Chaotic wave packet spreading in one-dimensional disordered nonlinear lattices

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/**

Outline

- **Disordered 1D lattices:**
  - ✓ **The quartic disordered Klein-Gordon (DKG) model**
  - ✓ **The disordered discrete nonlinear Schrödinger equation (DDNLS)**
  - ✓ **Different dynamical behaviors**

- **Chaotic behavior of the DKG and DDNLS models**
  - ✓ **Lyapunov exponents**
  - ✓ **Deviation Vector Distributions**

- **The Peyrard-Bishop-Dauxois (PBD) model of DNA**

- **Summary**

Work in collaboration with

Bob Senyange (PhD student): DKG model

Bertin Many Manda (PhD student): DDNLS model

Malcolm Hillebrand (PhD student): DNA model

The
DKG and DDNLS models

Interplay of disorder and nonlinearity

Waves in disordered media – Anderson localization [Anderson, Phys. Rev. (1958)]. **Experiments on BEC** [Billy et al., Nature (2008)]

Waves in nonlinear disordered media – localization or delocalization?

Theoretical and/or numerical studies [Shepelyansky, PRL (1993) – Molina, Phys. Rev. B (1998) – Pikovsky & Shepelyansky, PRL (2008) – Kopidakis et al., PRL (2008) – Flach et al., PRL (2009) – S. et al., PRE (2009) – Mulansky & Pikovsky, EPL (2010) – S. & Flach, PRE (2010) – Laptyeva et al., EPL (2010) – Mulansky et al., PRE & J.Stat.Phys. (2011) – Bodyfelt et al., PRE (2011) – Bodyfelt et al., IJBC (2011)]

Experiments: propagation of light in disordered 1d waveguide lattices [Lahini et al., PRL (2008)]
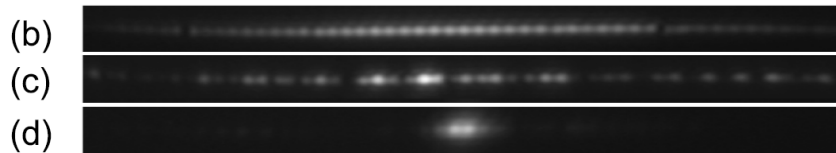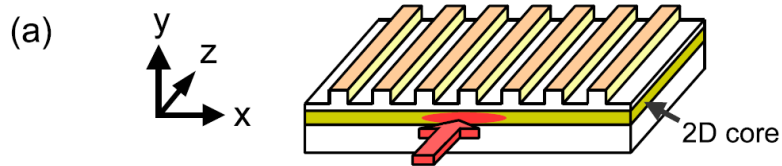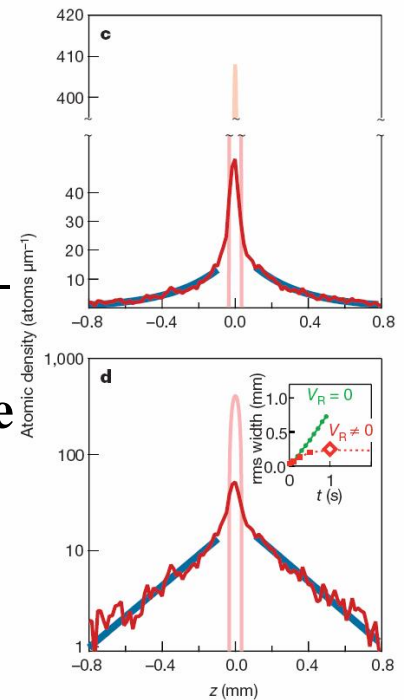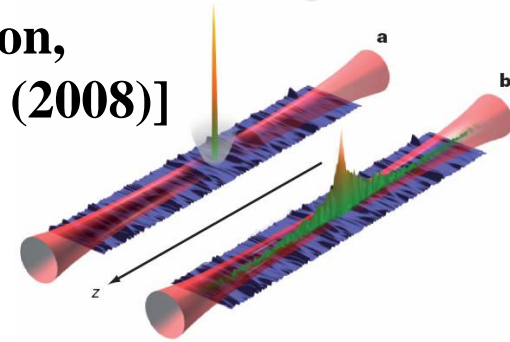
The disordered Klein – Gordon (DKG) model

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

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** $\left[\dfrac{1}{2}, \dfrac{3}{2} \right]$.

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 disordered discrete nonlinear Schrödinger (DDNLS) 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** $\left[-\dfrac{W}{2}, \dfrac{W}{2} \right]$ **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** $z_v \equiv \dfrac{E_v}{\sum_m E_m}$

with $E_v = \dfrac{p_v^2}{2} + \dfrac{\tilde{\varepsilon}_v}{2} u_v^2 + \dfrac{1}{4} u_v^4 + \dfrac{1}{4W}\left(u_{v+1} - u_v\right)^2$ for the DKG model,

and **norm distributions** $z_v \equiv \dfrac{|\psi_v|^2}{\sum_l |\psi_l|^2}$ for the DDNLS system.

Second moment: $m_2 = \sum_{v=1}^{N}\left(v - \bar{v}\right)^2 z_v$ with $\bar{v} = \sum_{v=1}^{N} v z_v$

Participation number: $P = \dfrac{1}{\sum_{v=1}^{N} z_v^2}$

measures the number of stronger excited modes in z_v.

Single site $P=1$. 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: $\delta < d$, $m_2 \propto t^{1/3}$

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: $d < \delta < \Delta$, $m_2 \propto t^{1/2} \longrightarrow m_2 \propto t^{1/3}$

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

DDNLS W=4, β= **0.1, 1, 4.5** **DKG** W = 4, E = **0.05, 0.4, 1.5**
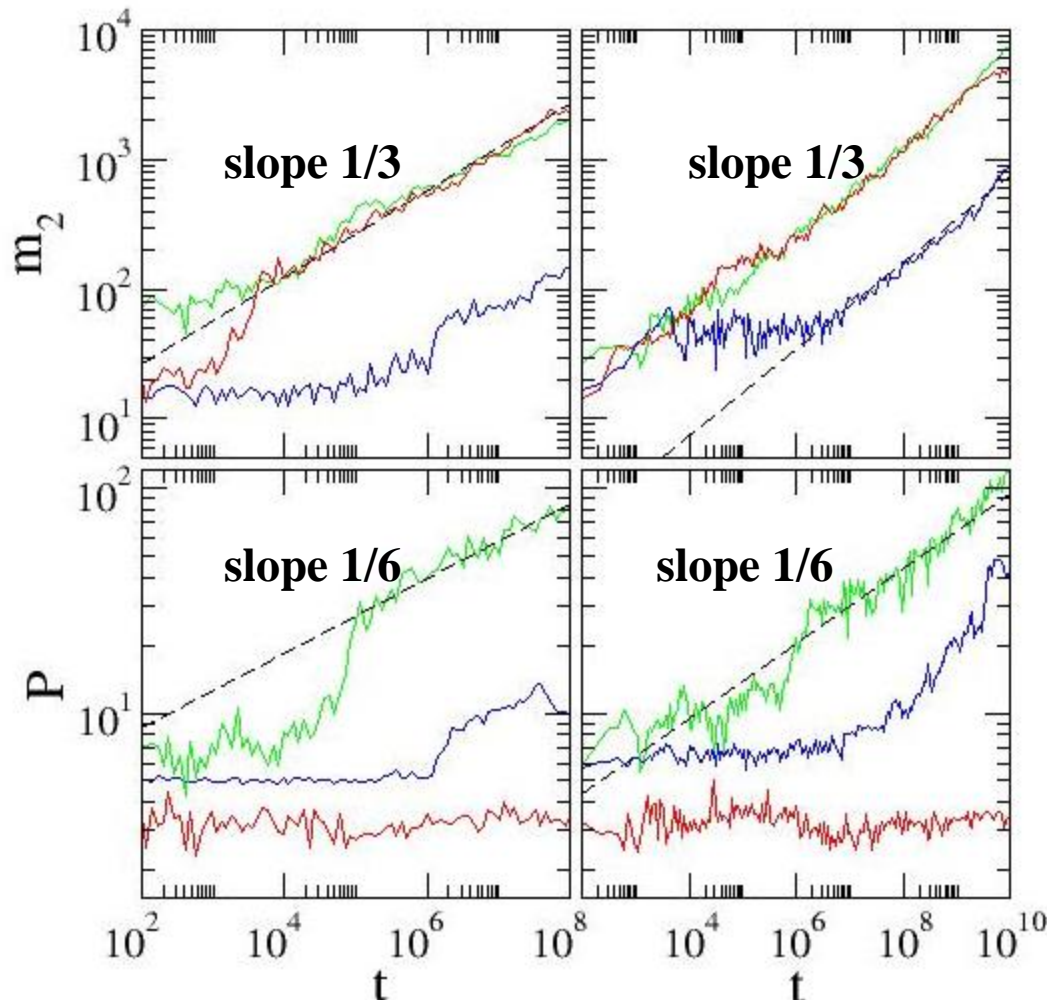
No strong chaos regime

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

α=0.33±0.05 (DKG)
α=0.33±0.02 (DDLNS)

Flach et al., PRL (2009)
S. et al., PRE (2009)

DKG: Different spreading regimes
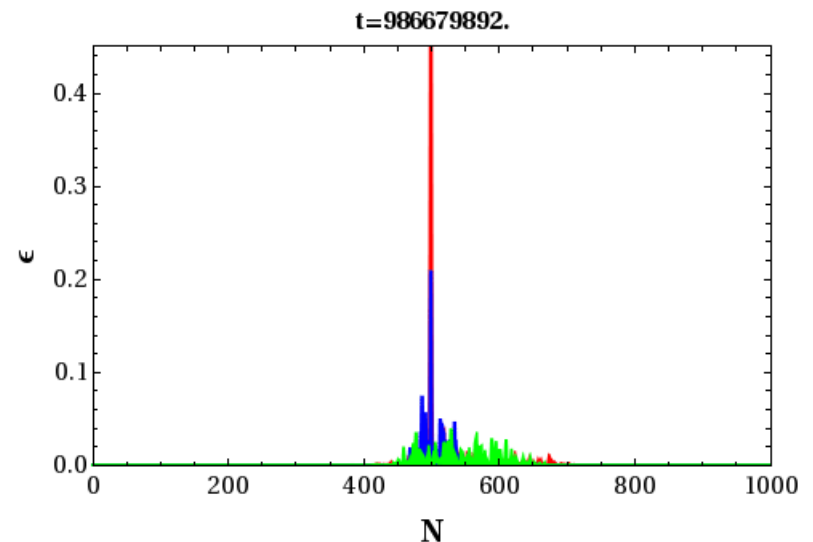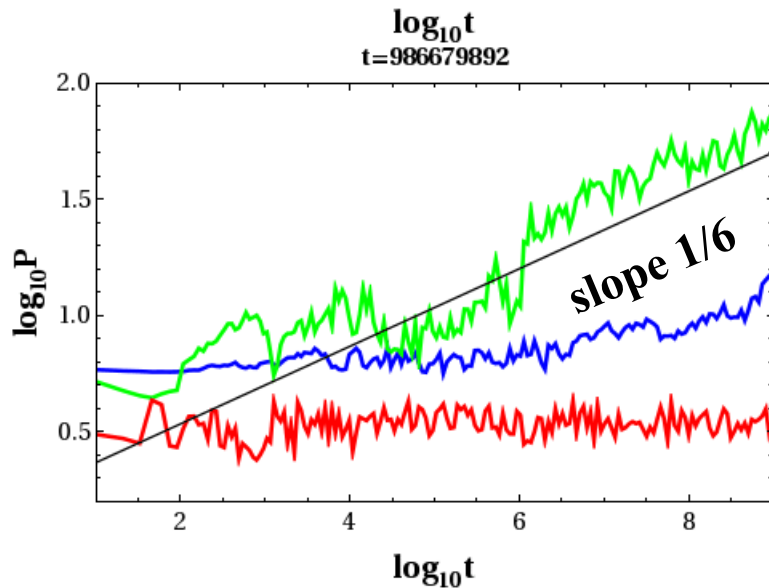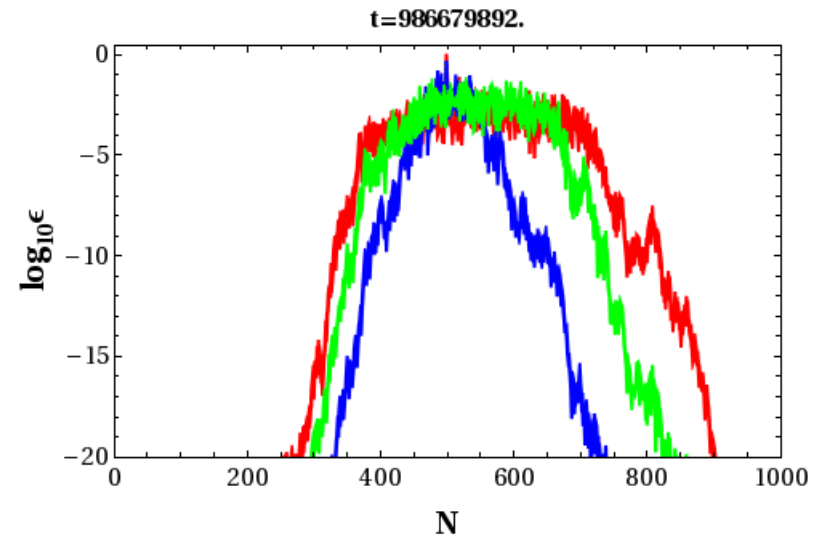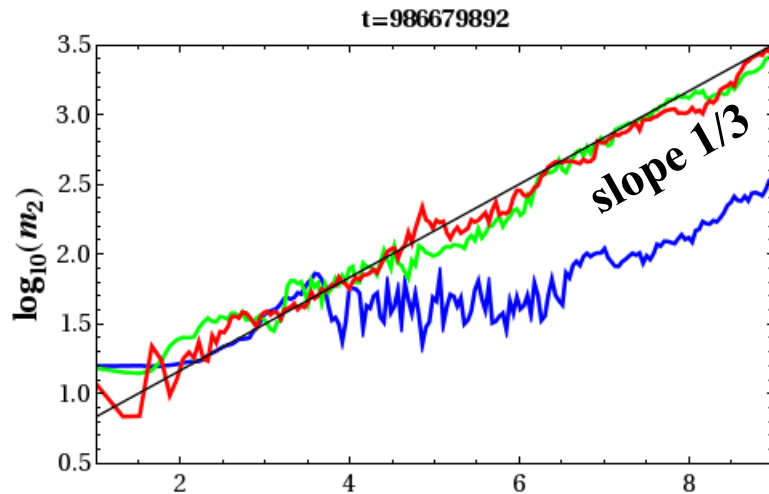
Crossover from strong to weak chaos (block excitations)

DDNLS β= 0.04, 0.72, 3.6   DKG E= 0.01, 0.2, 0.75

W=4

Average over 1000 realizations!

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

α=1/2
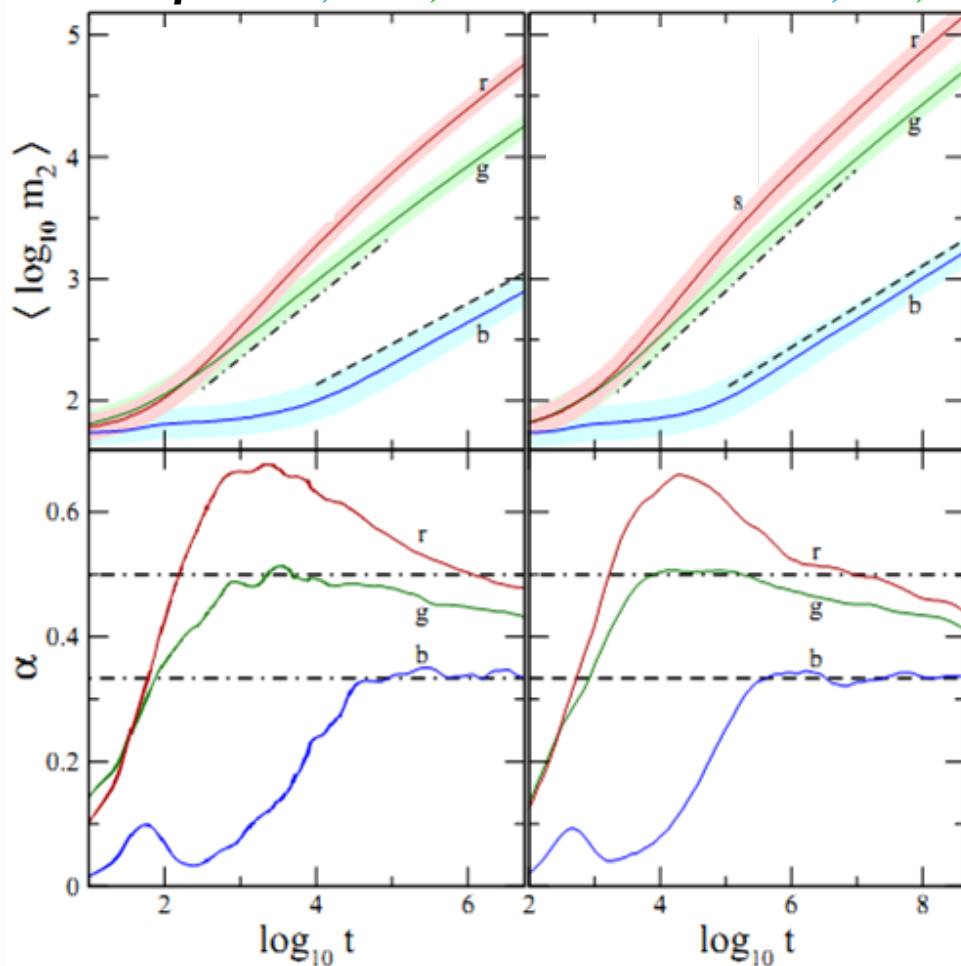
α=1/3

Laptyeva et al., EPL (2010)

Bodyfelt et al., PRE (2011)

Variational Equations

We use the notation $x = (q_1, q_2, \ldots, q_N, p_1, p_2, \ldots, p_N)^T$. The **deviation vector** from a given orbit is denoted by

$$v = (\delta x_1, \delta x_2, \ldots, \delta x_n)^T \text{, with n=2N}$$

The time evolution of **v** is given by the so-called **variational equations:**

$$\frac{dv}{dt} = -J \cdot P \cdot v$$

where

$$J = \begin{pmatrix} 0_N & -I_N \\ I_N & 0_N \end{pmatrix} \, , \quad P_{ij} = \frac{\partial^2 H}{\partial x_i \partial x_j} \quad i, j = 1, 2, \ldots, n$$

Benettin & Galgani, 1979, in Laval and Gressillon (eds.), op cit, 93
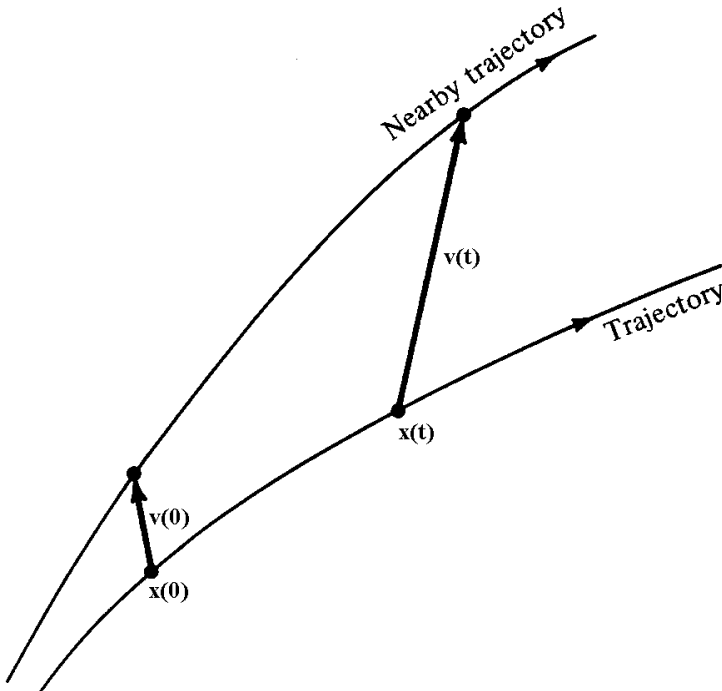
Maximum Lyapunov Exponent

Chaos: sensitive dependence on initial conditions.

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 x(0)** and **an initial deviation vector from it v(0).** Then the mean exponential rate of divergence is:

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

$$\lambda_1 = 0 \rightarrow \textbf{Regular motion}$$
$$\lambda_1 \neq 0 \rightarrow \textbf{Chaotic motion}$$
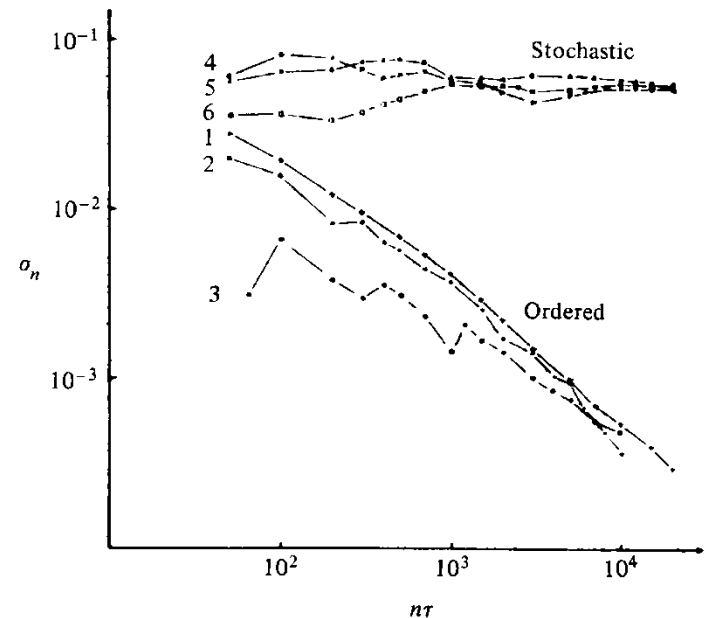
Figure 5.7. Behavior of σ_n at the intermediate energy $E = 0.125$ for initial points taken in the ordered (curves 1–3) or stochastic (curves 4–6) regions (after Benettin et al., 1976).

Symplectic integration

We apply **the 2-part splitting integrator ABA864** [Blanes et al., Appl. Num. Math. (2013) – Senyange & S., EPJ ST (2018)] to the DKG 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) – Danieli et al., MinE (2019)] to the DDNLS system:

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

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

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)].

DKG: Weak Chaos

**Block excitation
L=37 sites,
E=0.37, W=3**

Second Moment

Slope = 1/3

Participation Number

Slope = 1/6

mLCE

Slope = -1

Energy Distribution
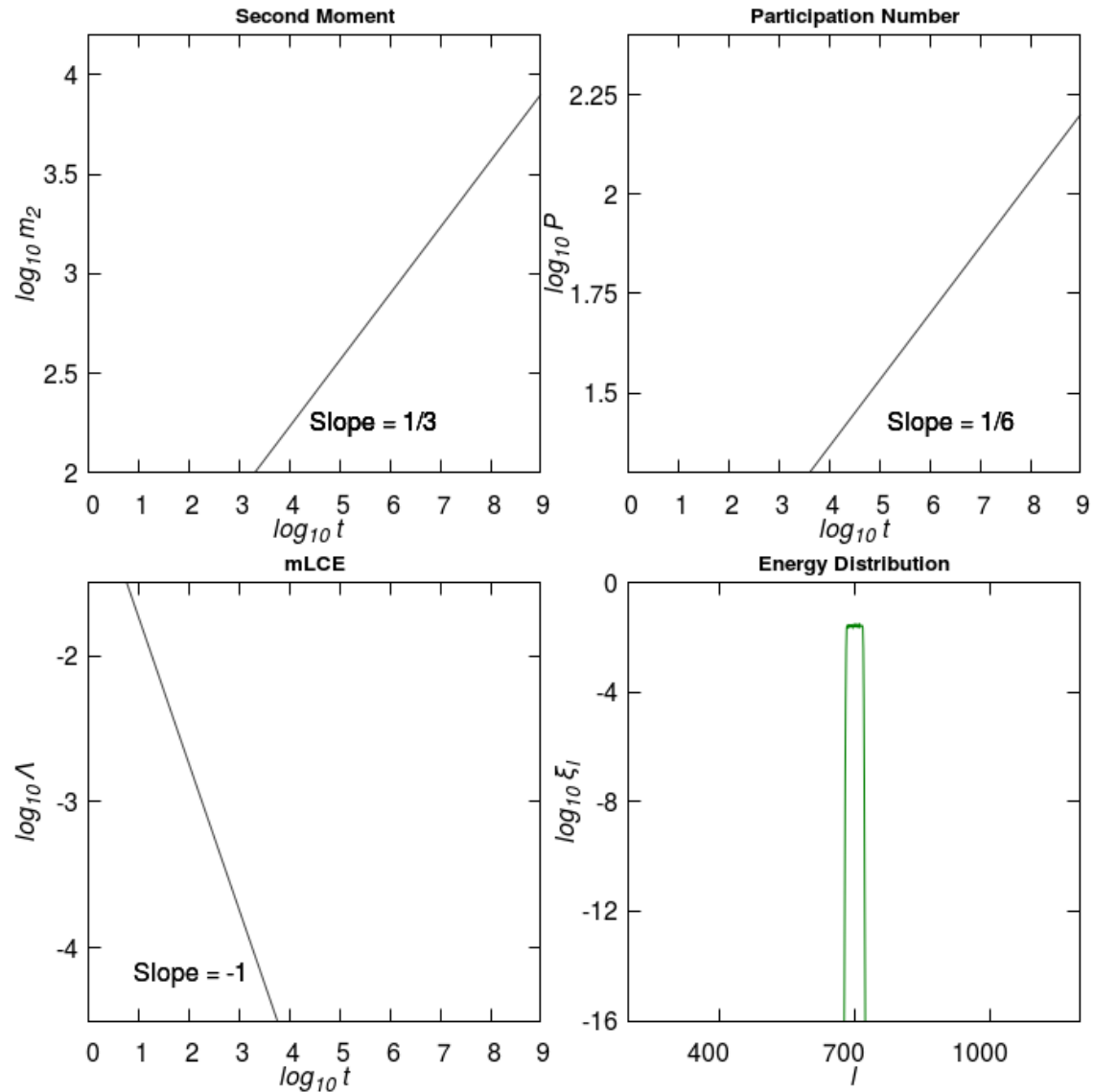
DKG: Weak Chaos

Block excitation L=37 sites, E=0.37, W=3
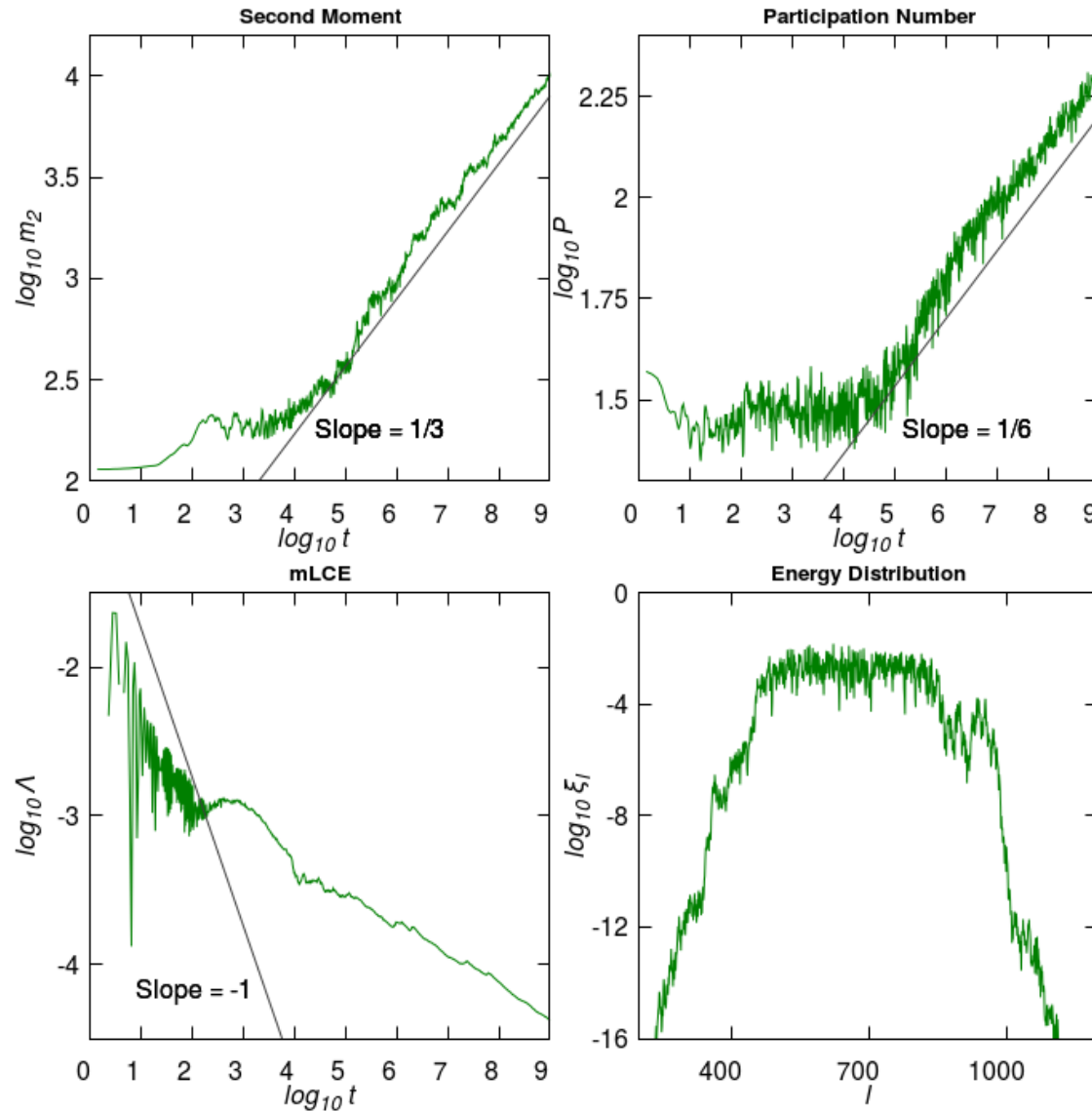
DKG: Weak Chaos

Individual runs
Linear case
E=0.4, W=4
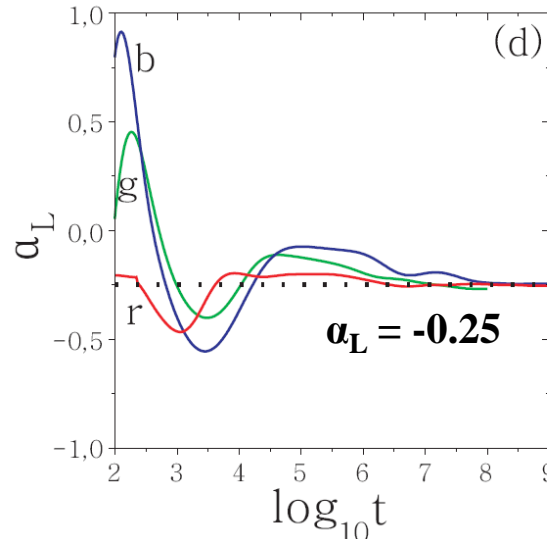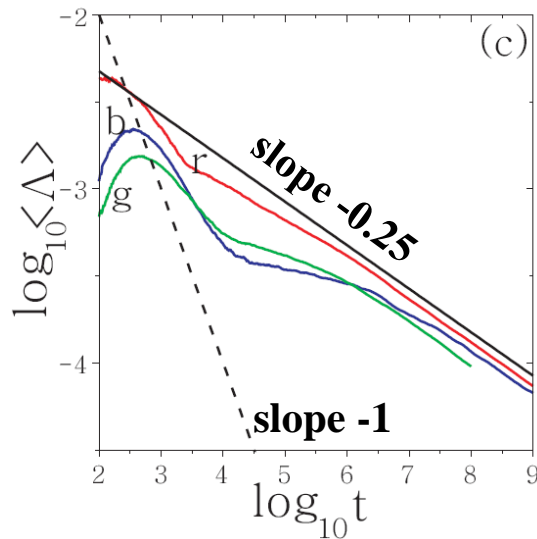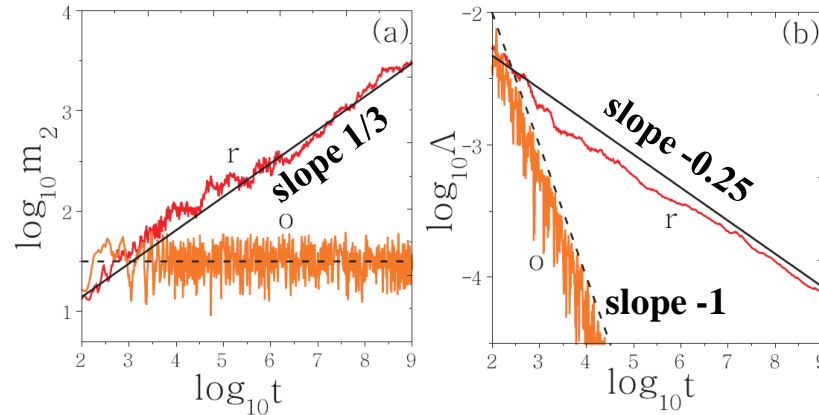
Average over 50 realizations

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

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

S. et al., PRL (2013)

Weak Chaos: DKG and DDNLS
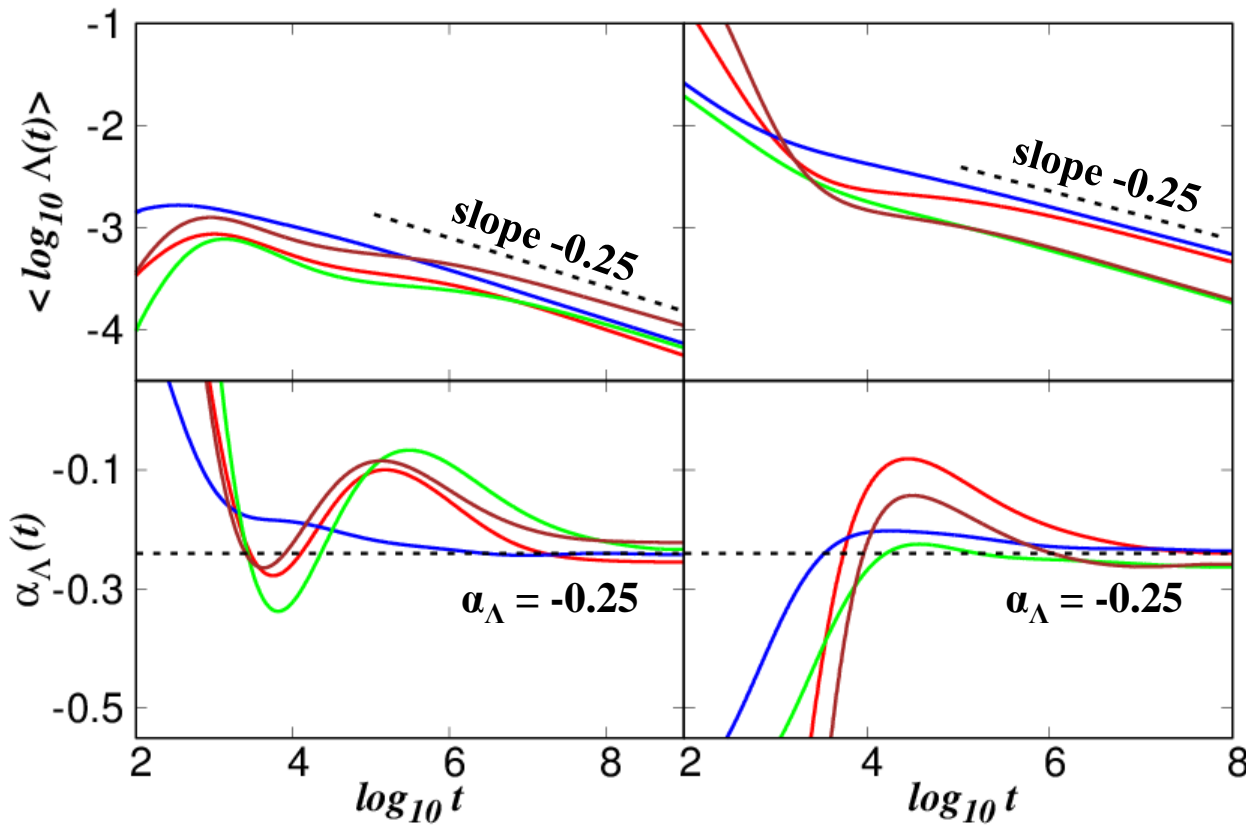
DKG

DDNLS

Average over 100 realizations [Senyange, Many Manda & S., PRE (2018)]

Block excitation (L=37 sites) E=0.37, W=3
Single site excitation E=0.4, W=4
Block excitation (L=21 sites) E=0.21, W=4
Block excitation (L=13 sites) E=0.26, W=5

Block excitation (L=21 sites) β=0.04, W=4
Single site excitation β=1, W=4
Single site excitation β=0.6, W=3
Block excitation (L=21 sites) β=0.03, W=3

Strong Chaos: DKG and DDNLS
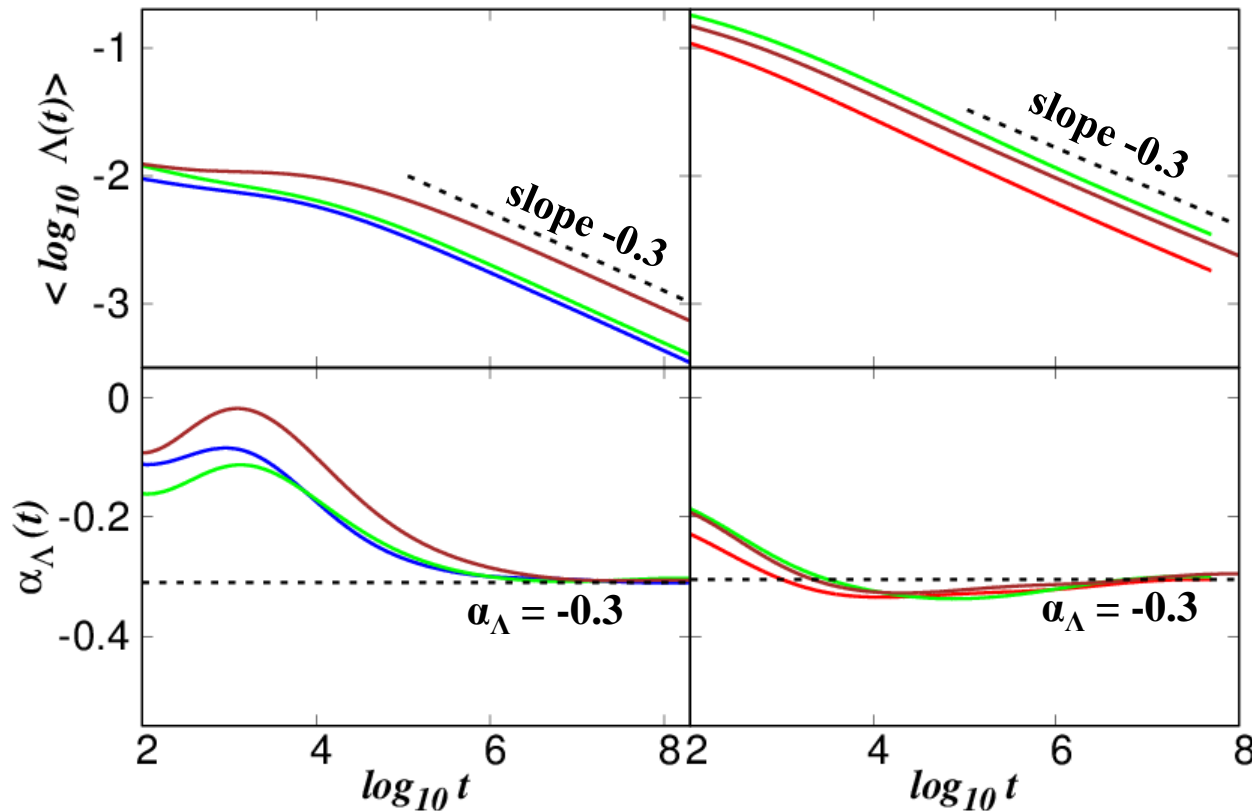
DKG

DDNLS

Average over 100 realizations [Senyange, Many Manda & S., PRE (2018)]

Block excitation (L=83 sites) E=0.83, W=2   Block excitation (L=21 sites) β=0.62, W=3.5
Block excitation (L=37 sites) E=0.37, W=3   Block excitation (L=21 sites) β=0.5, W=3
Block excitation (L=83 sites) E=0.83, W=3   Block excitation (L=21 sites) β=0.72, W=3.5

Deviation Vector Distributions (DVDs)

Energy
DVD

DKG
weak chaos
L=37 sites,
E=0.37, W=3

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

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

Deviation Vector Distributions (DVDs)

Energy
DVD

DKG
weak chaos
L=37 sites,
E=0.37, W=3

Deviation vector:
$$\mathbf{v}(t)=(\delta u_1(t),\ \delta u_2(t),\ldots,\ \delta u_N(t),\ \delta p_1(t),\ \delta p_2(t),\ldots,\ \delta p_N(t))$$
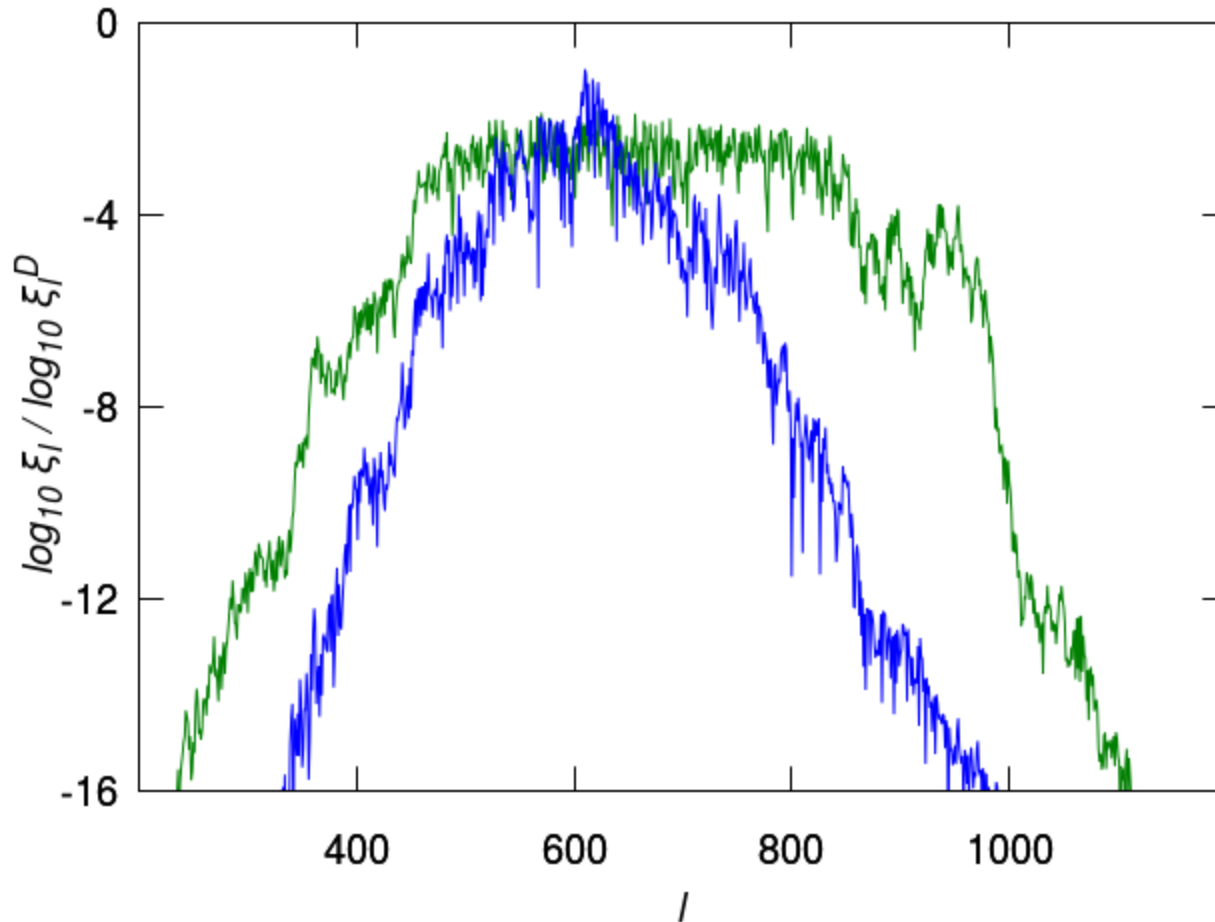
$$\text{DVD:}\ \xi_l^D = \frac{\delta u_l^2 + \delta p_l^2}{\sum_l \left(\delta u_l^2 + \delta p_l^2 \right)}$$

Deviation Vector Distributions (DVDs)

DKG: weak chaos. L=37 sites, E=0.37, W=3

Deviation Vector Distributions (DVDs)

DKG: weak chaos. L=37 sites, E=0.37, W=3

Energy
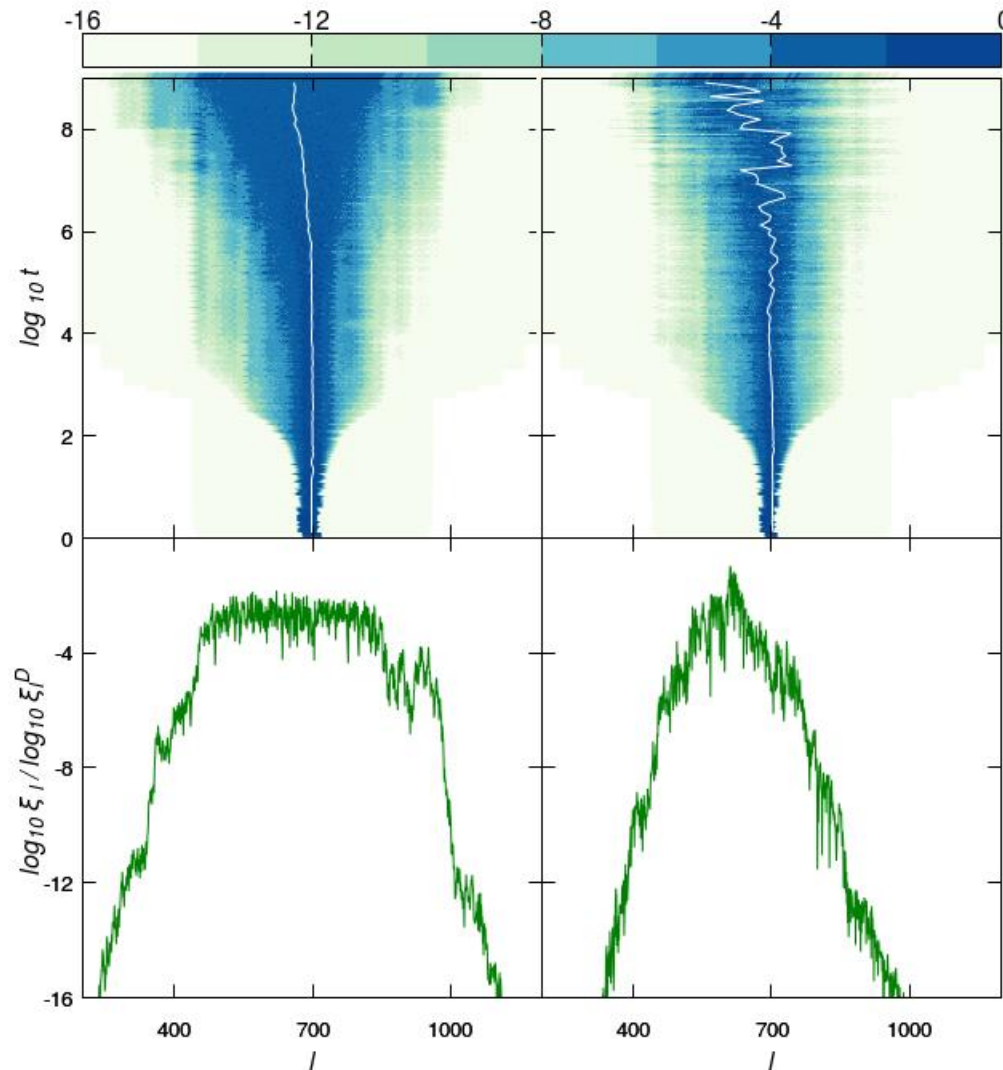
DVD

Weak Chaos: DKG and DDNLS
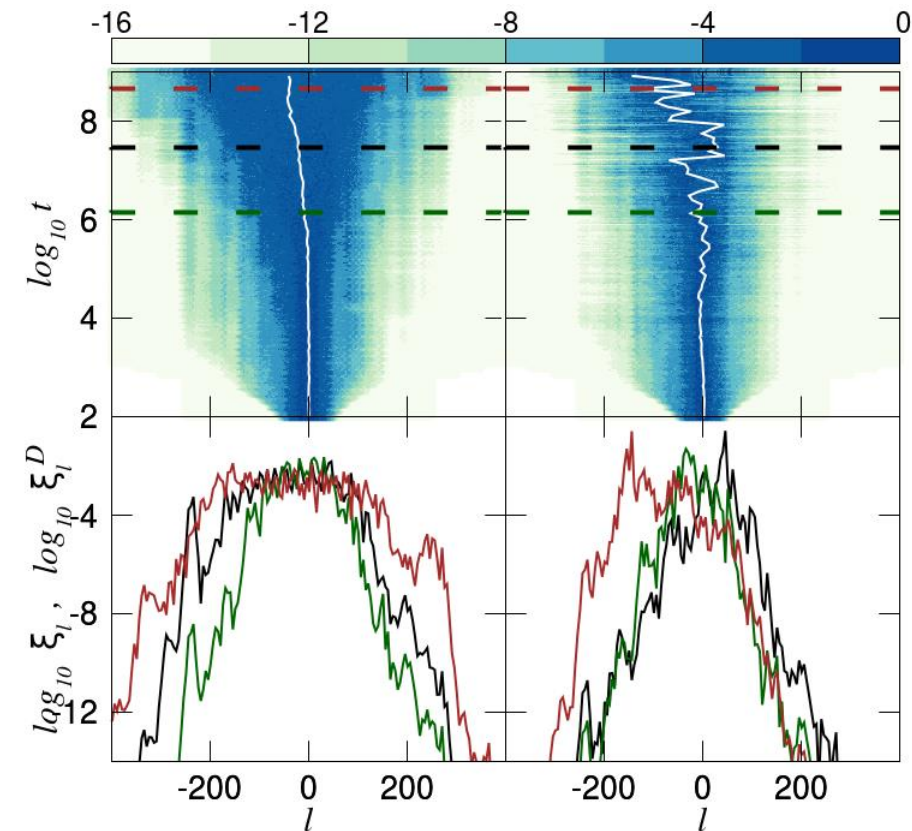
DKG: W=3, L=37, E=0.37
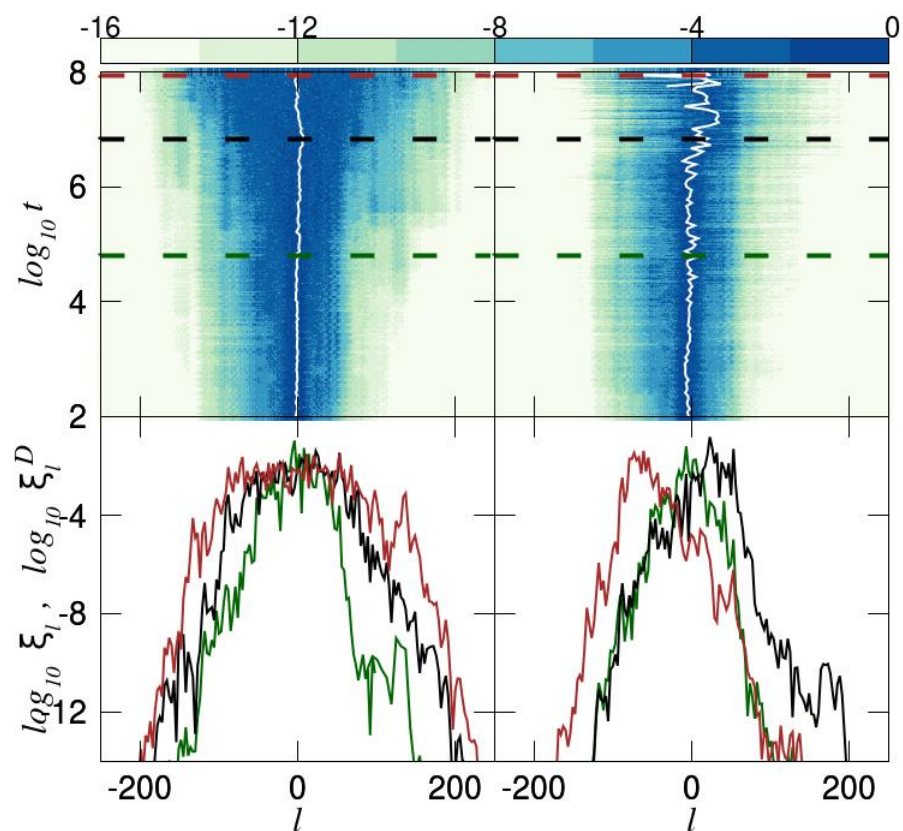
DDNLS: W=4, L=21, β=0.04

Deviation Vector Distributions (DVDs)

DDNLS: strong chaos W=3.5, L=21, β=0.72
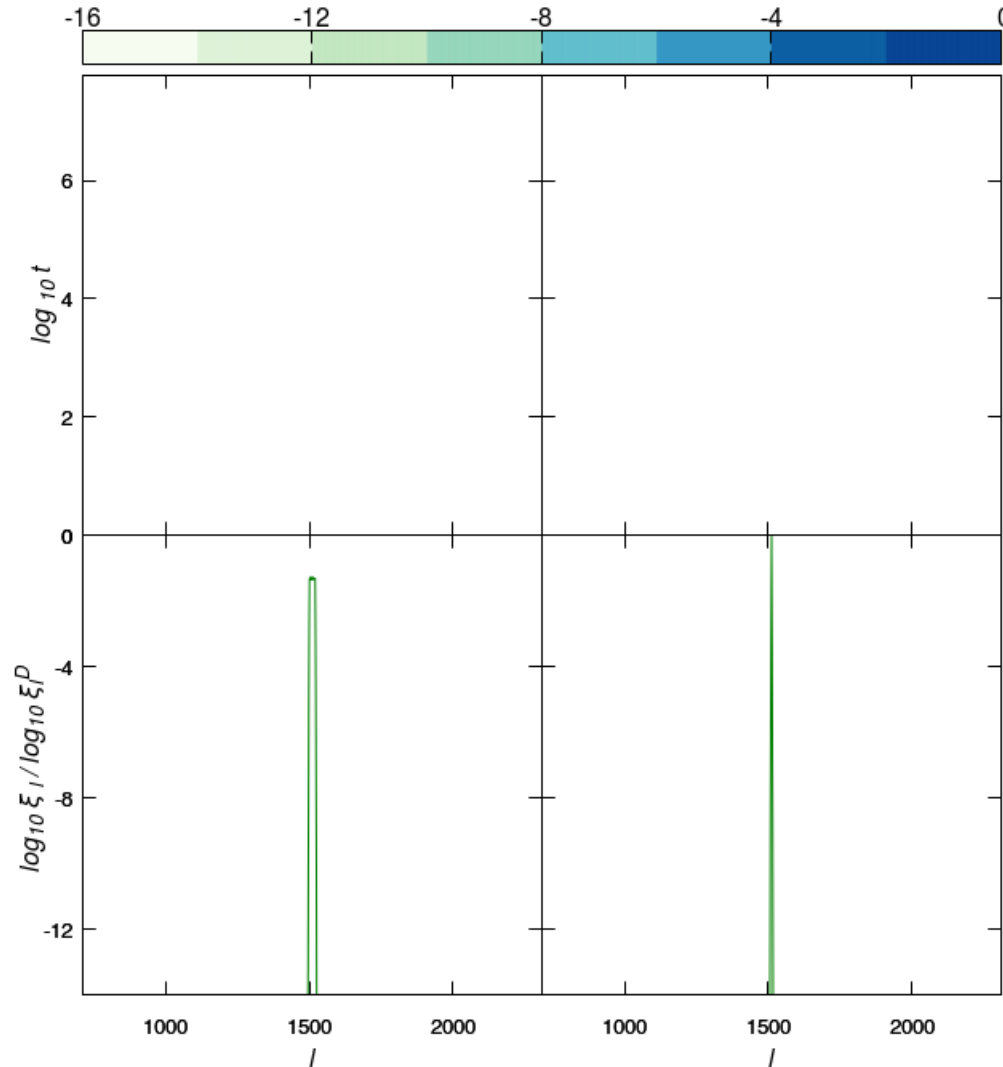
Norm

DVD

Deviation Vector Distributions (DVDs)

DDNLS: strong chaos W=3.5, L=21, β=0.72

Norm

DVD
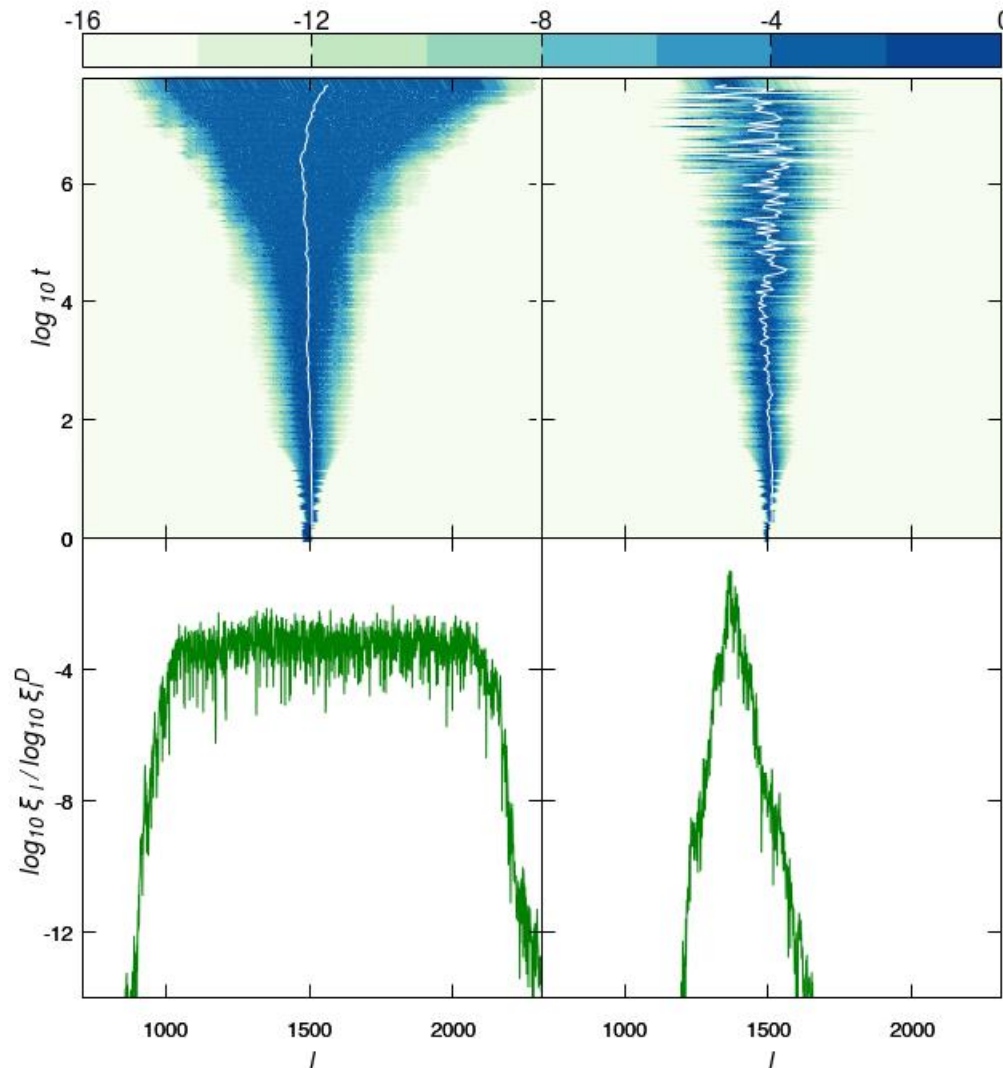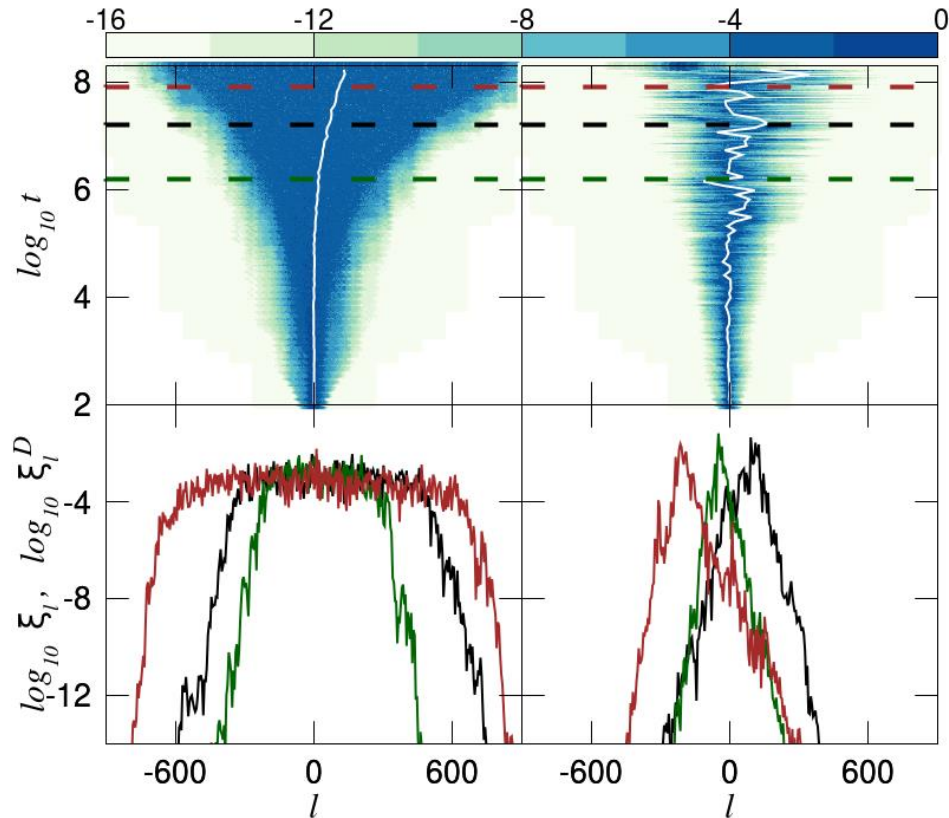
Strong Chaos: DKG and DDNLS

DKG: W=3, L=83, E=8.3
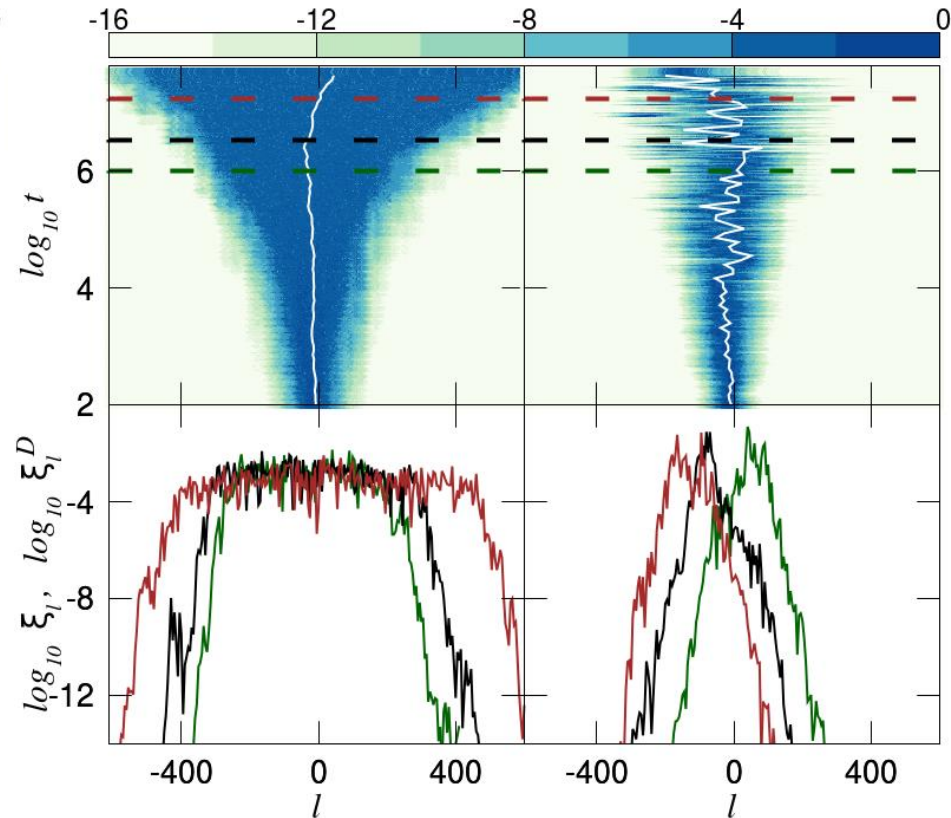
DDNLS: W=3.5, L=21, β=0.72
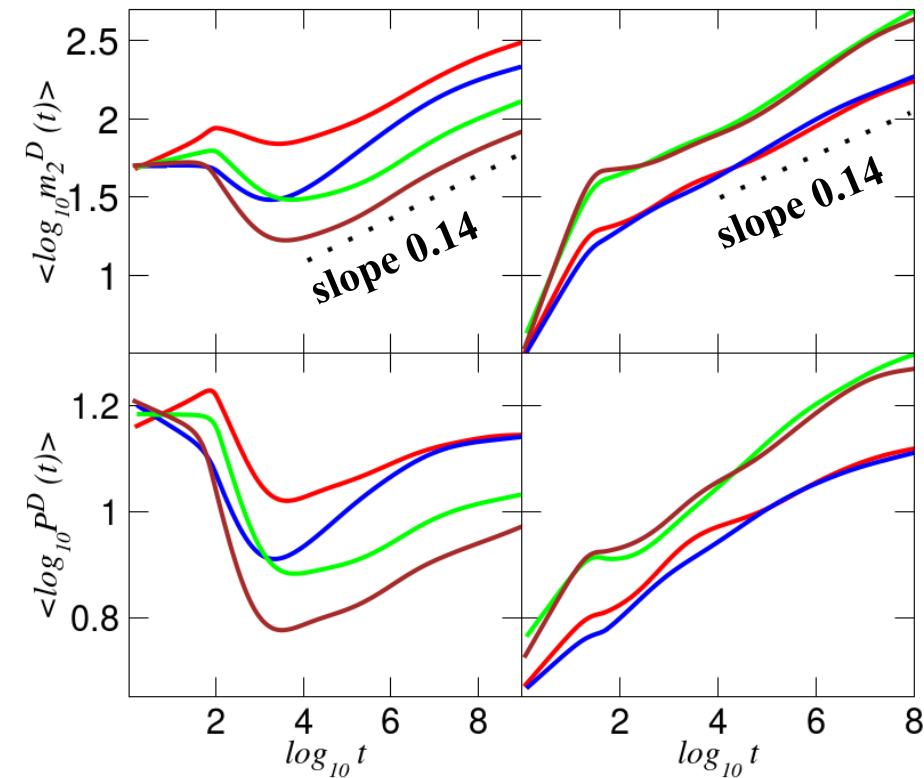
Characteristics of DVDs
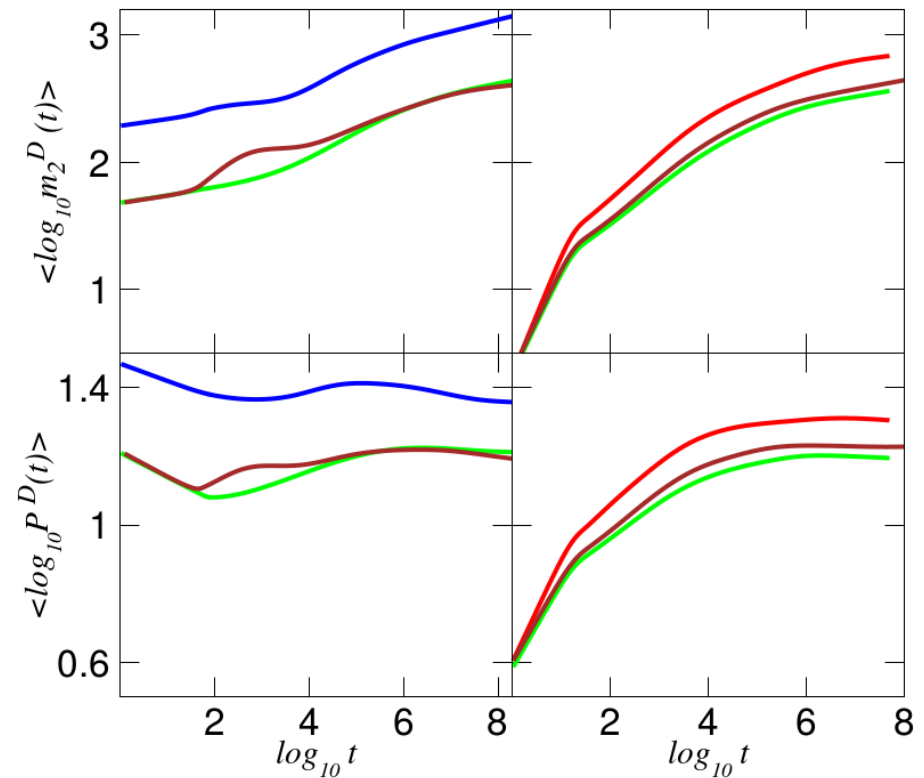
Characteristics of DVDs

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

DKG **DDNLS**

Weak chaos

slope 0.24 slope 0.24
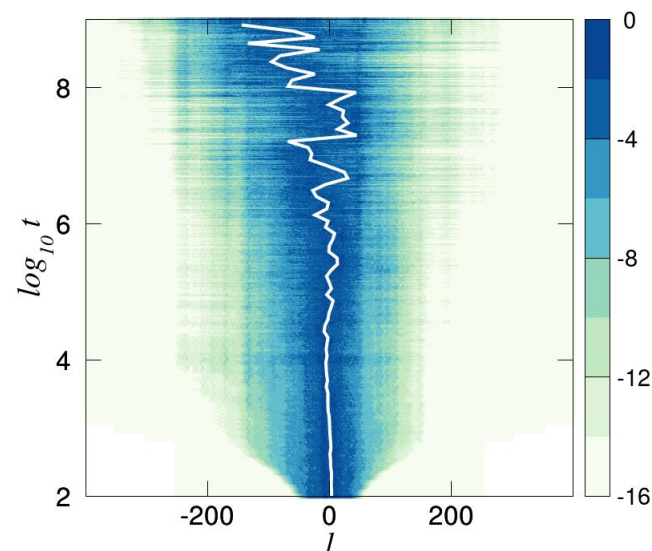
Strong chaos

Range of the lattice visited by the DVD

$$R(t) = \max_{[0,t]} \left\{ \overline{l}_w(t) \right\} - \min_{[0,t]} \left\{ \overline{l}_w(t) \right\}$$

$$\overline{l}_w = \sum_{l=1}^{N} l \xi_l^D$$
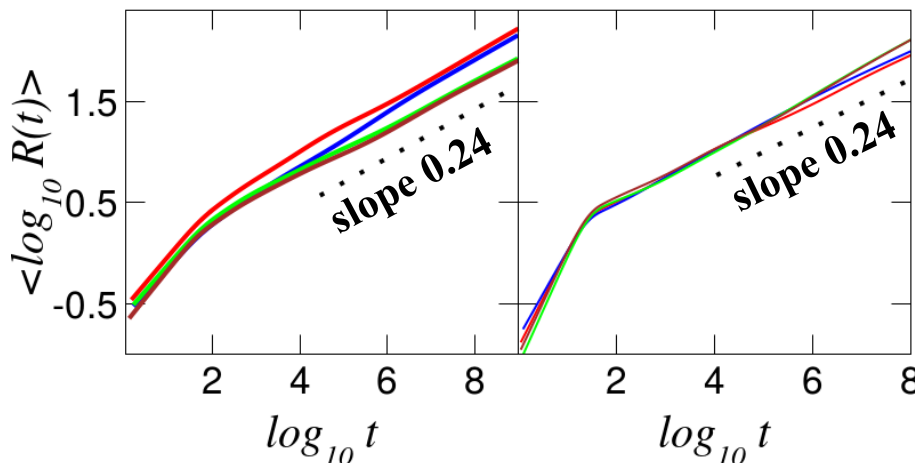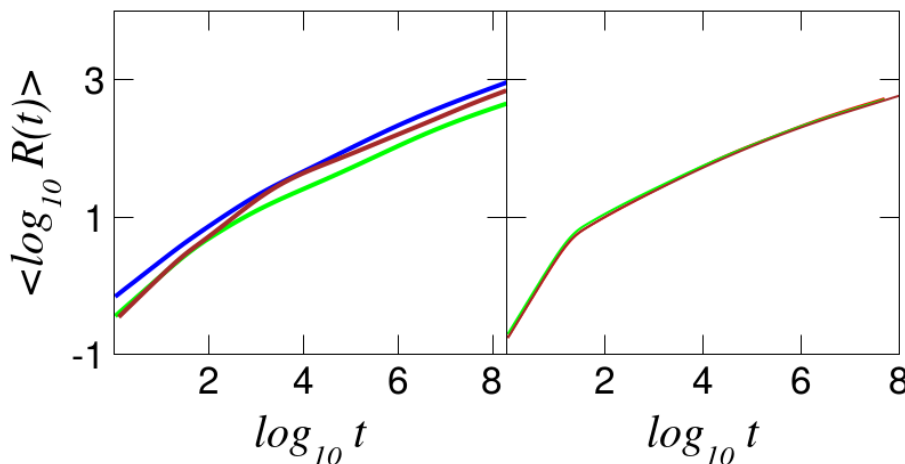
The

PBD model of DNA

DNA structure

Double helix with two types of bonds:

- **Adenine-thymine (AT) – two hydrogen bonds**
- **Guanine-cytosine (GC) – three hydrogen bonds**
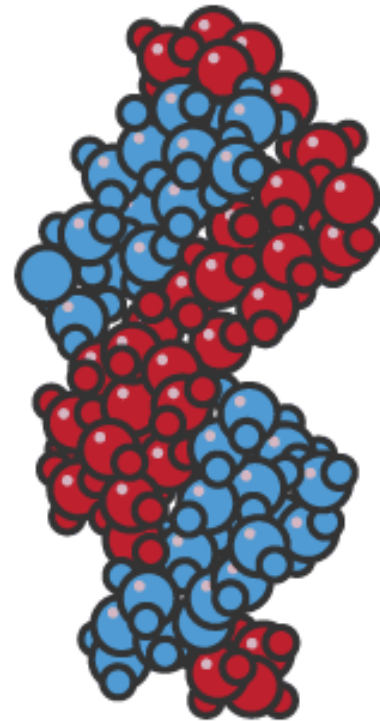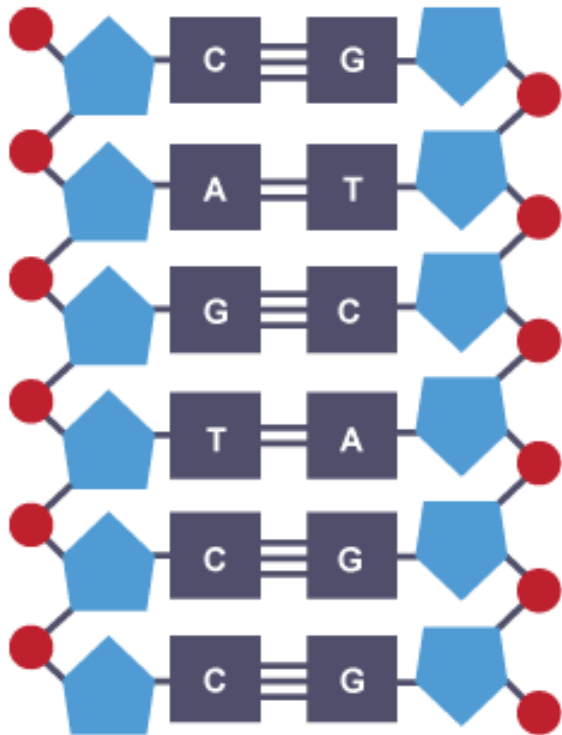
Hamiltonian model

Peyrard-Bishop-Dauxois (PBD) model
[Dauxois, Peyrard, Bishop, PRE (1993)]

$$H_N = \sum_{n=1}^{N} \left[\frac{1}{2m} p_n^2 + D_n (e^{-a_n y_n} - 1)^2 + \frac{K}{2} (1 + \rho e^{-b(y_n + y_{n-1})})(y_n - y_{n-1})^2 \right]$$

Bond potential energy (Morse potential)
GC: D=0.075 eV, a=6.9 Å^{-1}
AT: D=0.05 eV, a=4.2 Å^{-1}

Nearest neighbors coupling potential
K=0.025 eV/Å^2, ρ=2, b=0.35 Å^{-1}

Disorder realizations

Different arrangements of AT and GC bonds.

AT AT AT AT AT AT AT AT AT AT

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$P_{AT}=1$ (100% AT bonds)

Disorder realizations

Different arrangements of AT and GC bonds.

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$P_{AT}=1$ **(100% AT bonds)**

GC AT AT GC GC GC GC AT AT GC

🔵 🔴 🔴 🔵 🔵 🔵 🔵 🔴 🔴 🔵

$P_{AT}=0.4$ **(40% AT bonds)**

Disorder realizations

Different arrangements of AT and GC bonds.

AT AT AT AT AT AT AT AT AT AT
● ● ● ● ● ● ● ● ● ● $P_{AT}=1$ (100% AT bonds)

GC AT AT GC GC GC GC AT AT GC
● ● ● ● ● ● ● ● ● ● $P_{AT}=0.4$ (40% AT bonds)

GC AT AT AT GC AT GC GC GC GC
● ● ● ● ● ● ● ● ● ●

Disorder realizations

Different arrangements of AT and GC bonds.

AT AT AT AT AT AT AT AT AT AT

● ● ● ● ● ● ● ● ● ●

$P_{AT}=1$ (100% AT bonds)

GC AT AT GC GC GC GC AT AT GC

● ● ● ● ● ● ● ● ● ●

$P_{AT}=0.4$ (40% AT bonds)

GC AT AT AT GC AT GC GC GC GC

● ● ● ● ● ● ● ● ● ●
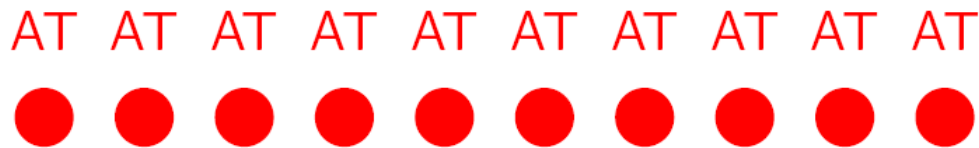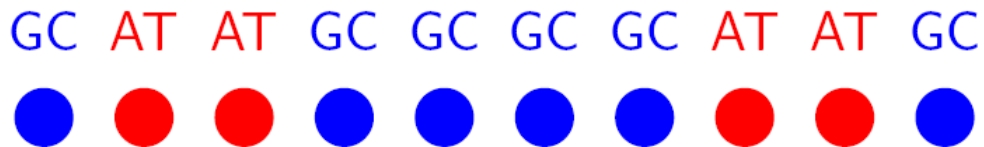
Periodic boundary conditions
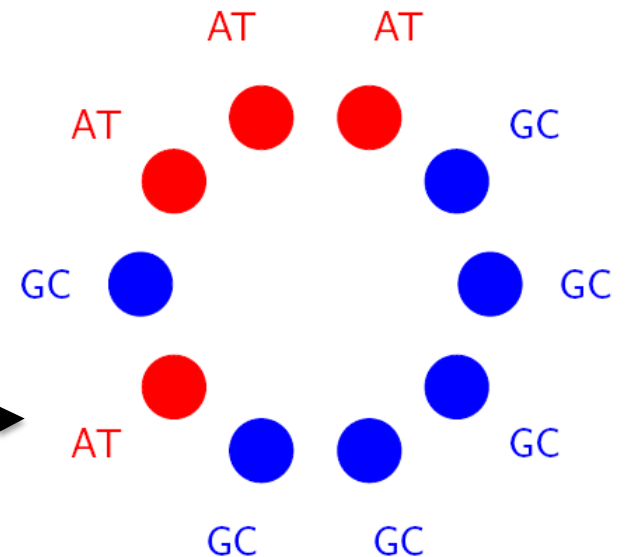
Lyapunov exponents (E/n=0.04, P_{AT}=0.3)
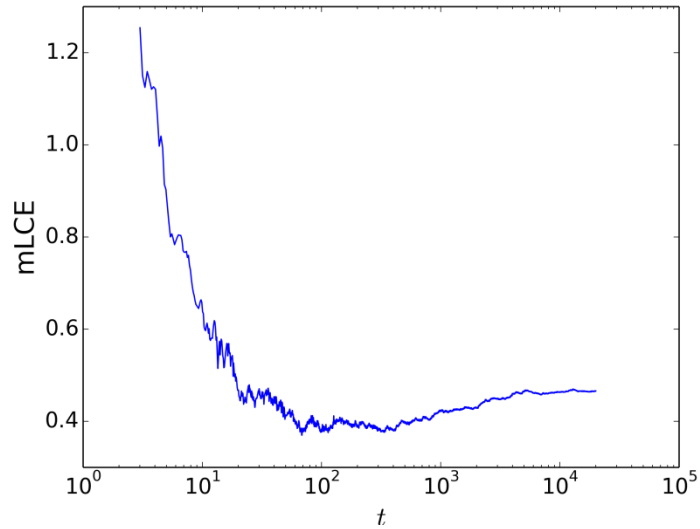
1 realization, 1 initial condition

Lyapunov exponents (E/n=0.04, P_{AT}=0.3)
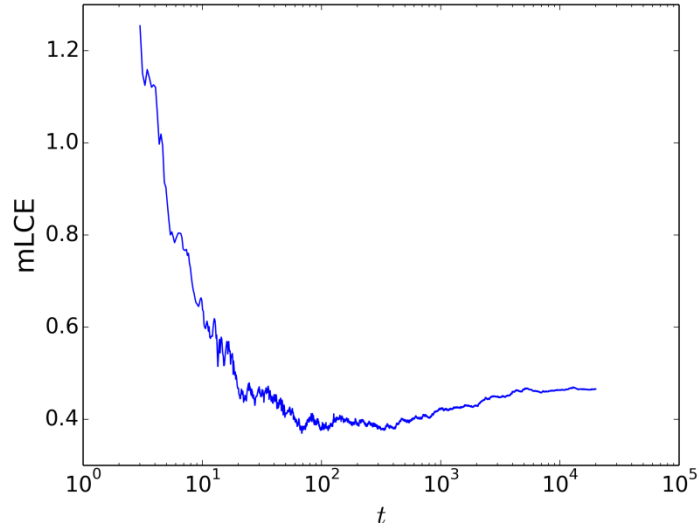
1 realization, 1 initial condition

1 realization, 10 initial conditions
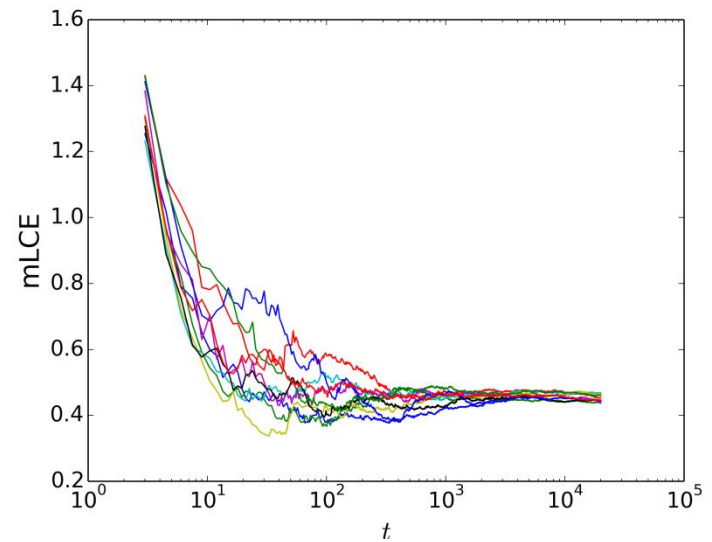
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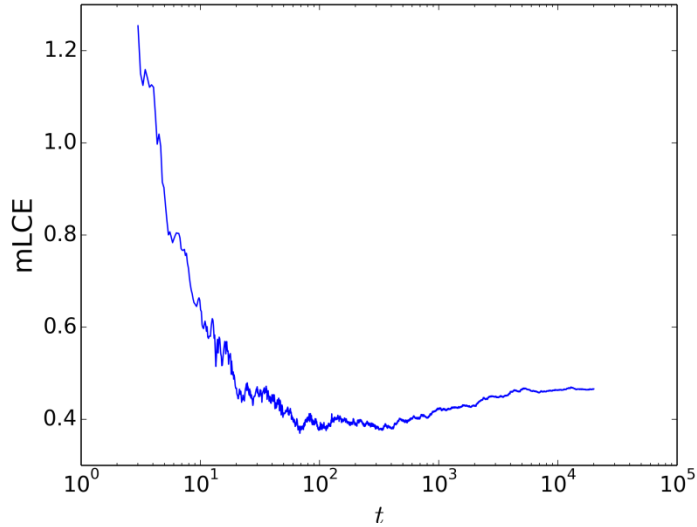
1 realization, 1 initial condition

1 realization, 10 initial conditions
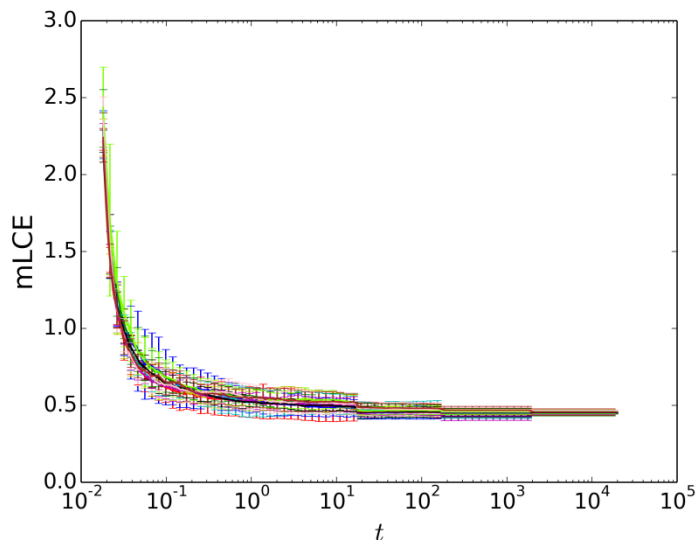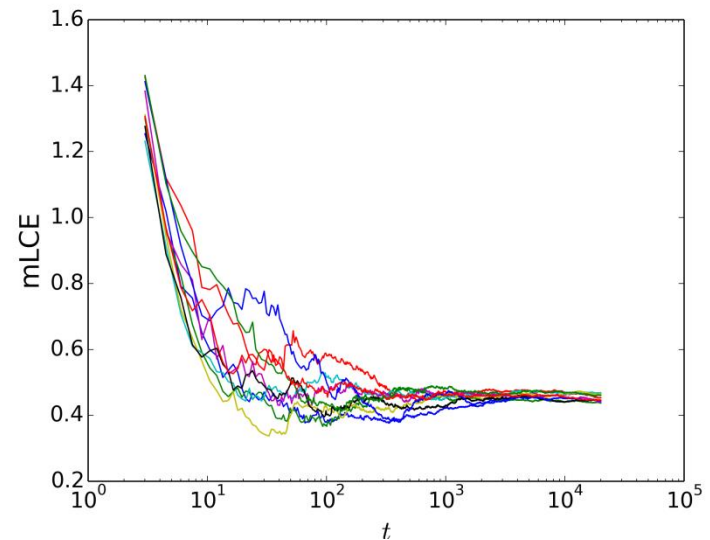
10 realizations, 10 initial conditions
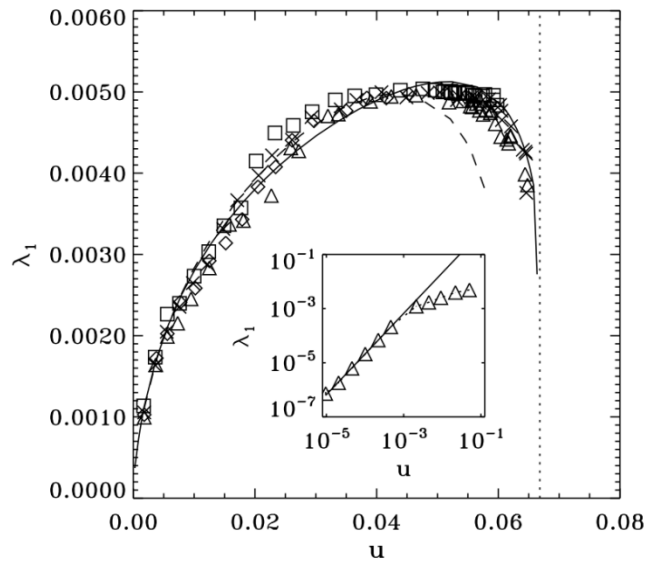
Lyapunov exponent vs. energy per particle

**Homogeneous chain
[Barré & Dauxois,
EPL (2001)]**

Lyapunov exponent vs. energy per particle

Homogeneous chain [Barré & Dauxois, EPL (2001)]
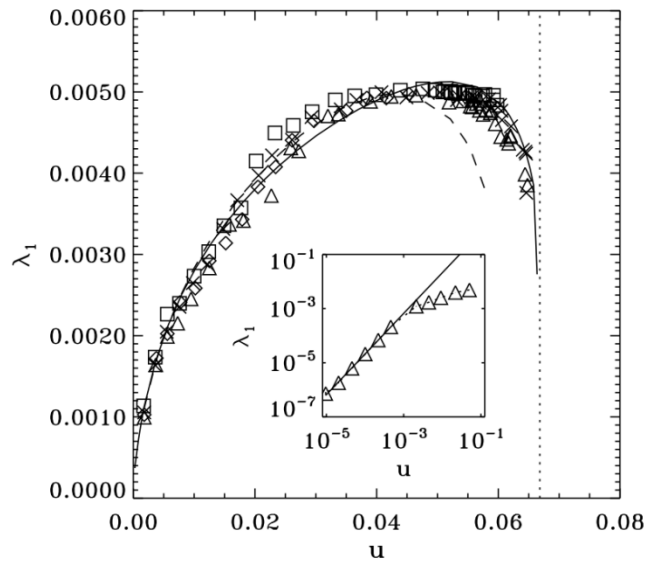
Lyapunov exponent vs. energy per particle
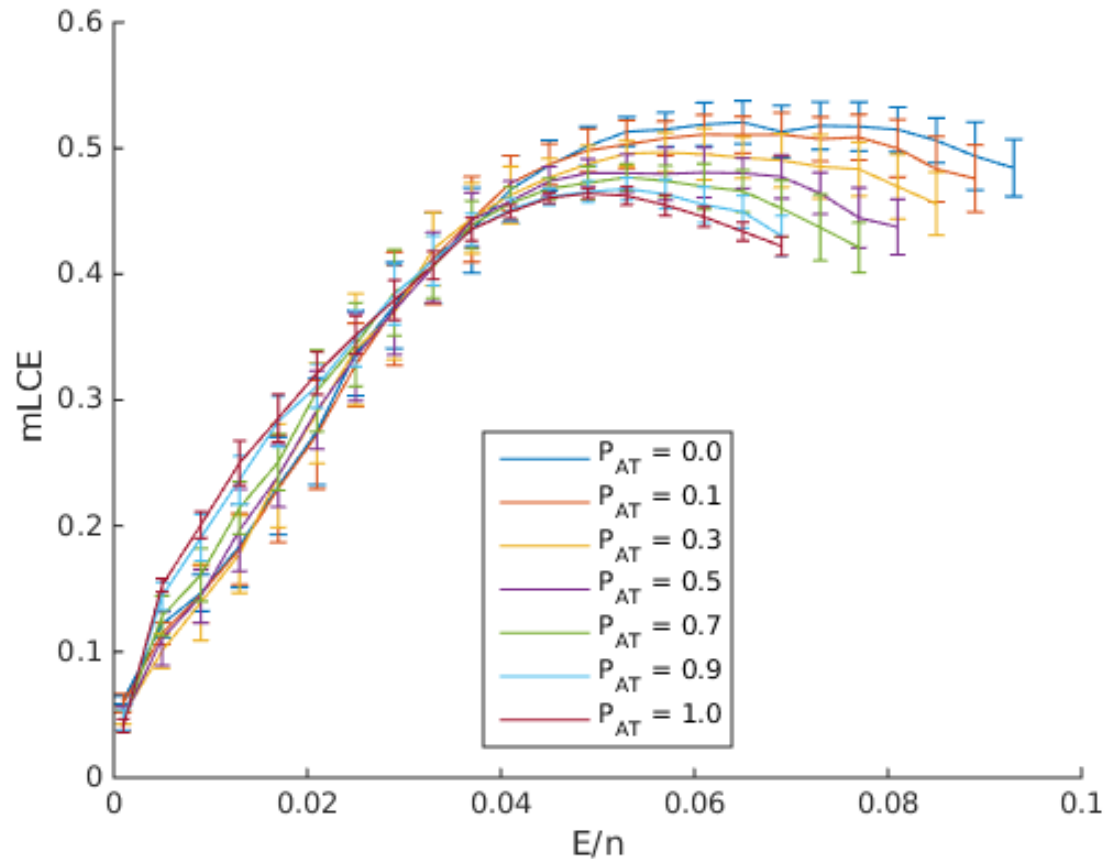
Homogeneous chain
[Barré & Dauxois,
EPL (2001)]
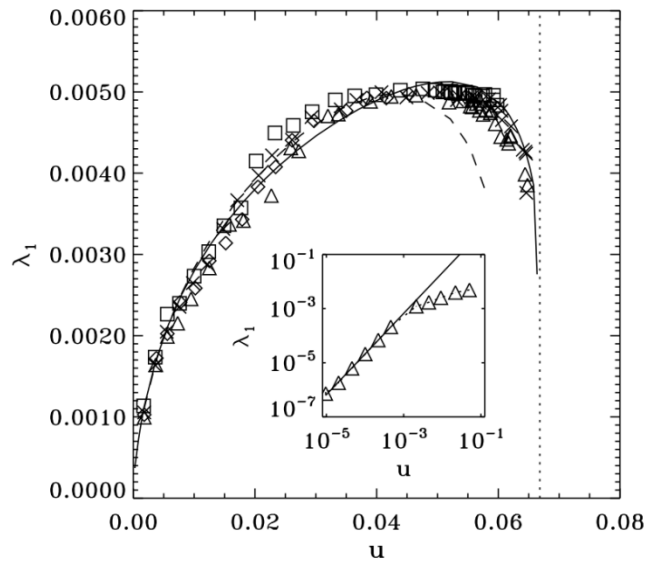
GC chains
more chaotic
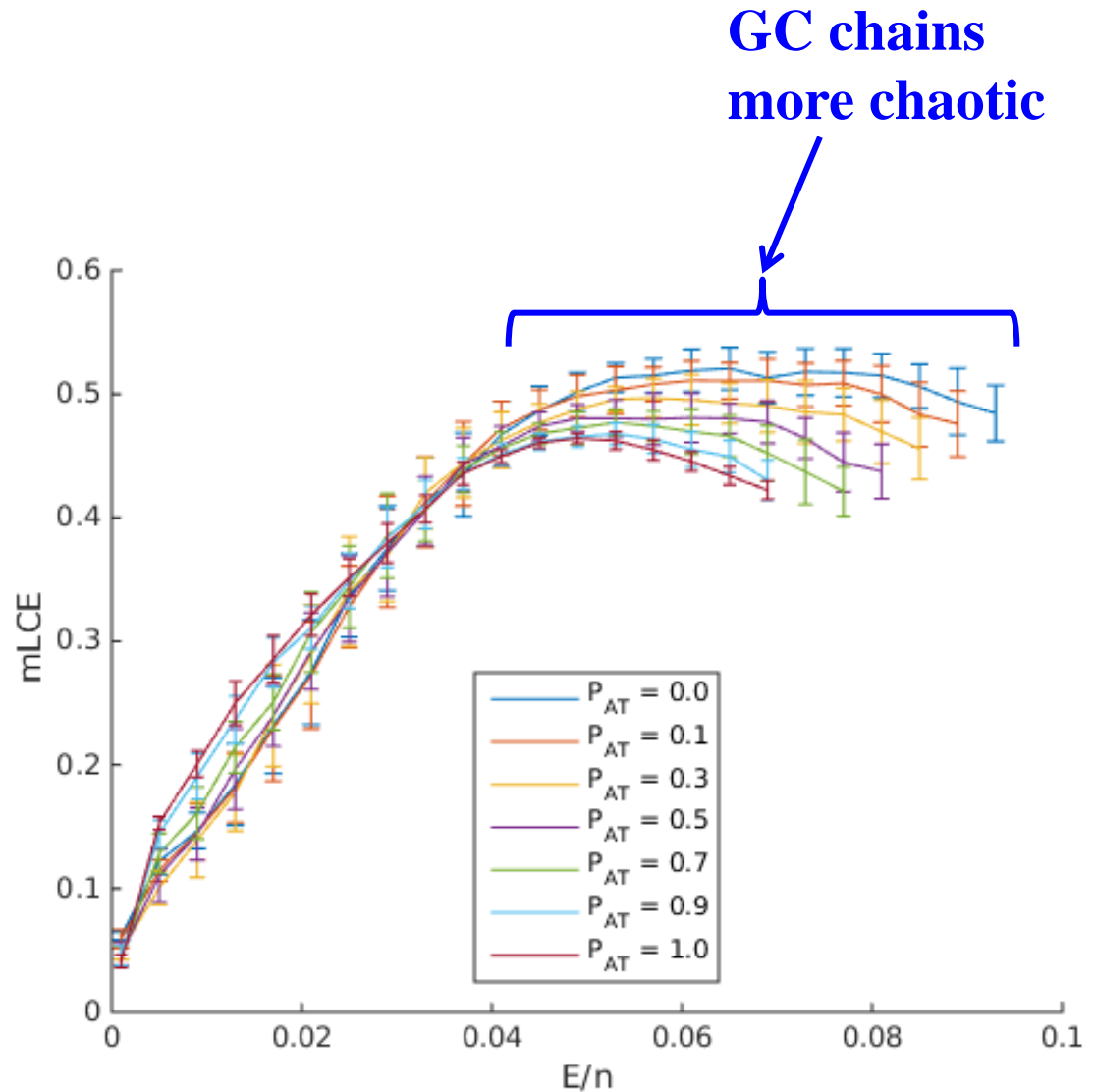
Lyapunov exponent vs. energy per particle

AT chains more chaotic

GC chains more chaotic
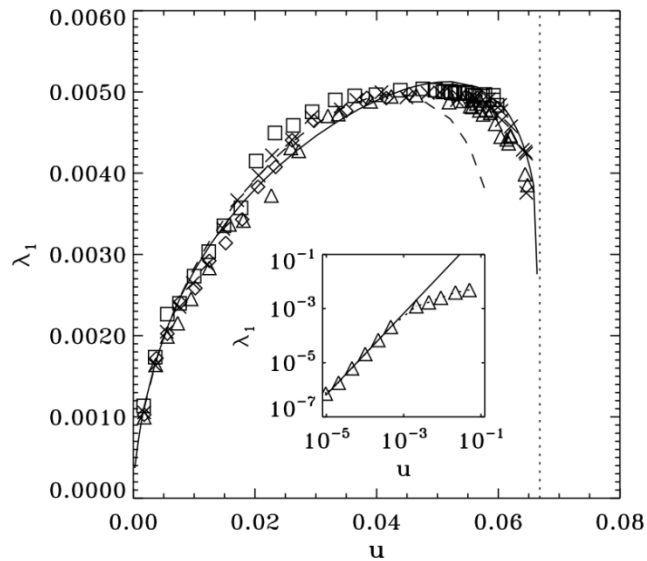
Homogeneous chain [Barré & Dauxois, EPL (2001)]

$P_{AT} = 0.0$
$P_{AT} = 0.1$
$P_{AT} = 0.3$
$P_{AT} = 0.5$
$P_{AT} = 0.7$
$P_{AT} = 0.9$
$P_{AT} = 1.0$
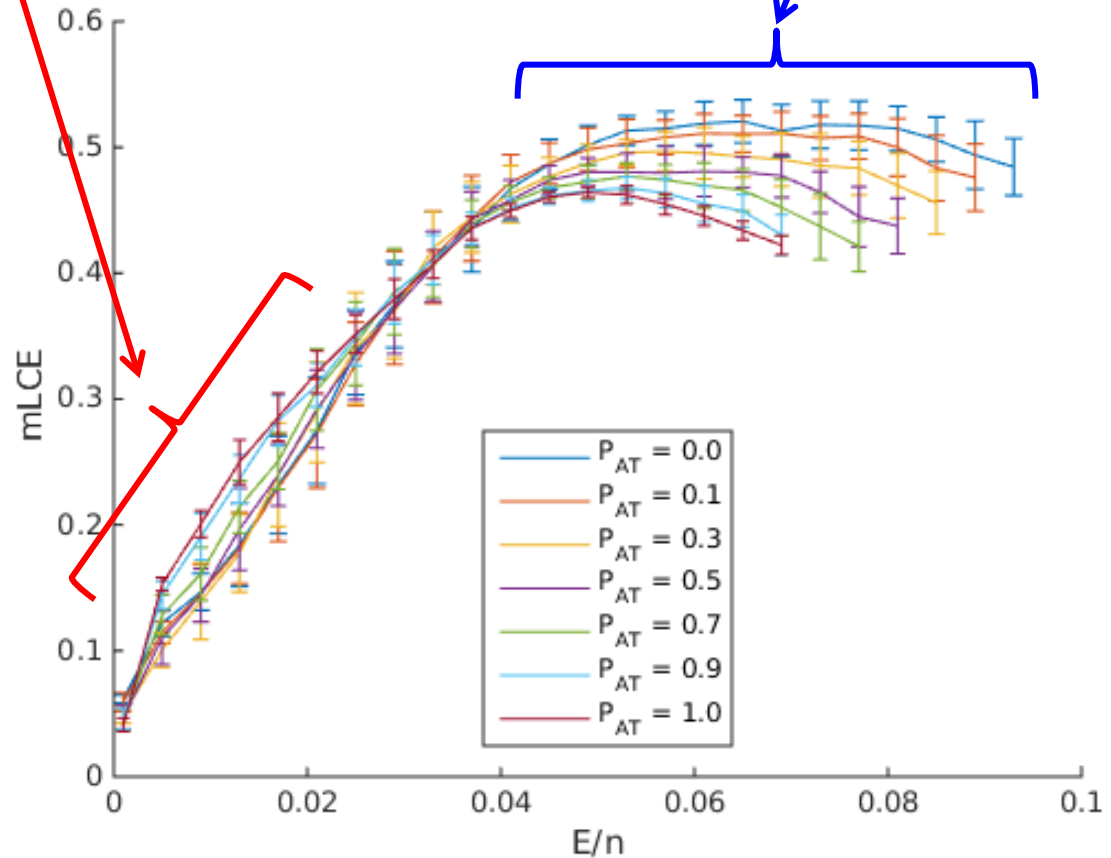
Lyapunov exponent vs. energy per particle

AT chains more chaotic

Type of chain does not play a role

GC chains more chaotic

Homogeneous chain
[Barré & Dauxois, EPL (2001)]

$P_{AT} = 0.0$
$P_{AT} = 0.1$
$P_{AT} = 0.3$
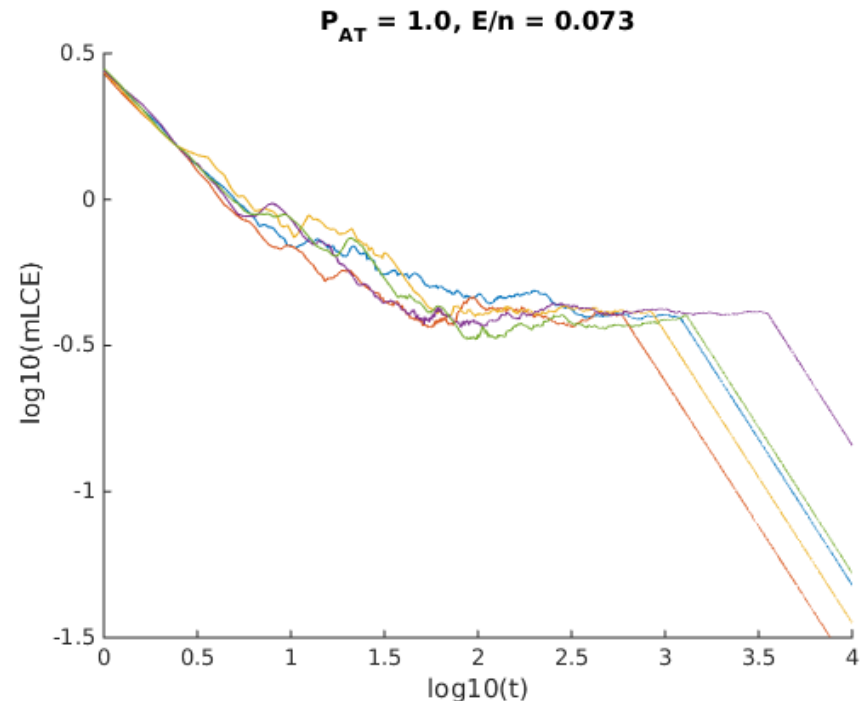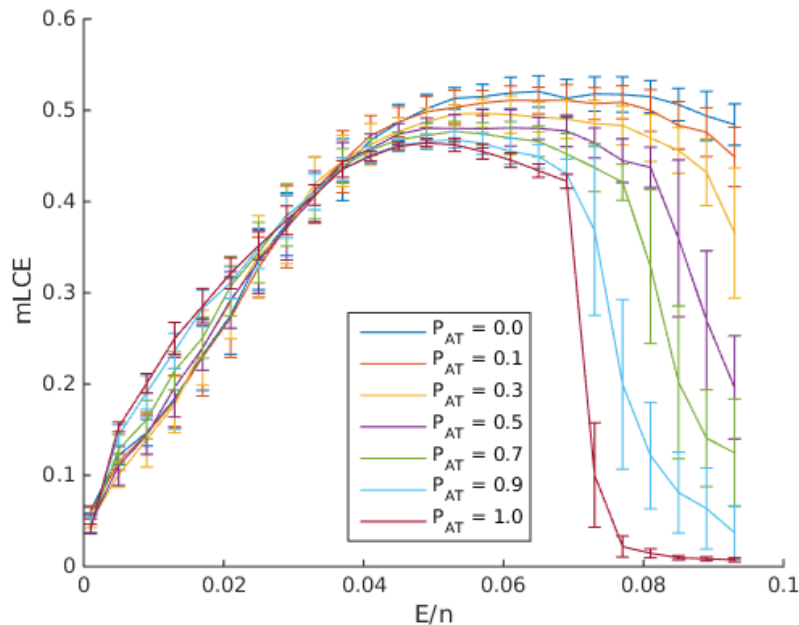$P_{AT} = 0.5$
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DNA denaturation (melting)

Melting: large bubbles forming in the DNA chain as bonds break
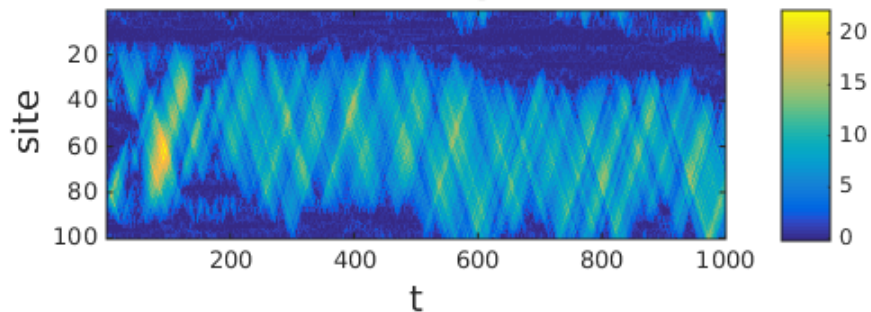

Temperature

As y_n increases the exponentials in

$$D_n(e^{-a_n y_n} - 1)^2 + \frac{K}{2}(1 + \rho e^{-b(y_n + y_{n-1})})(y_n - y_{n-1})^2$$

tend to 0, the system becomes effectively linear and the mLCE →0.

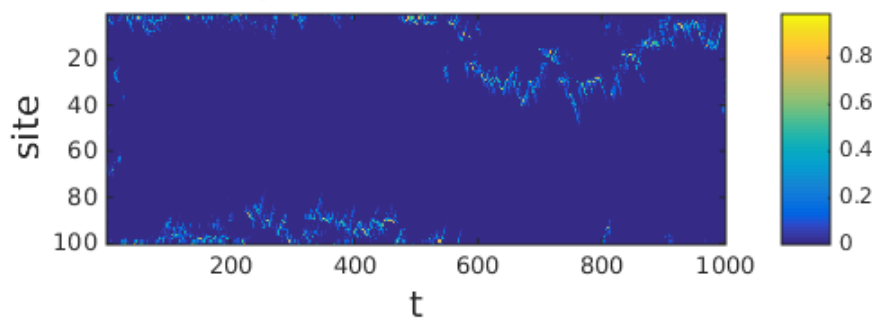# DNA denaturation (melting)

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$P_{AT} = 1.0, E/n = 0.073$

DVD and the formation of bubbles

DVD and the formation of bubbles
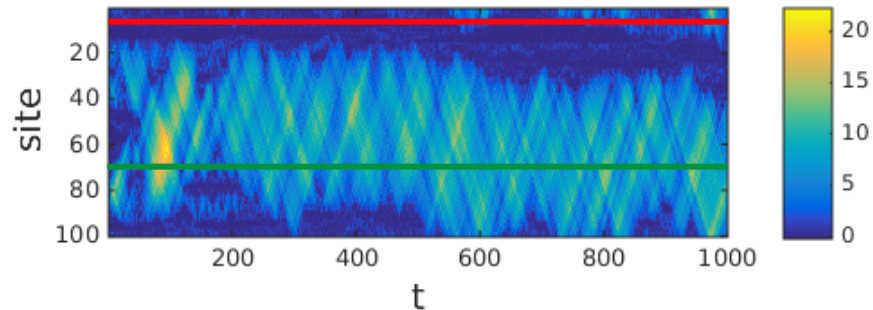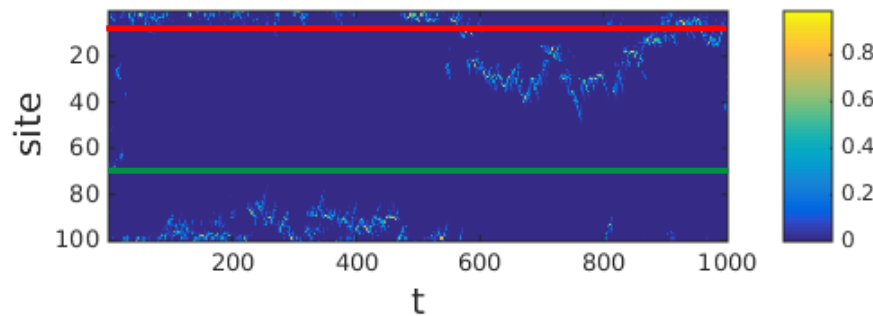
DVD and the formation of bubbles

DVD and the formation of bubbles

Relation between the concentration of the deviation vector at a site and the formation of a bubble at that site.
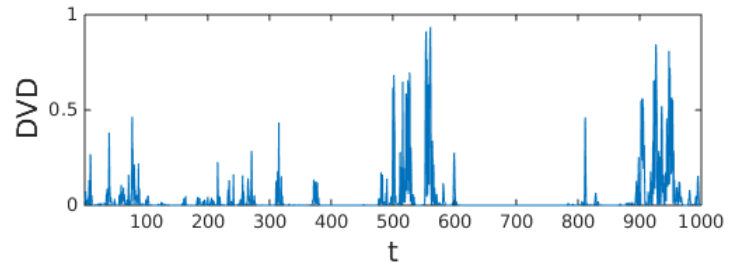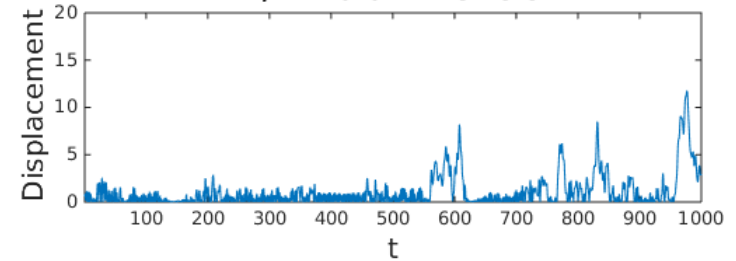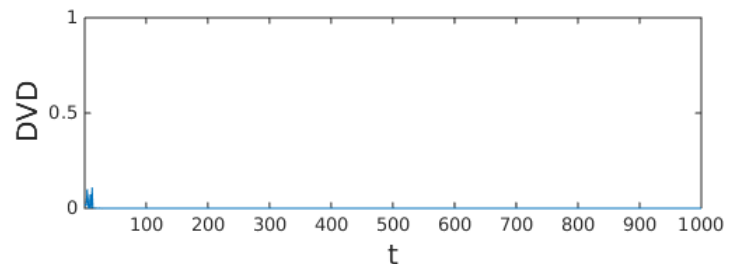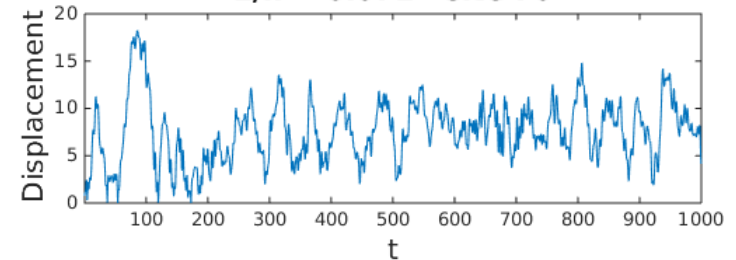
Future works

- **DKG and DDNLS models in 2 spatial dimensions**

- **Extended, sequence-dependent PBD models of DNA**

- **Models of granular material**

- **Graphene models**

Future works

DDNLS in 2 spatial dimensions (strong chaos)

Norm　　　**DVD**　　　　　**Norm**　　　　**DVD**

Future works

DDNLS in 2 spatial dimensions (strong chaos)

Norm   **DVD**   **Norm**   **DVD**

Summary

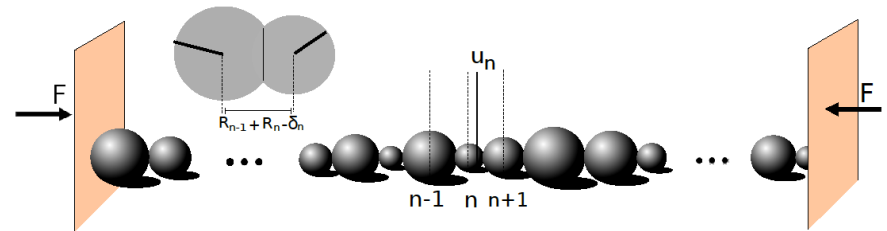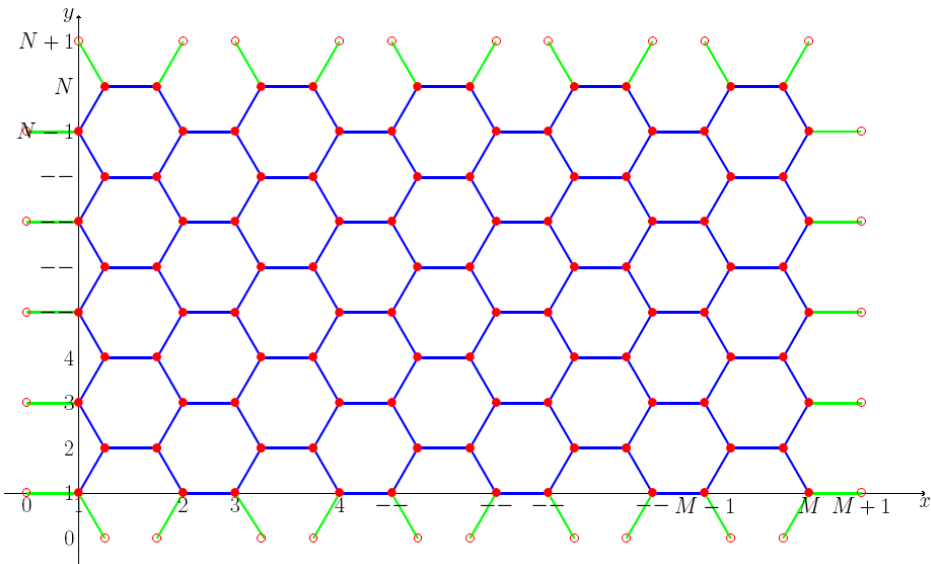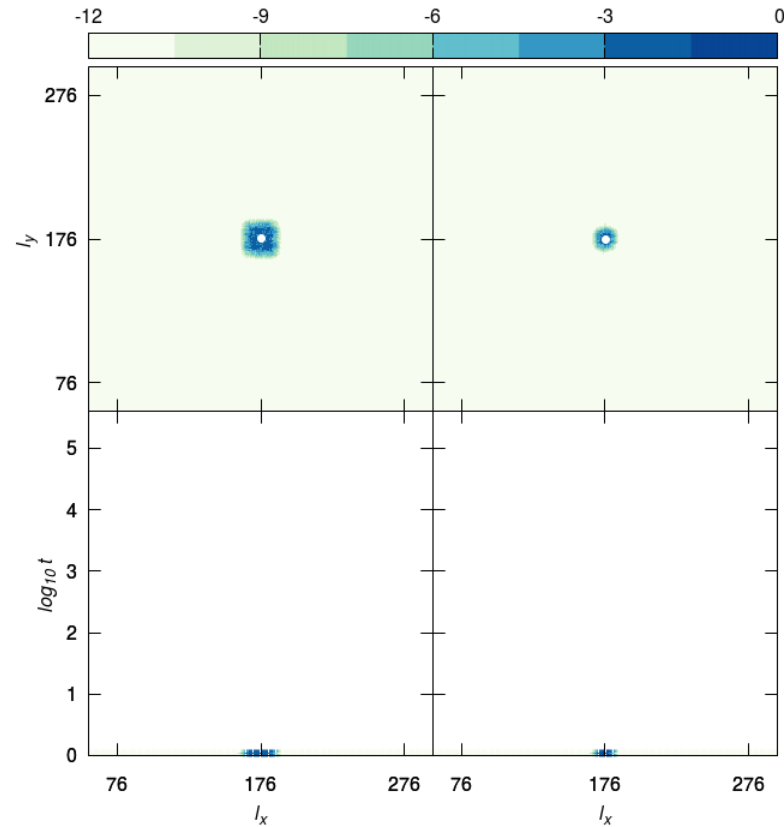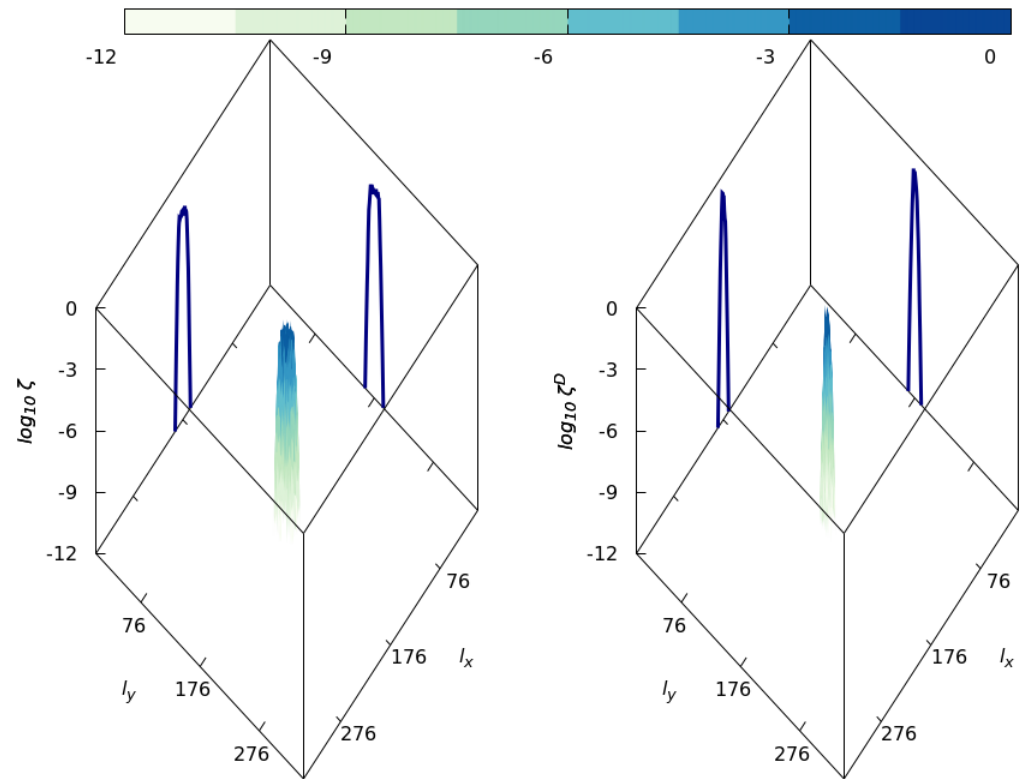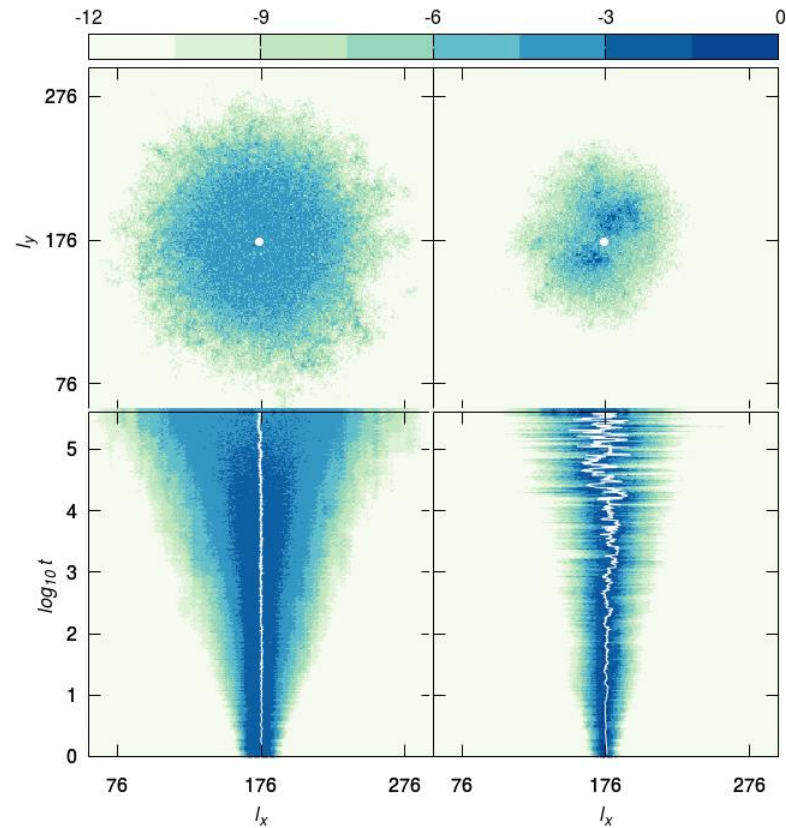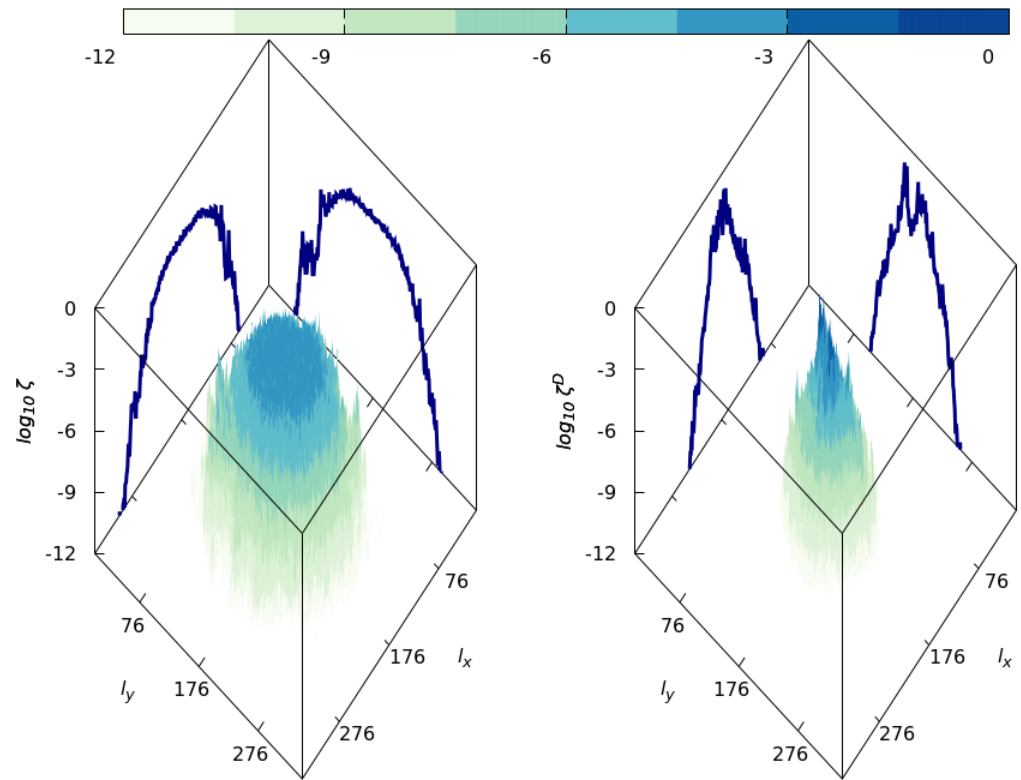- **Both the DKG and the DDNLS models show similar chaotic behaviors**

- **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.

- **Heterogeneity influences the chaotic behavior of the DNA** chaotic behavior.

- There seems to be a **relation between the concentration of the DVD at a site and the formation of a bubble**

B. Senyange, B. Many Manda & Ch. S.: Phys. Rev. E, **98**, 052229 (2018) 'Characteristics of chaos evolution in one-dimensional disordered nonlinear lattices'

M. Hillebrand, G. Kalosakas, A. Schwellnus & Ch. S.: Phys. Rev. E, **99**, 022213 (2019) 'Heterogeneity and chaos in the Peyrard-Bishop-Dauxois DNA model '

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