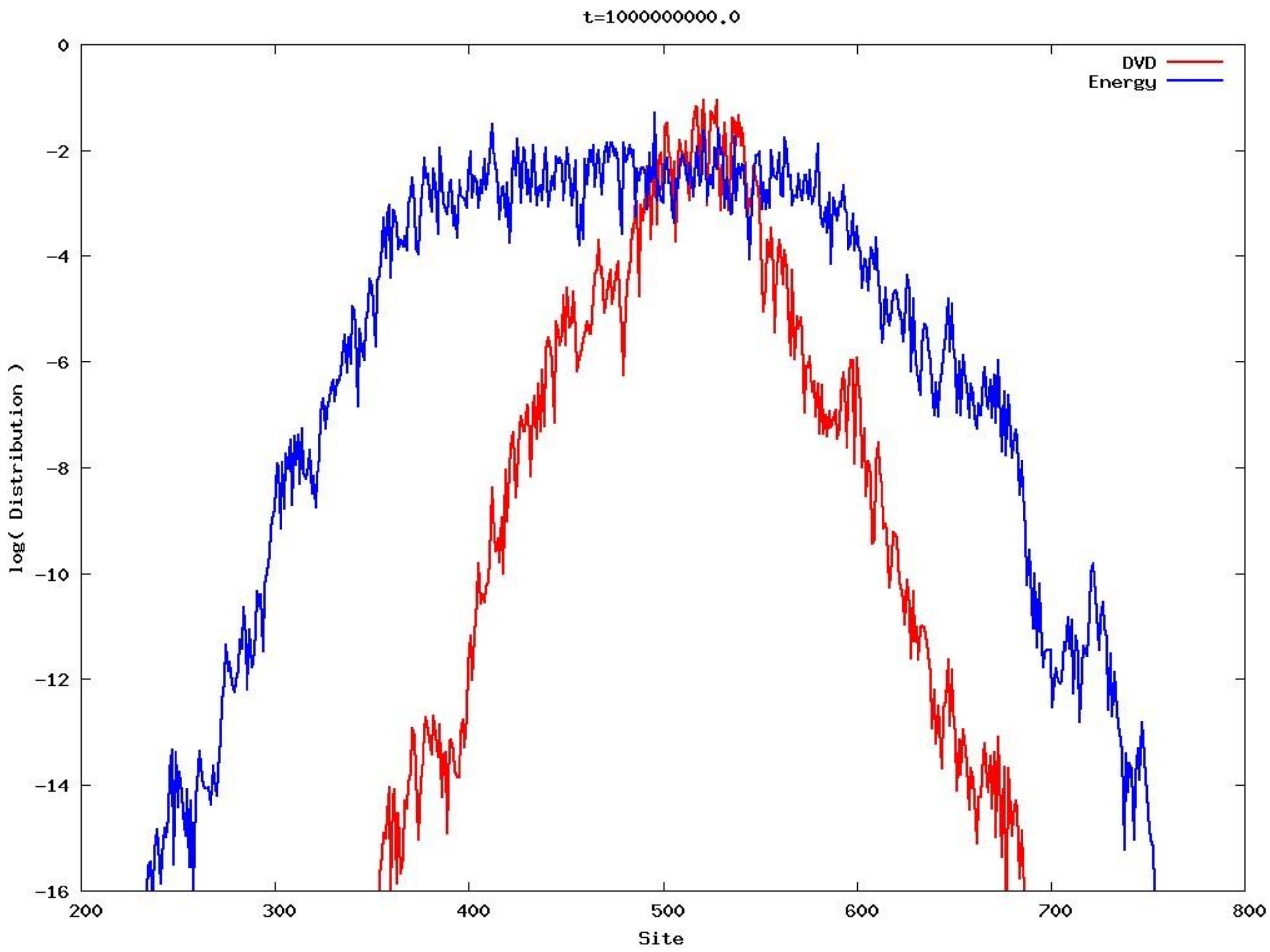
Block excitation (L=83 sites) E=0.83, W=3

Block excitation (L=21 sites) β=0.62, W=3.5

Block excitation (L=21 sites) β=0.5, W=3

Block excitation (L=21 sites) β=0.72, W=4

Deviation Vector Distributions (DVDs)

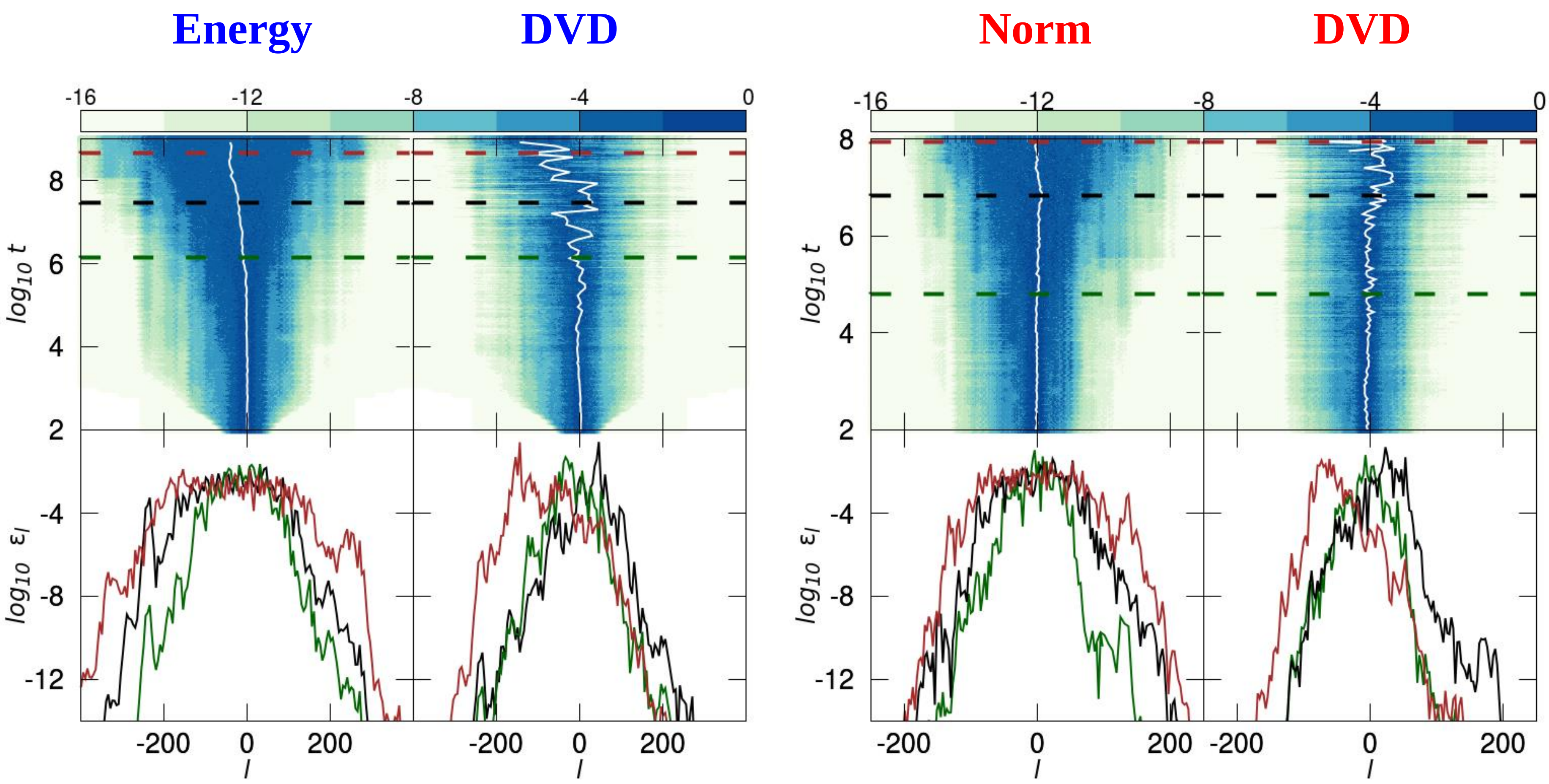


Deviation vector:

$v(t)=(\delta u_1(t), \delta u_2(t), \ldots, \delta u_N(t), \delta p_1(t), \delta p_2(t), \ldots, \delta p_N(t))$

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

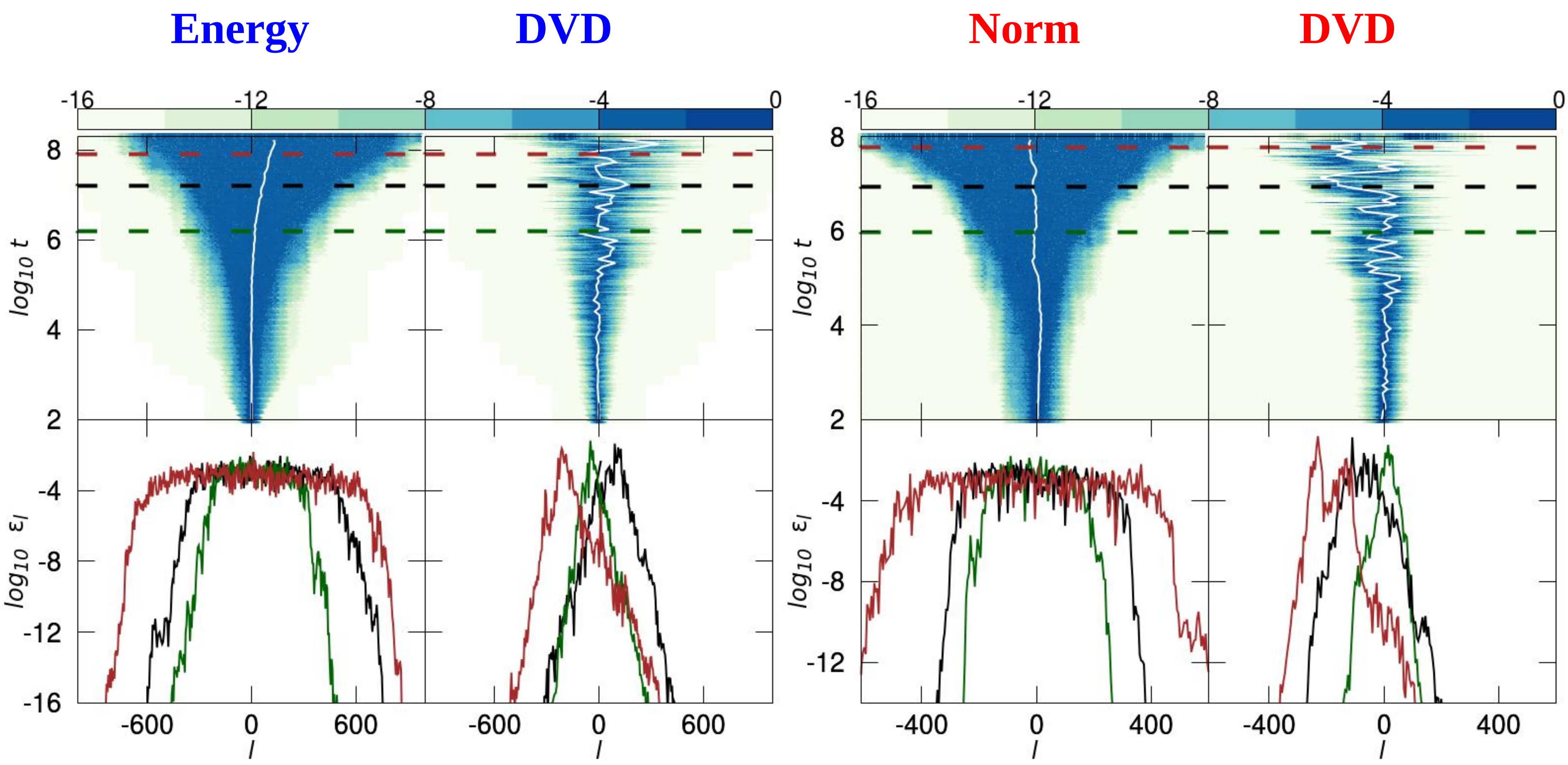
Weak Chaos: KG and DNLS



W=3, L=37, E=0.37

W=4, L=21, β=0.04

Strong Chaos: KG and DNLS



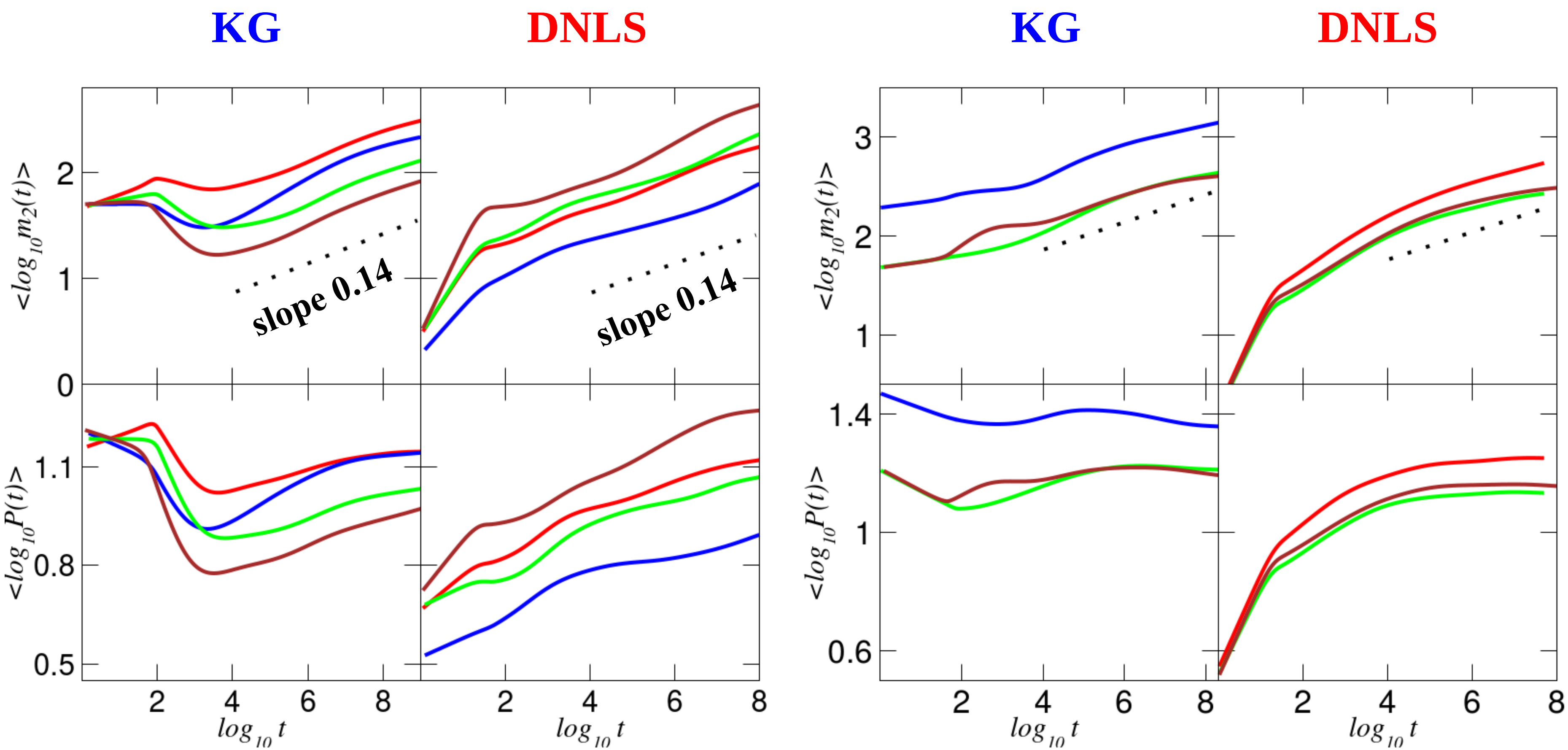
W=3, L=37, E=3.7

W=4, L=21, β=0.72

Characteristics of DVDs

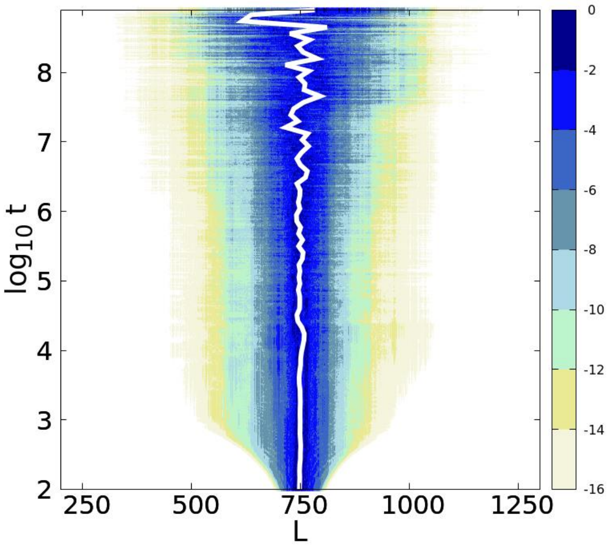
Weak chaos

Strong chaos

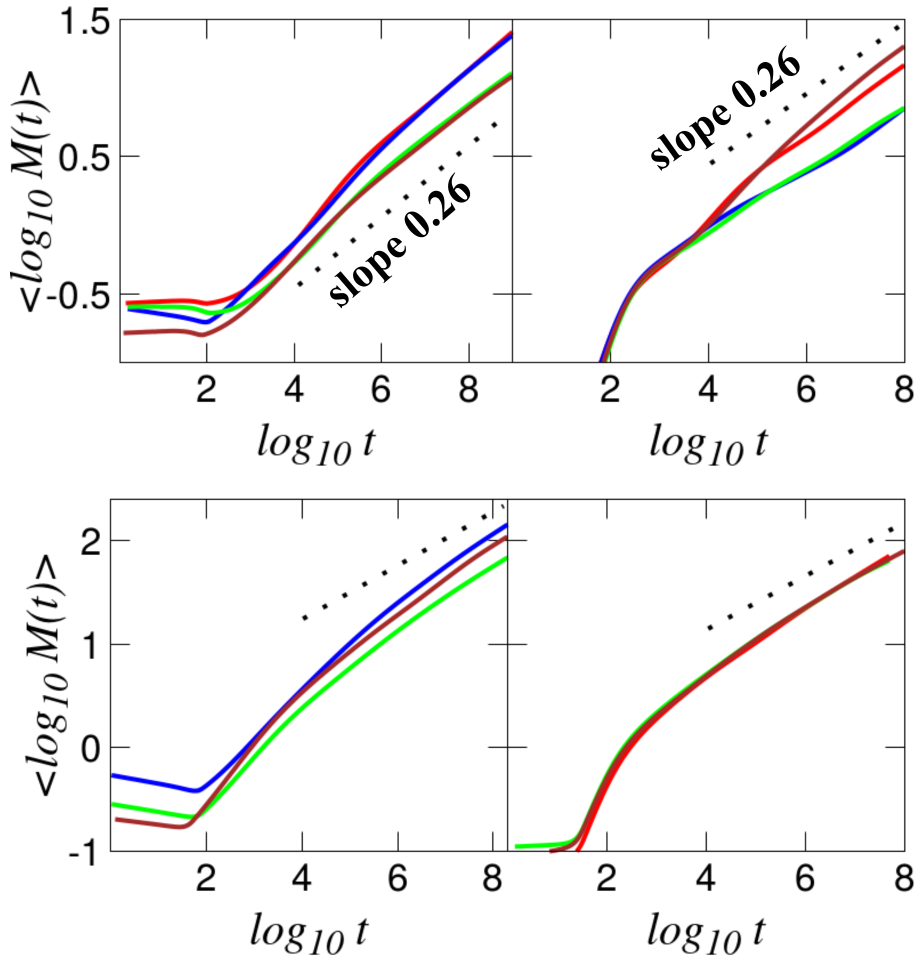


Characteristics of DVDs

KG weak chaos
L=37, E=0.37, W=3



KG **DNLS**



Weak chaos

Strong chaos

Maximum absolute deviation of DVD's mean position

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

Summary

- Both the KG and the DNLS models show similar chaotic behaviors
- The mLCE and the DVDs show different behaviors for the weak and the strong chaos regimes.
- Lyapunov exponent computations show that:
  - ✓ Chaos not only exists, but also persists.
  - ✓ Slowing down of chaos does not cross over to regular dynamics.
  - ✓ Weak chaos: mLCE ~ $t^{-0.25}$
  - ✓ Strong chaos: mLCE ~ $t^{-0.3}$
- The behavior of DVDs can provide information about the chaoticity of a dynamical system.
  - ✓ Chaotic hot spots meander through the system, supporting a homogeneity of chaos inside the wave packet.

Posters on Hamiltonian lattices

Chaotic dynamics of one-dimensional disordered nonlinear lattices

Bob Senyange, Bertin Many Manda, Haris Skokos

Bob Senyange & Bertin Many Manda: KG and DNLS

Chaotic behaviour of the Peyrard-Bishop-Dauxois model of DNA

Malcolm Hillebrand[1], Adrian Schwellnus[1], George Kalosakas[2], Haris Skokos[1]

Malcolm Hillebrand: DNA

Dynamical behavior of a 2D planar model of graphene

B. Many Manda[†♠], G. Kalosakas[‡], Ch. Skokos[†]

Bertin Many Manda: graphene