Heterogeneity and chaos: Granular chains and DNA models

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Adrian Schwellnus, Malcolm Hillebrand, George Kalosakas

Outline

- **Chaotic behavior of granular chains**
  - ✓ **Weakly nonlinear regime: Long-lived chaotic Anderson-like localization**
  - ✓ **Highly nonlinear regime: equilibrium chaotic state**

- **DNA models**
  - ✓ **Lyapunov exponents**
  - ✓ **Different dynamical regimes**
  - ✓ **DNA melting**
  - ✓ **Deviation Vector Distributions**

- **Summary**

Energy Distributions

We consider normalized energy distributions

$$z_\nu \equiv \frac{E_\nu}{\sum_m E_m}$$ with E_ν being the energy of particle ν.

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

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

measures the number of stronger excited modes in z_ν.

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

Lyapunov Exponents (LEs) and Deviation Vector Distributions (DVDs)

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:

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

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

$\lambda_1 \neq 0 \rightarrow$ Chaotic motion

Deviation vector:

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

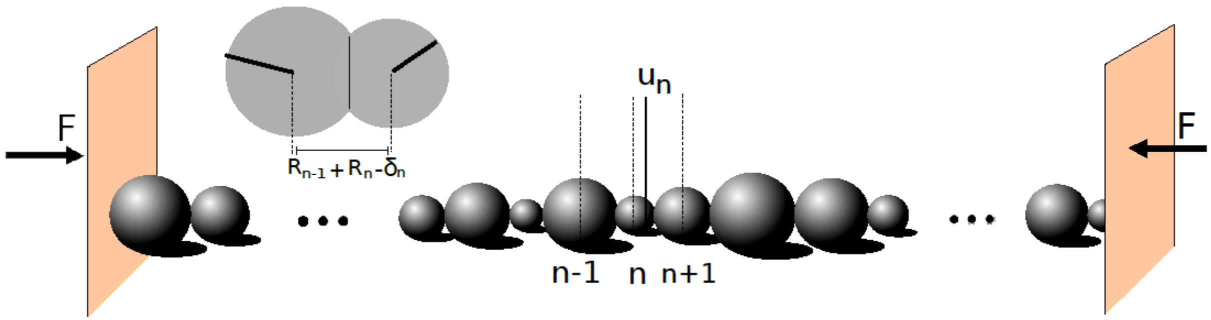
DVD: $w_l = \dfrac{\delta u_l^2 + \delta p_l^2}{\sum_l \left(\delta u_l^2 + \delta p_l^2 \right)}$

Granular media

Examples: coal, sand, rice, nuts, coffee etc.

1D granular chain (experimental control of nonlinearity and disorder)

Hamiltonian model



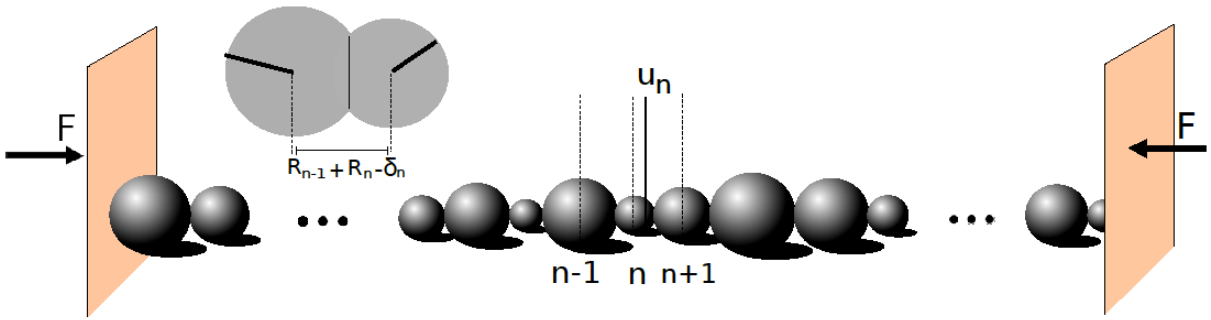
$$H=\sum_{n=1}^{N}\left(\frac{p_n^2}{2m_n}+\frac{2}{5}A_n[\delta_n+u_{n-1}-u_n]_+^{5/2}-\frac{2}{5}A_n\delta_n^{5/2}-A_n\delta_n^{3/2}(u_{n-1}-u_n)\right)$$

$$\delta_n=(F/A_n)^{2/3} \qquad A_n=(2/3)\mathcal{E}\sqrt{(R_{n-1}R_n)/(R_{n-1}+R_n)}/(1-\nu^2)$$

$[x]_+$=0 if x<0: formation of a gap. ν: Poisson's ratio, $\mathcal{E}$: Elastic modulus.

Hertzian forces between spherical beads. Fixed boundary conditions.

Hamiltonian model



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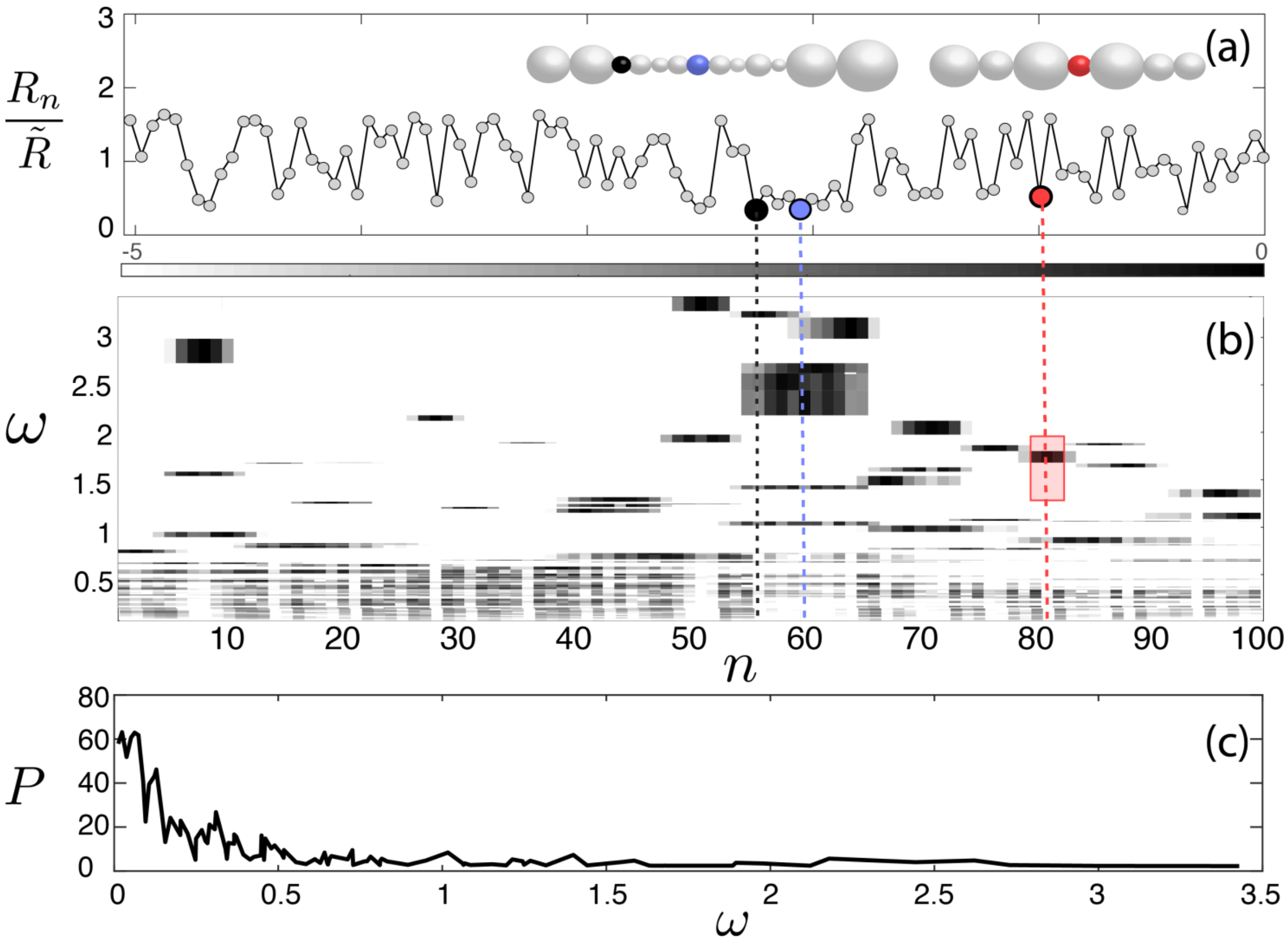
Disorder both in couplings and masses
$R_n \in [R, \alpha R]$ with $\alpha \geq 1$

Eigenmodes and single site excitations



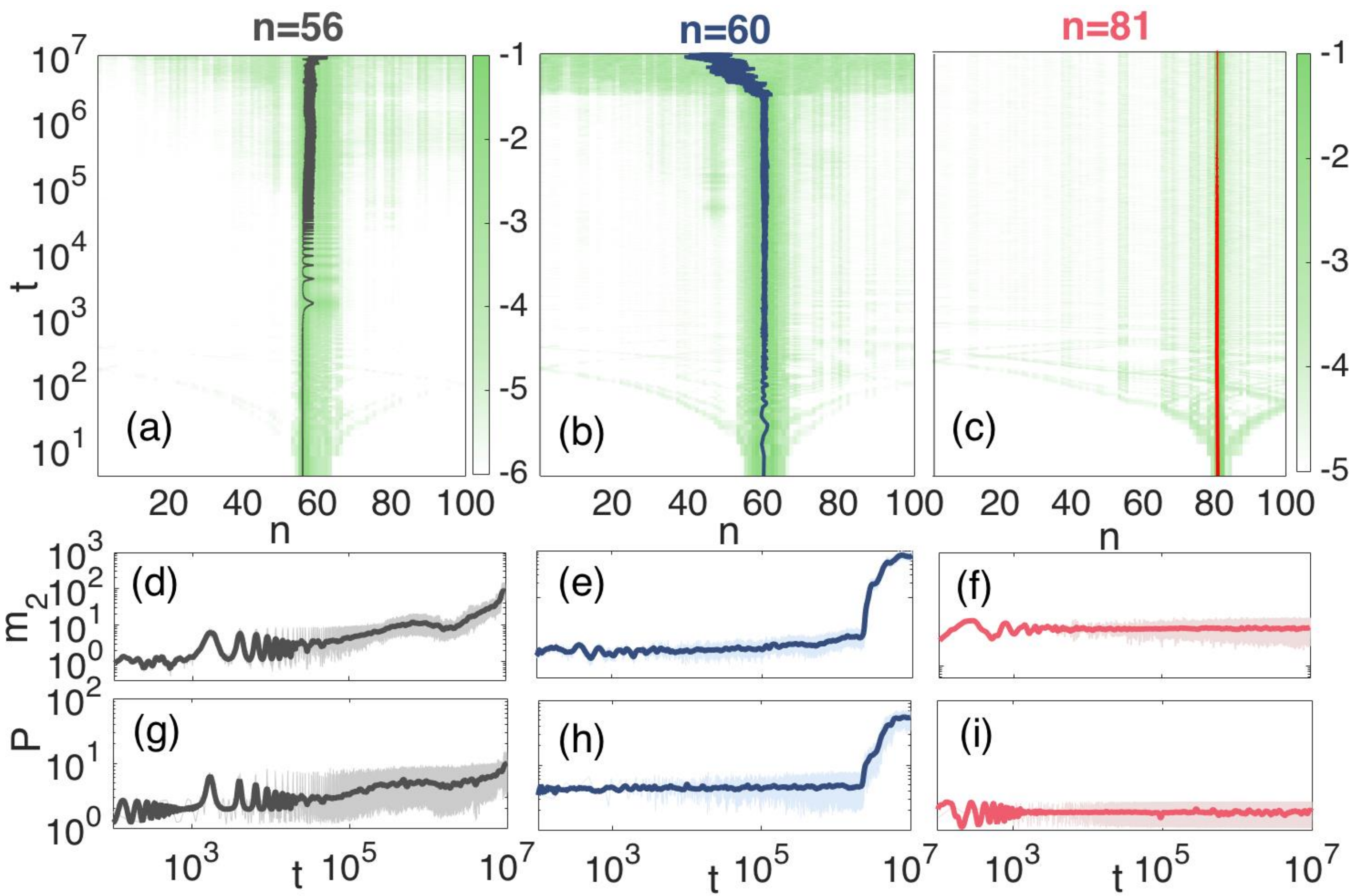
Disorder realization with N=100 beads

Displacement excitation of bead n

Participation number of eigenmodes. About 10 extended modes with P>40

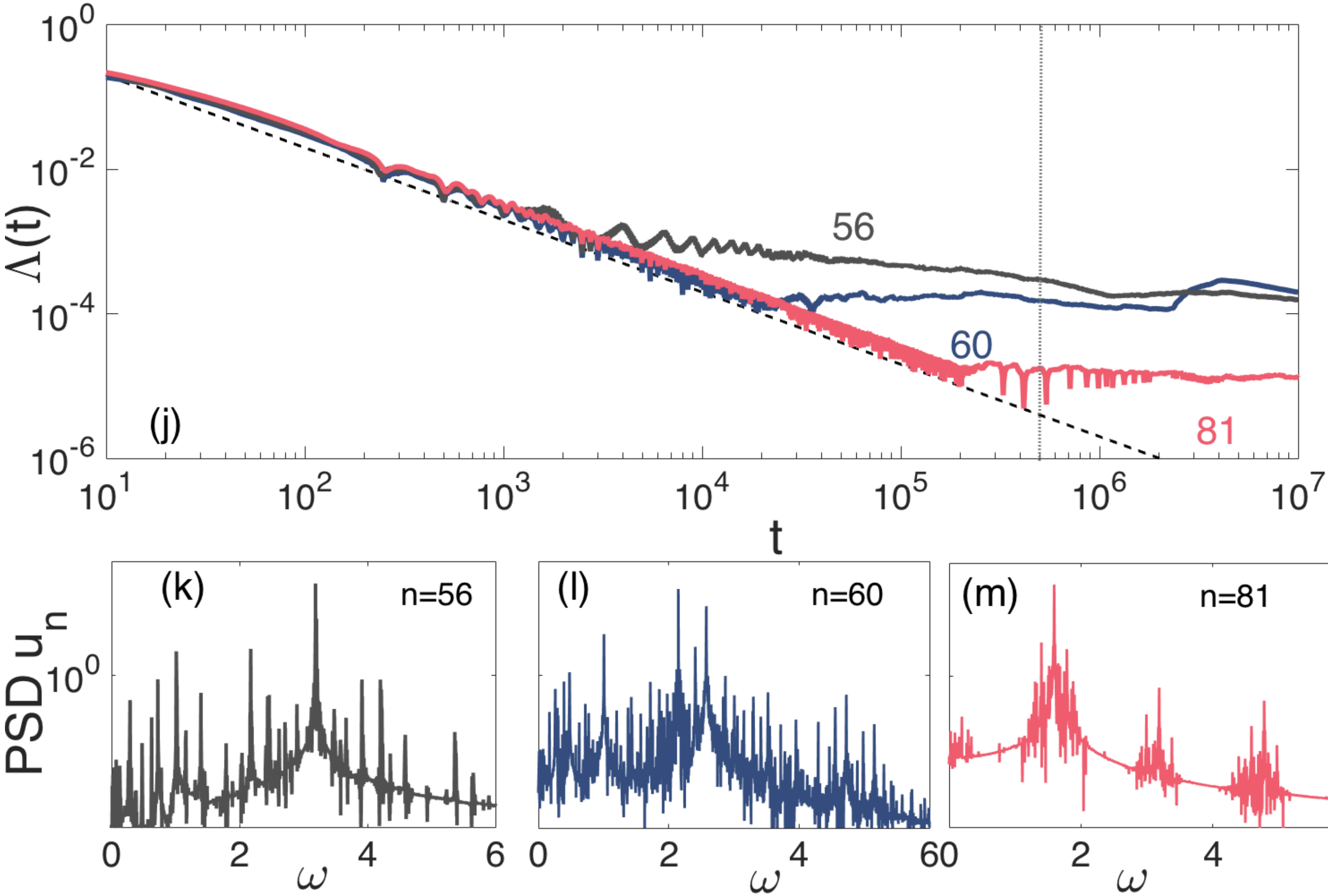
Achilleos et al. (2017) ArXiv:1707.03162

Weak nonlinearity: Long time evolution



Delocalization **Delocalization** **Localization**

Weak nonlinearity: Chaoticity



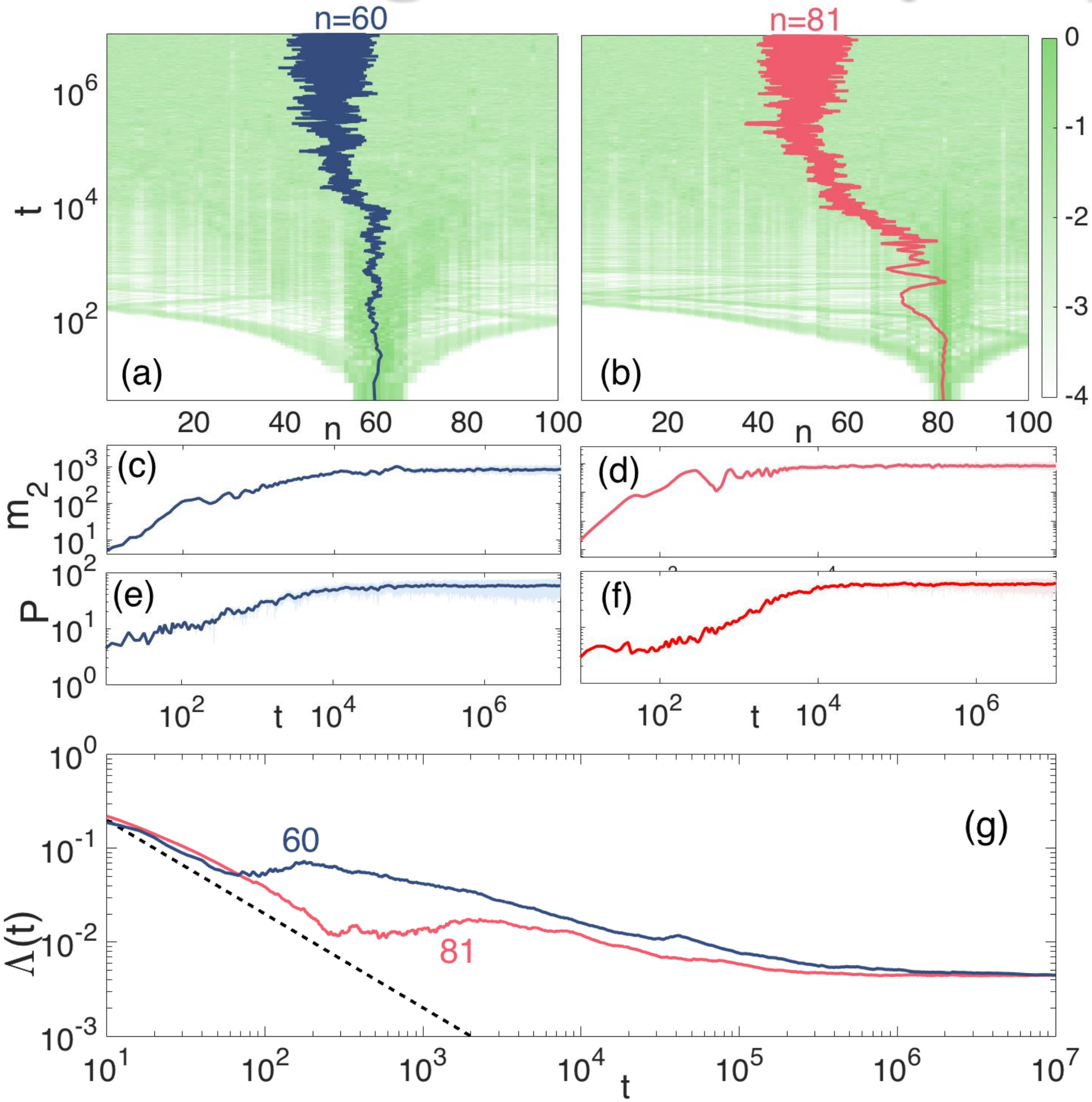
mLCE

Power Spectrum Distribution

Weakly chaotic motion: Delocalization

Long-lived chaotic Anderson-like Localization

Strong nonlinearity: Equipartition

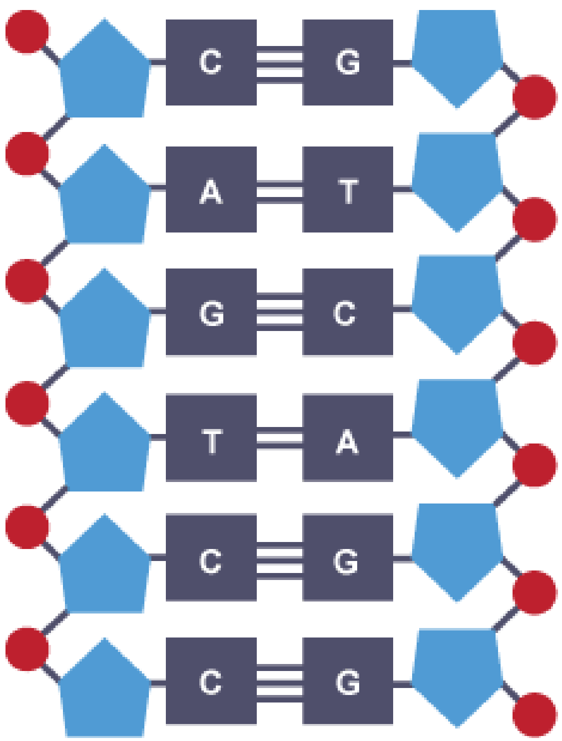


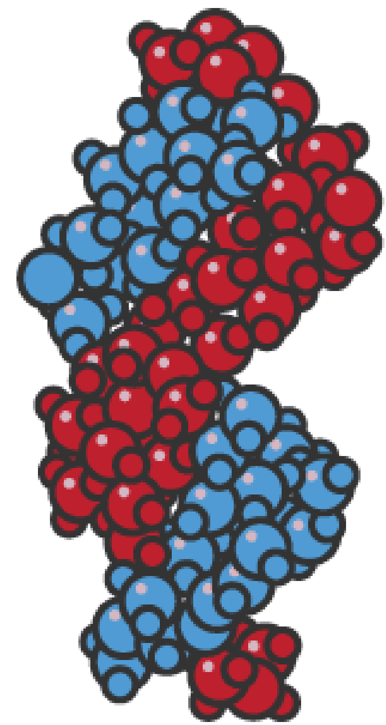
The granular chain reaches energy equipartition and an equilibrium chaotic state, independent of the initial position excitation.

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.

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

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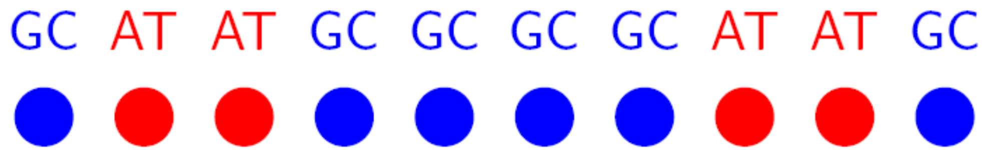

P_{AT}**=0.4 (40% AT bonds)**

Disorder realizations

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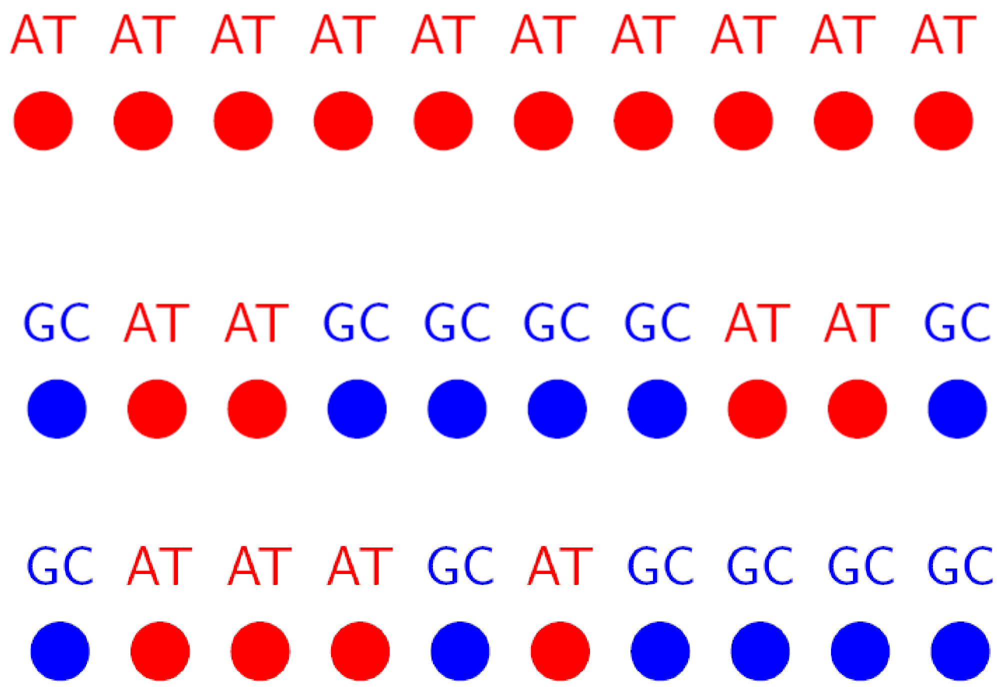

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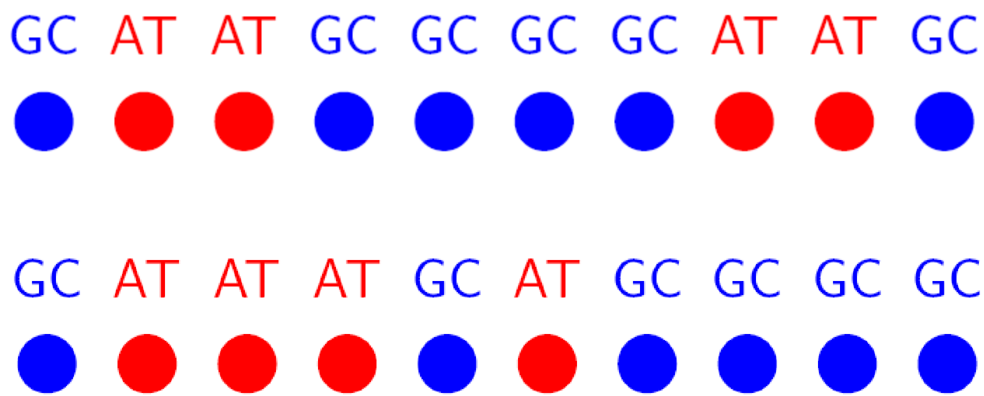

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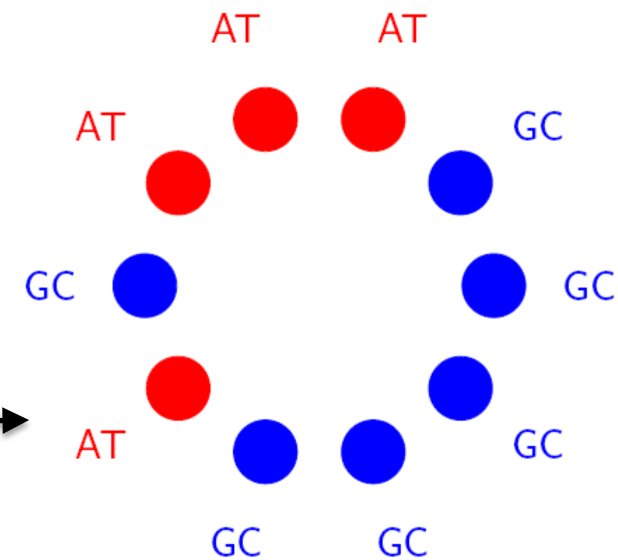
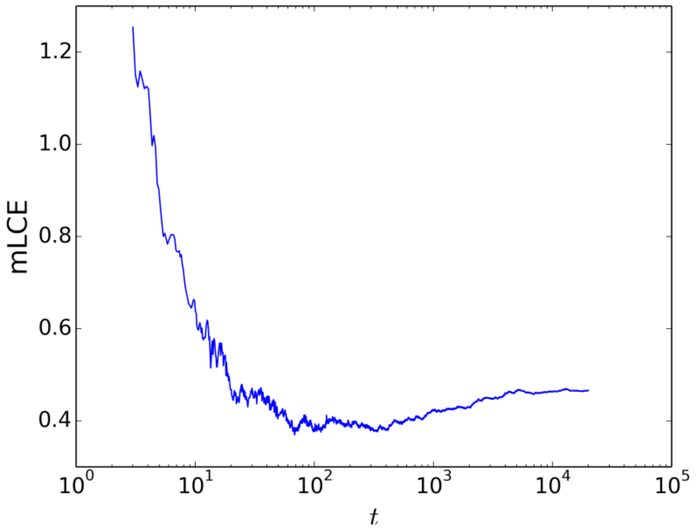
Periodic boundary conditions



Lyapunov exponents (E/n=0.04, P_{AT}=0.3)



1 realization, 1 initial condition

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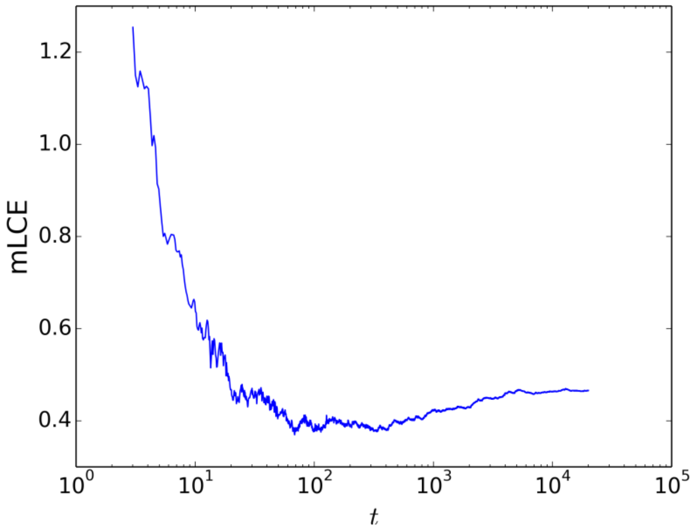
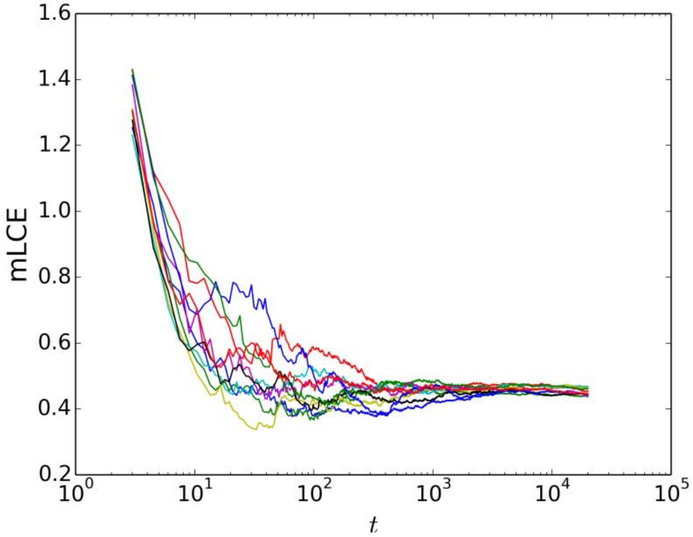


1 realization, 1 initial condition

1 realization, 10 initial conditions



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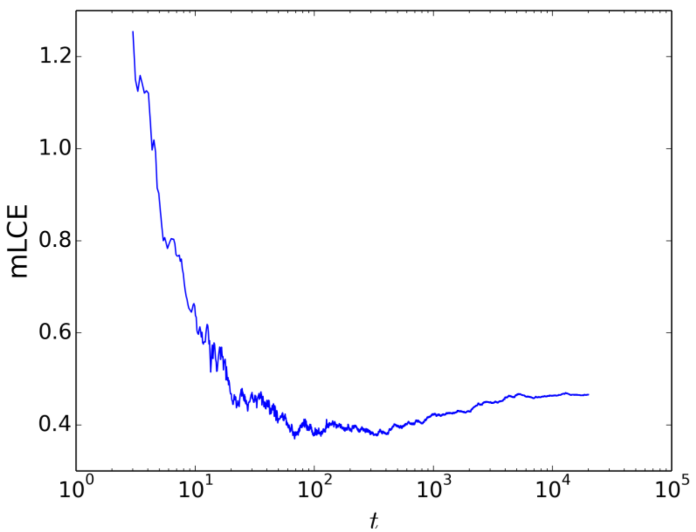

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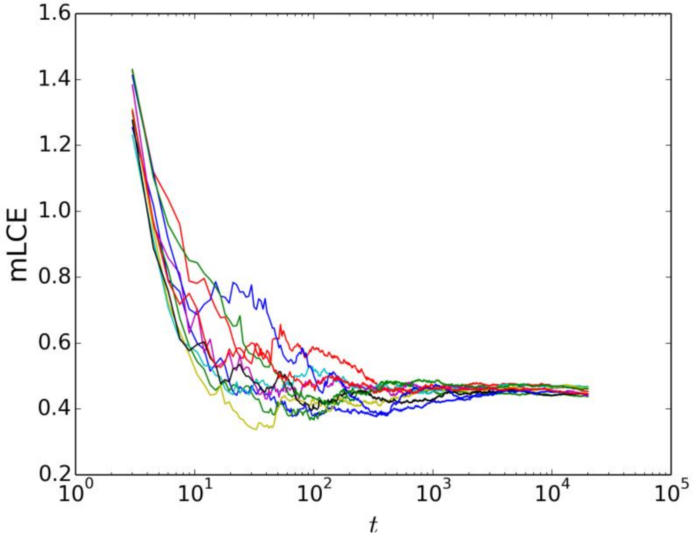
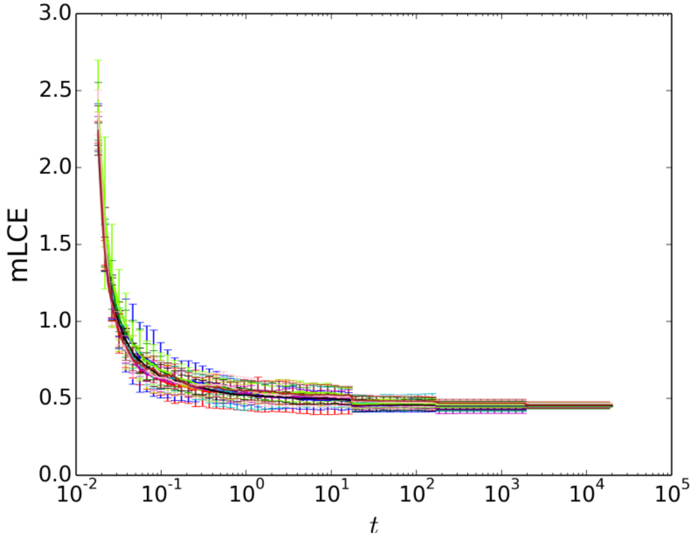
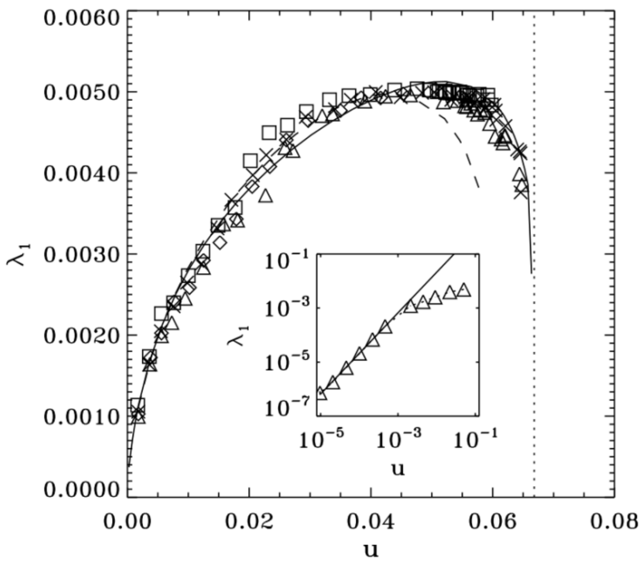




10 realizations, 10 initial conditions

Lyapunov exponent vs. energy per particle



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

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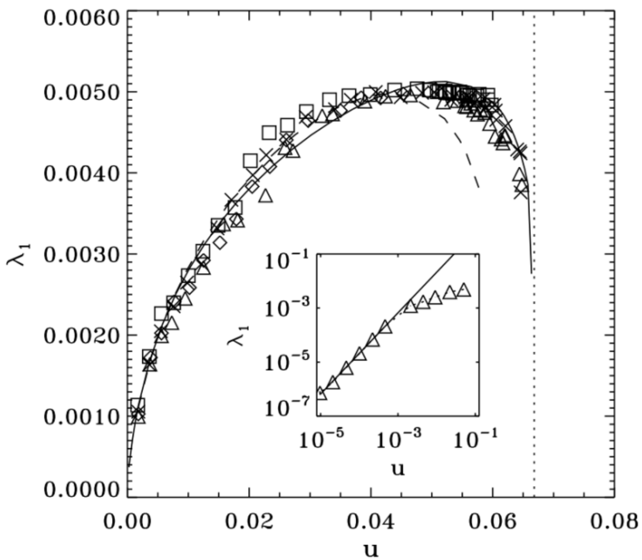

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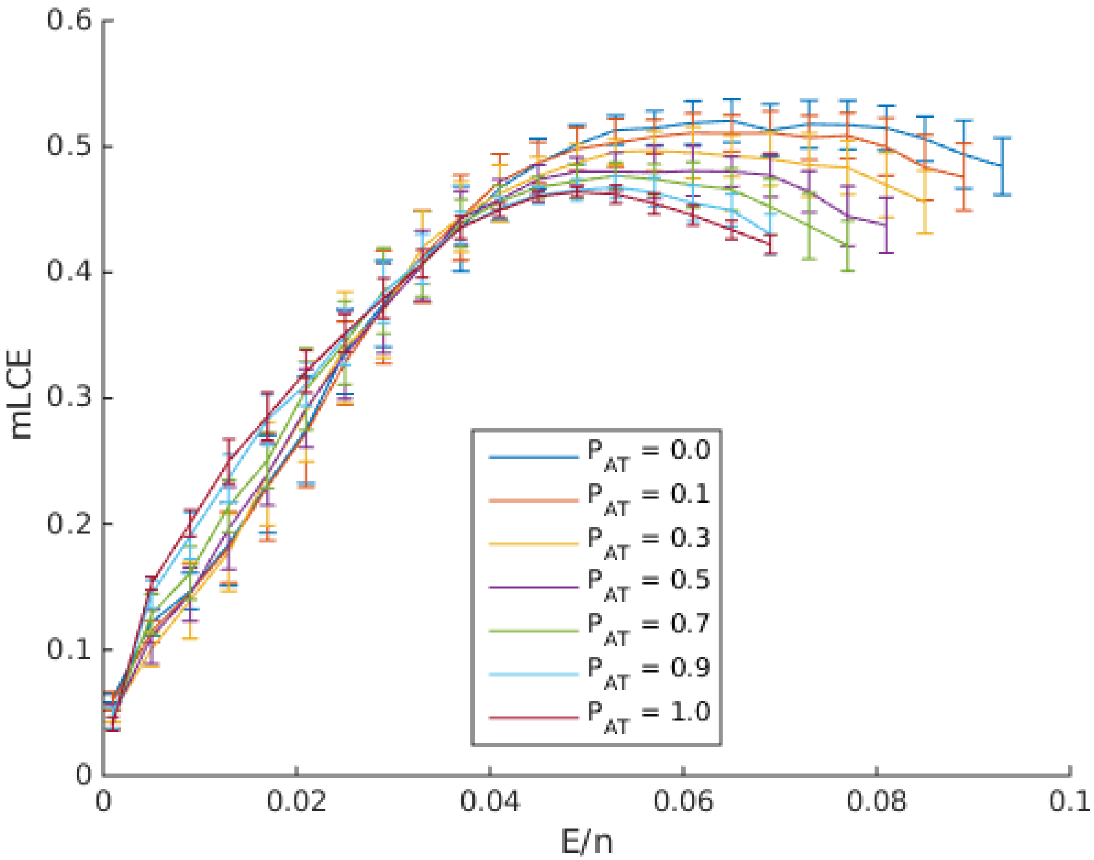

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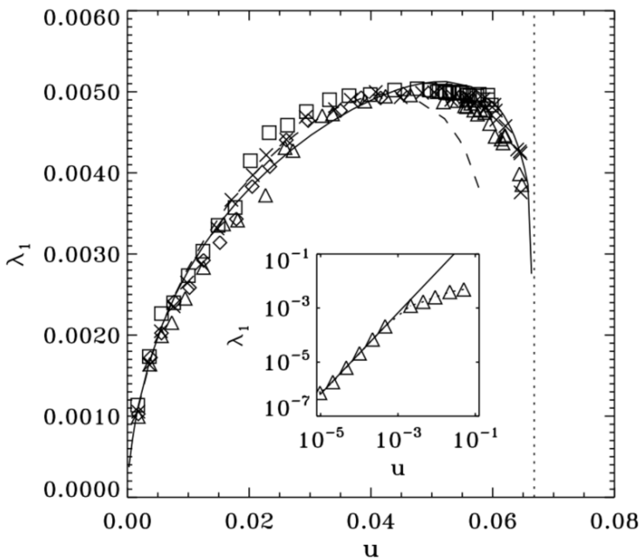

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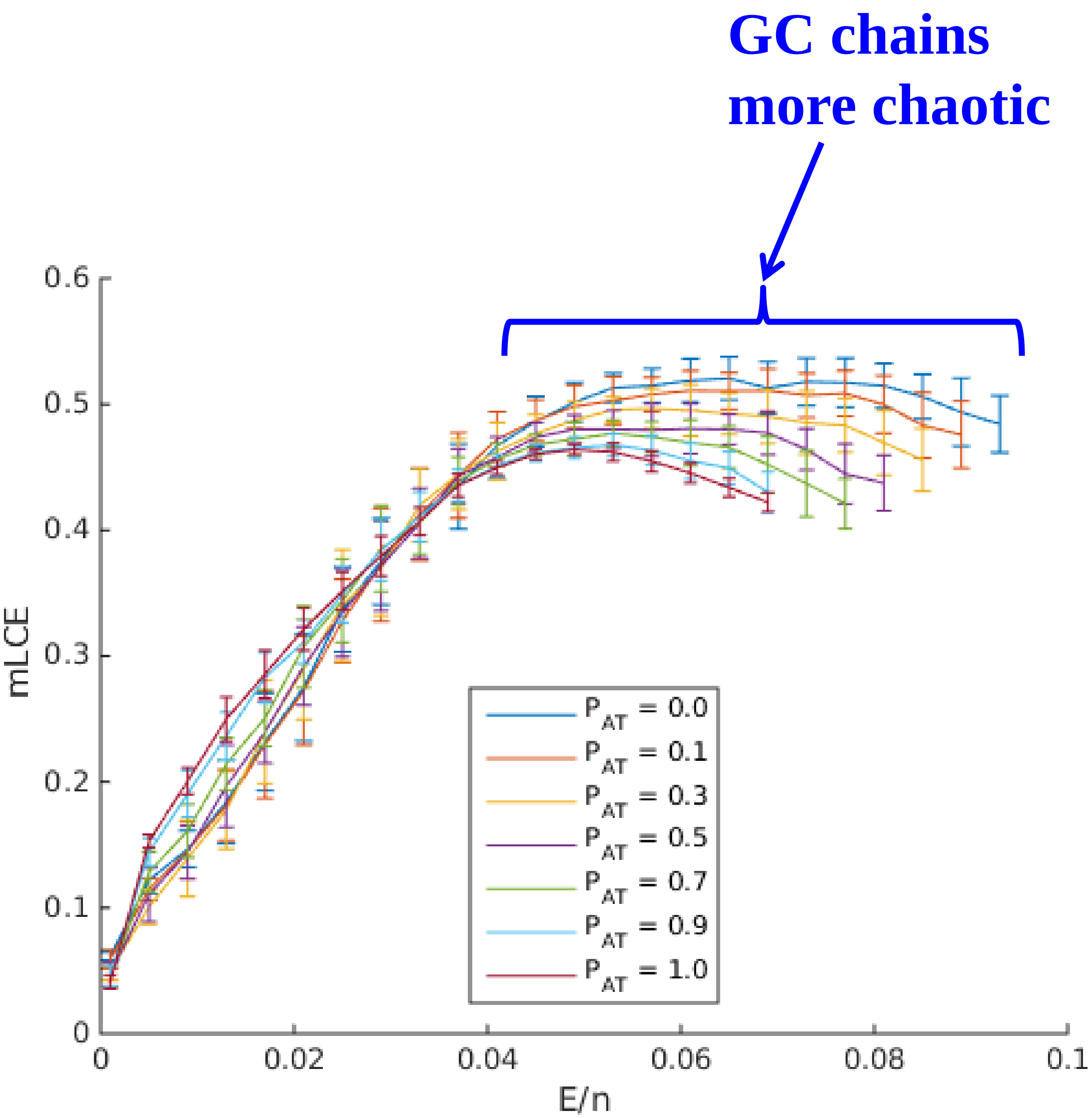

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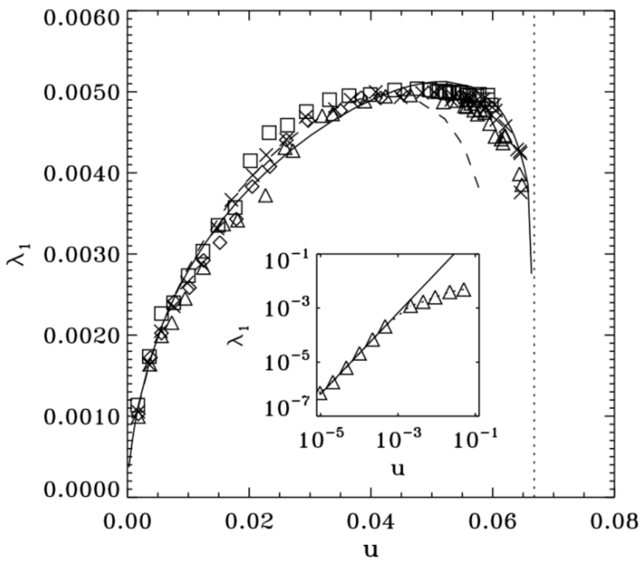

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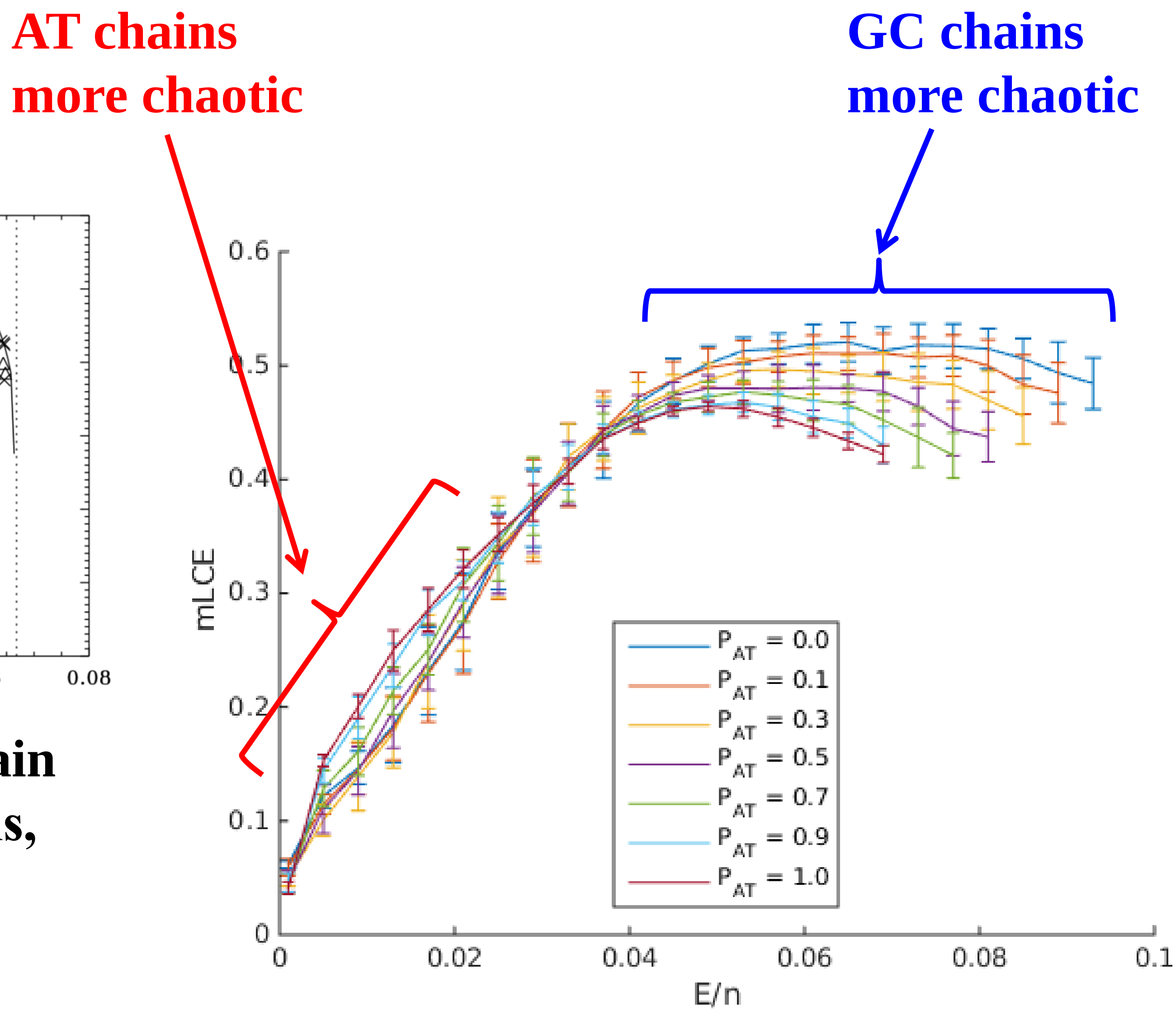

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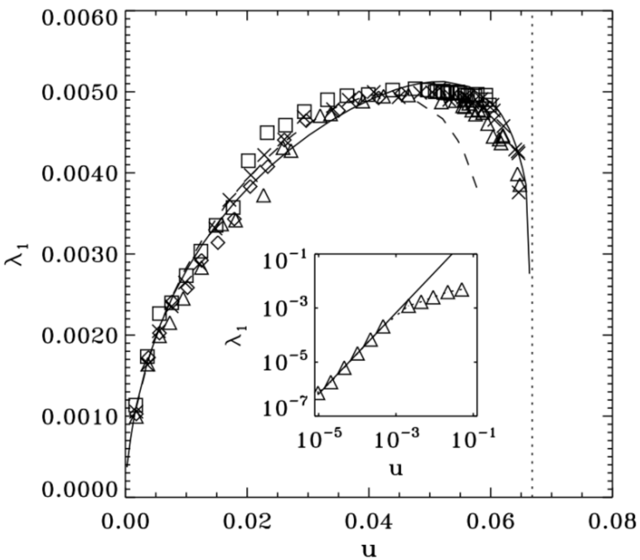
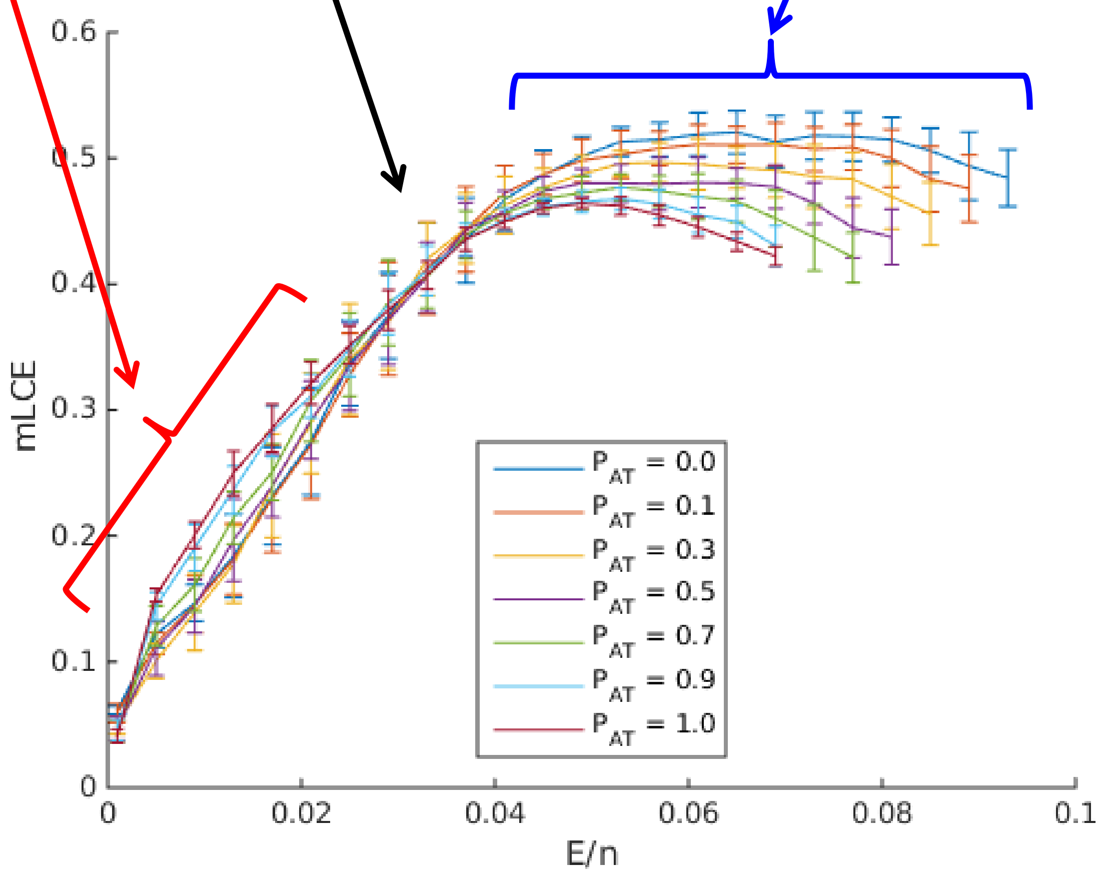


Homogeneous chain [Barré & Dauxois, EPL (2001)]

AT chains more chaotic

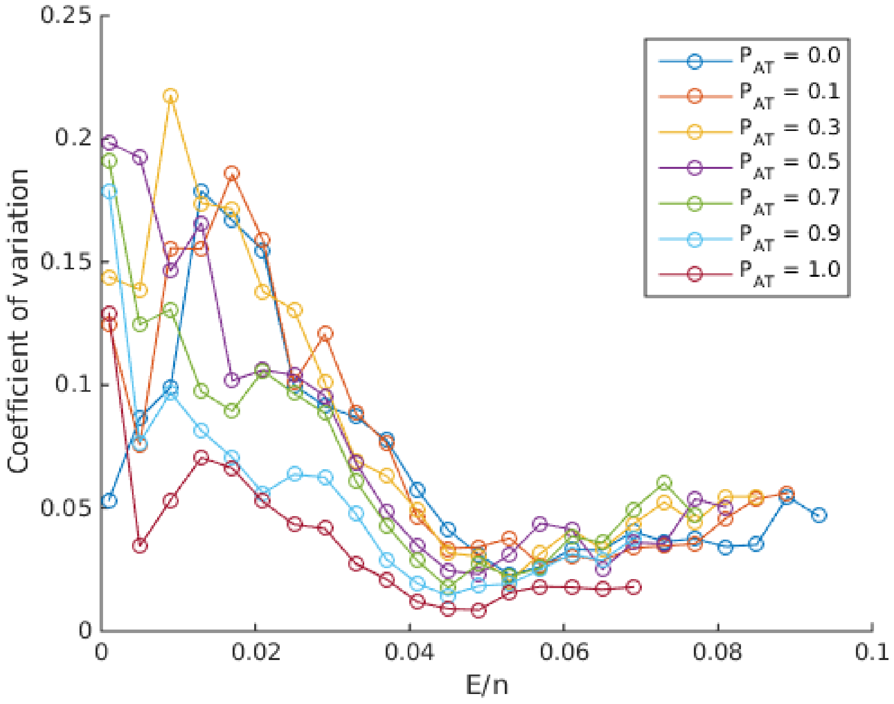
Type of chain does not play a role

GC chains more chaotic



Values of Lyapunov exponents

(Error of mLCE)/mLCE



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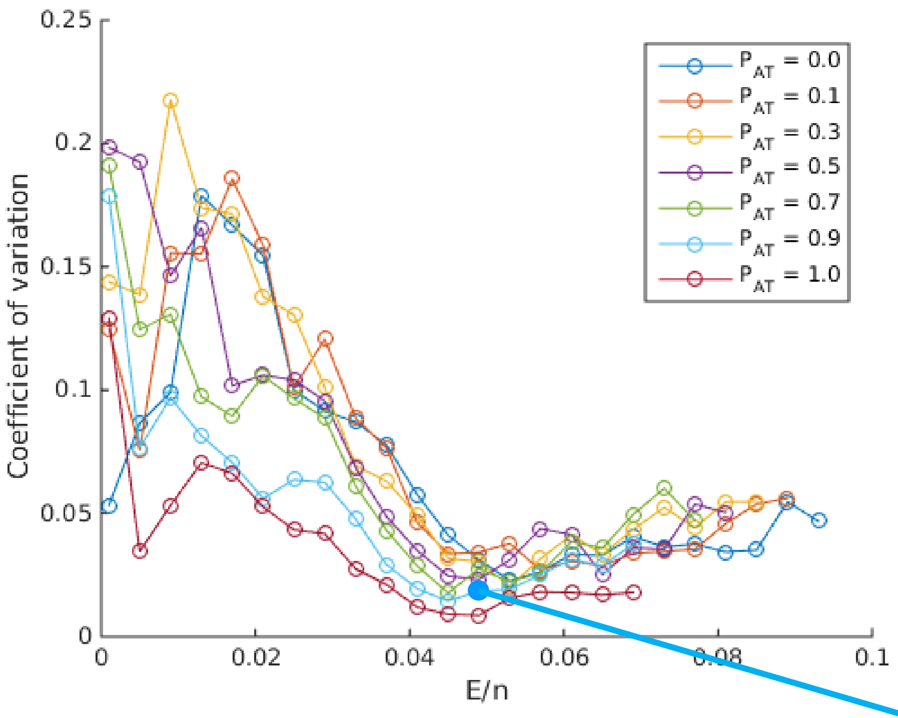

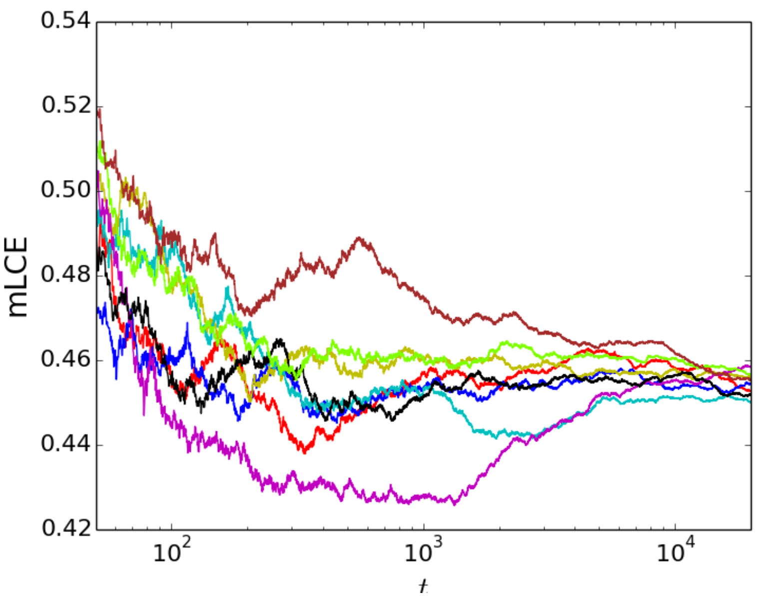

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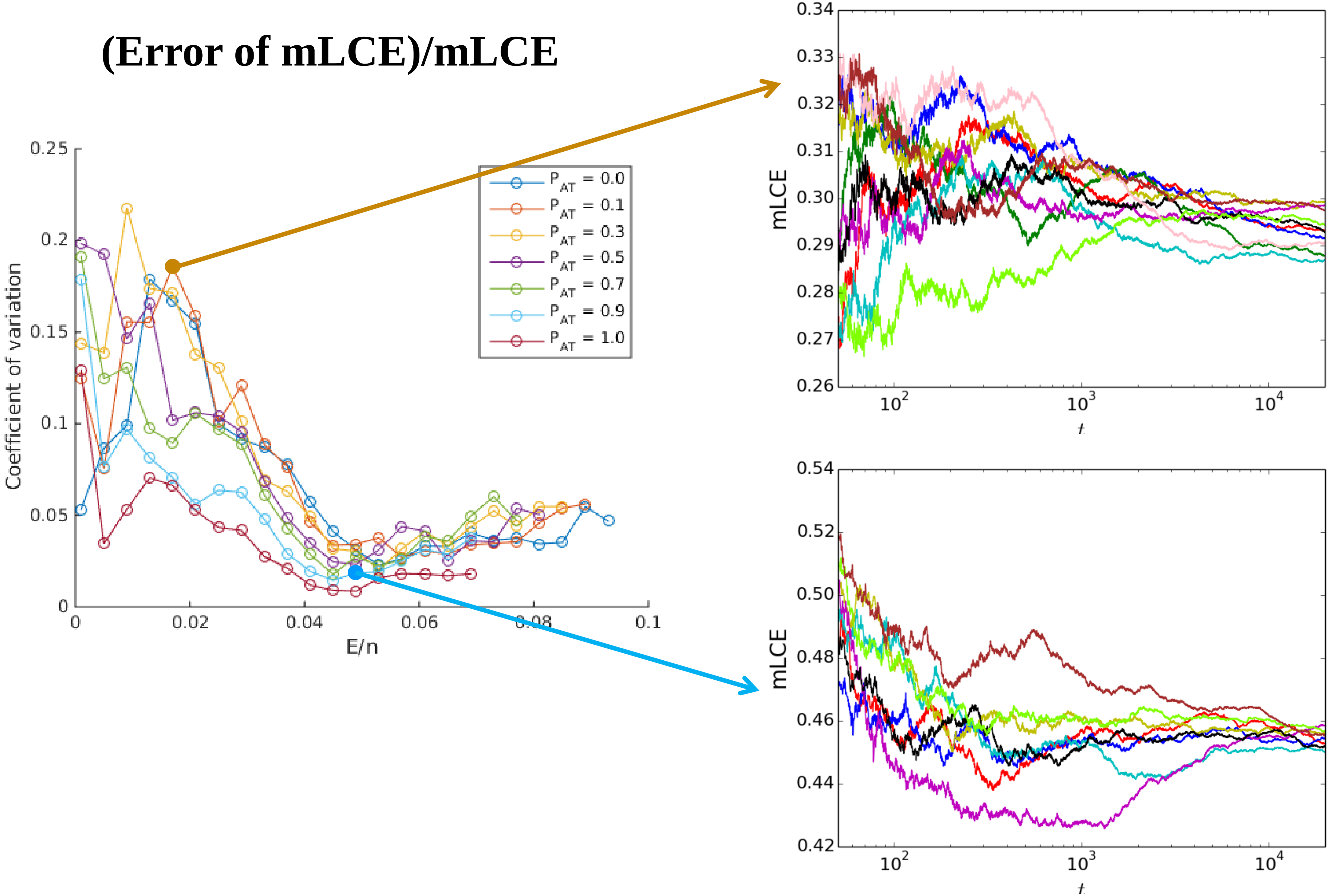
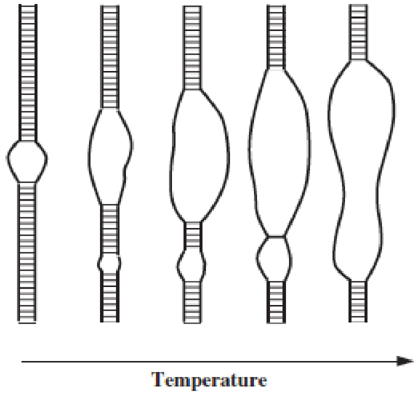


DNA denaturation (melting)

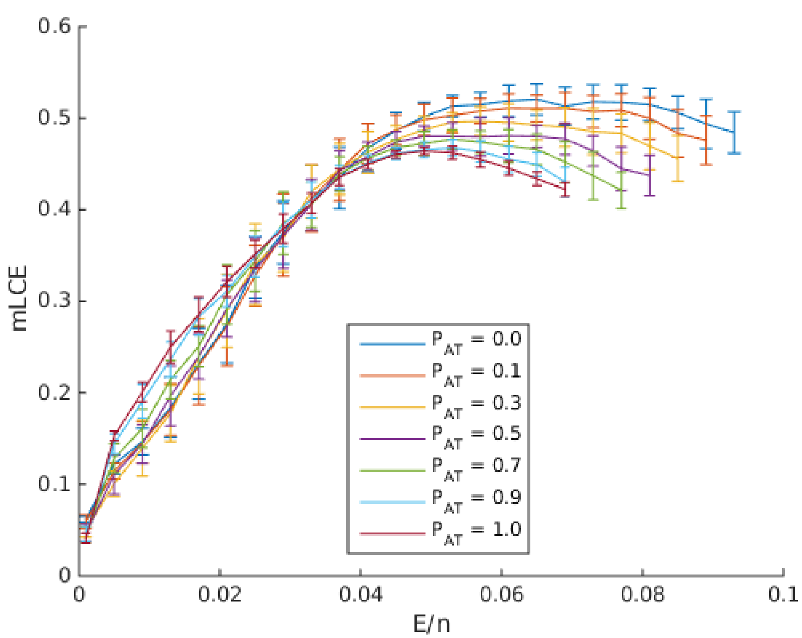
Melting: large bubbles forming in the DNA chain as bonds break



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.



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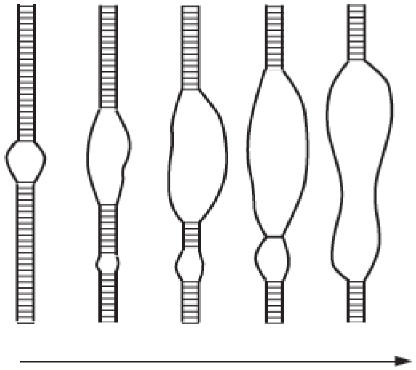

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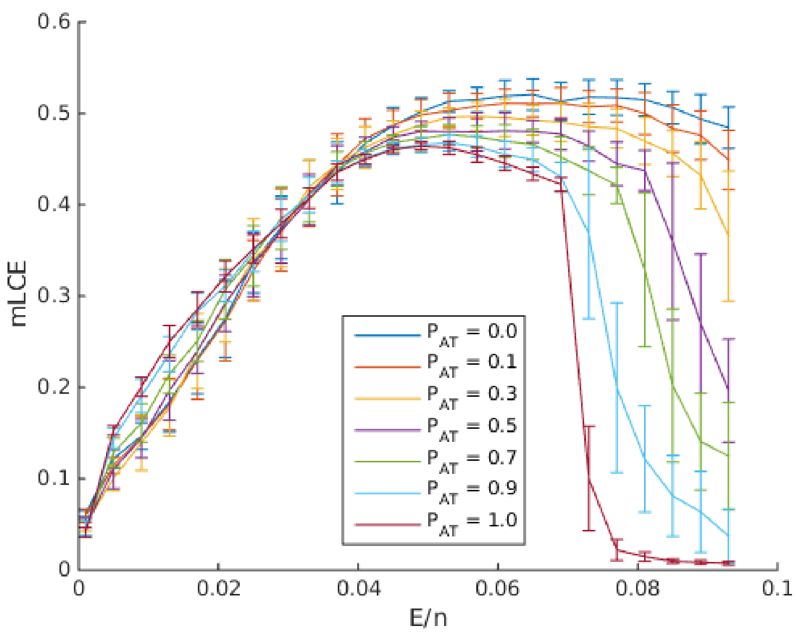

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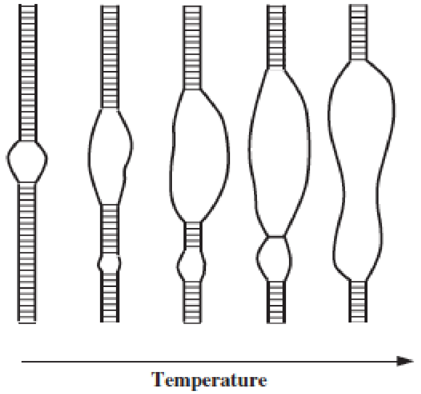

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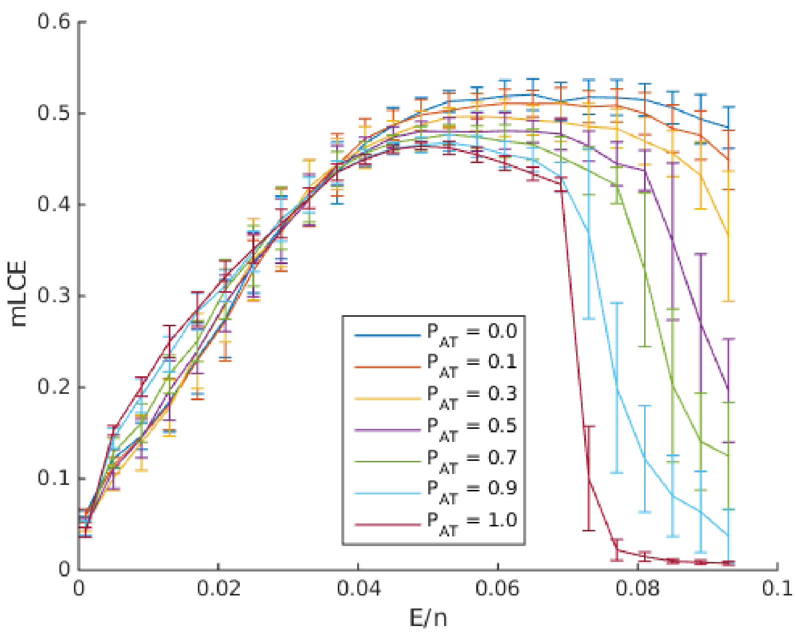
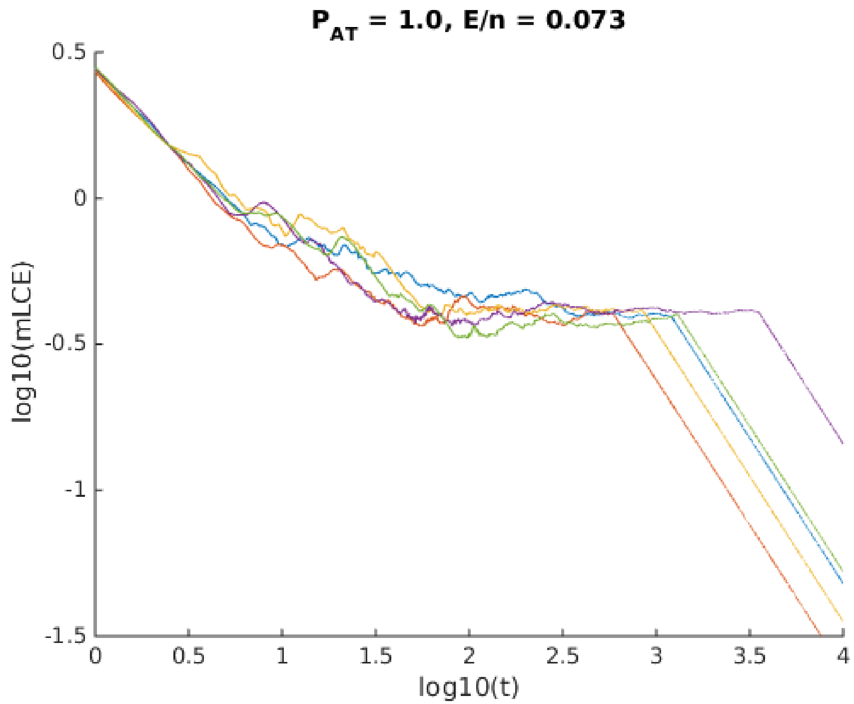
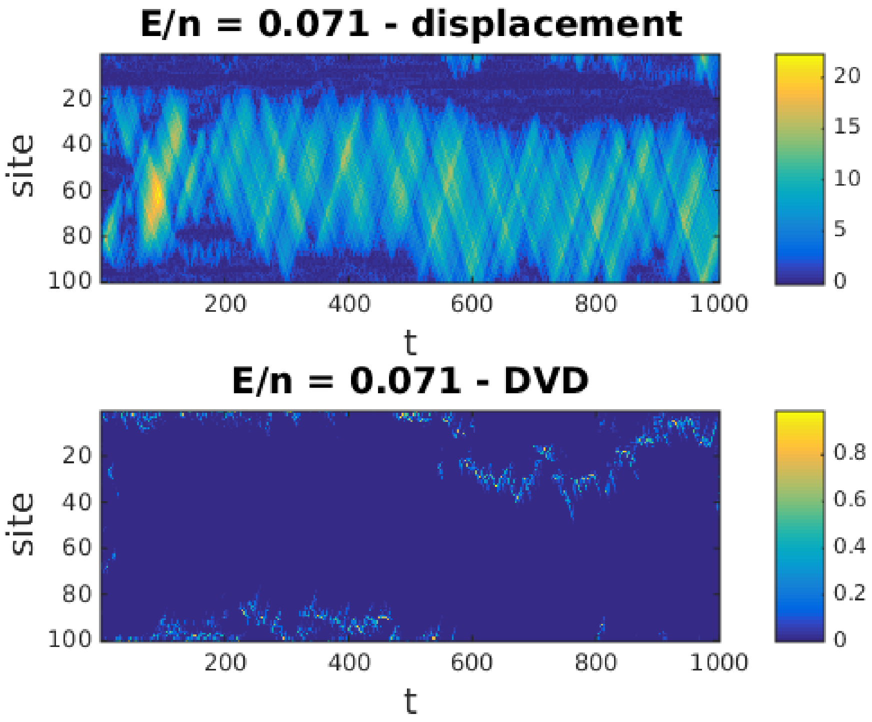




DVD and the formation of bubbles



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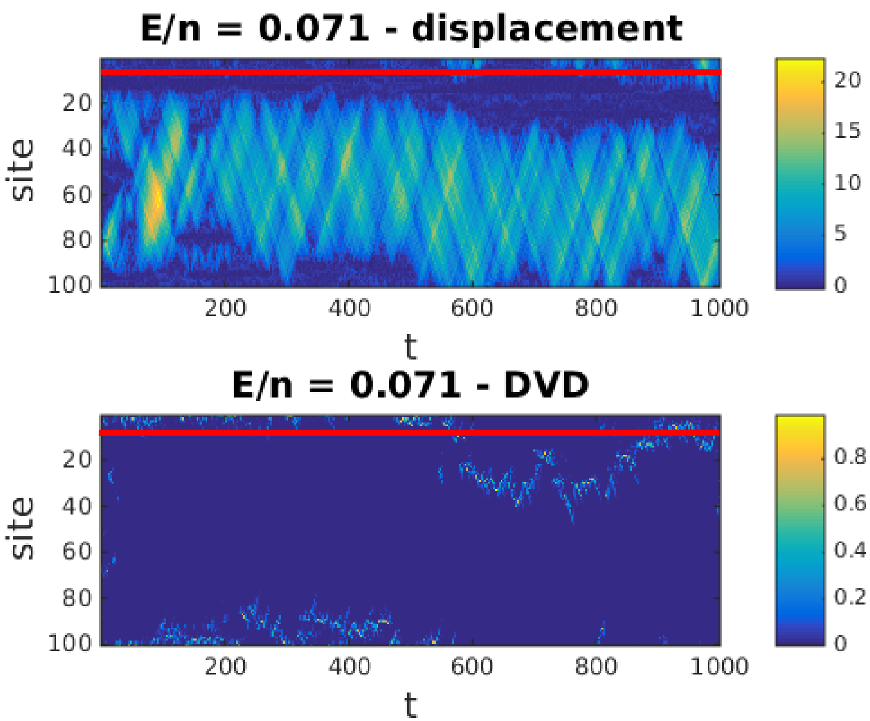

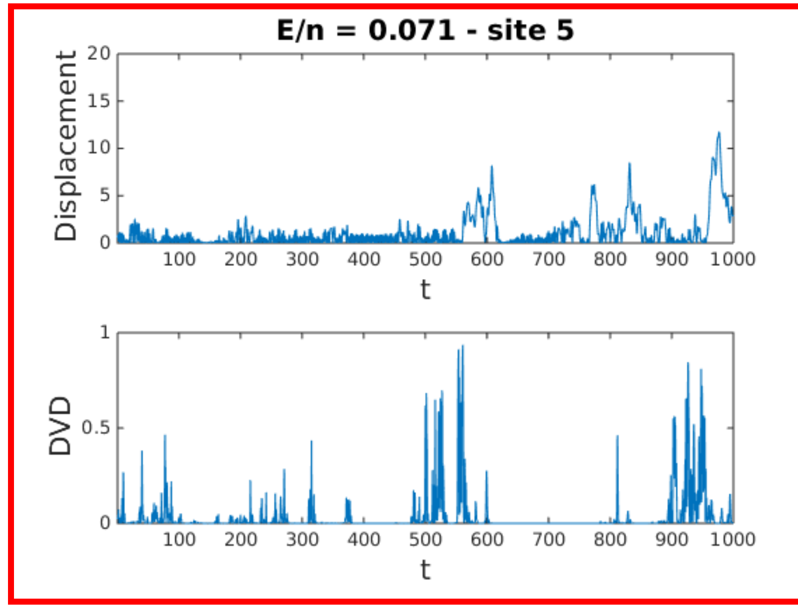

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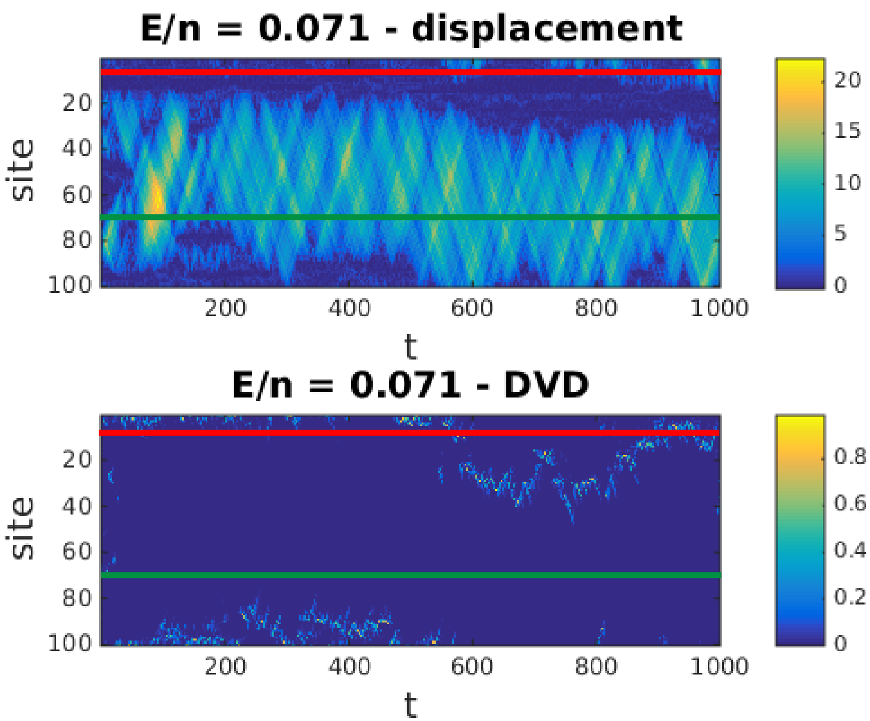
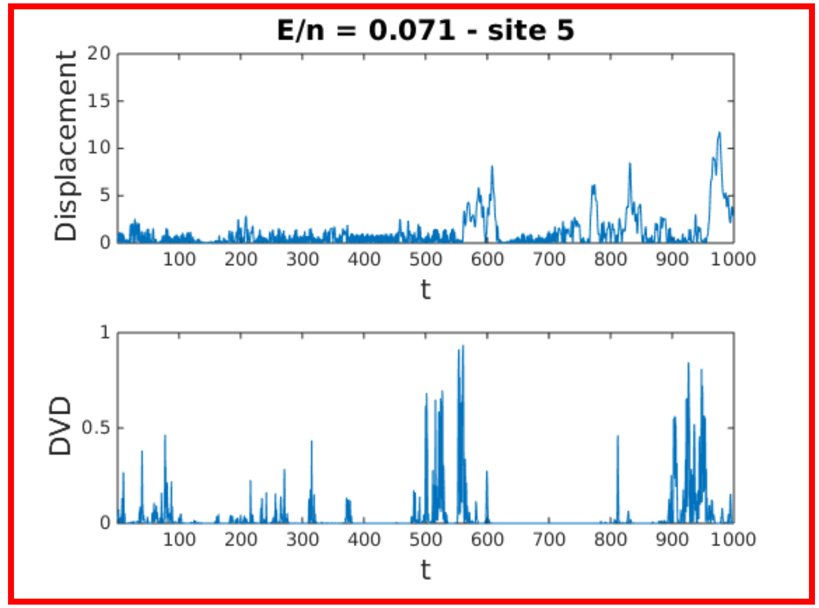
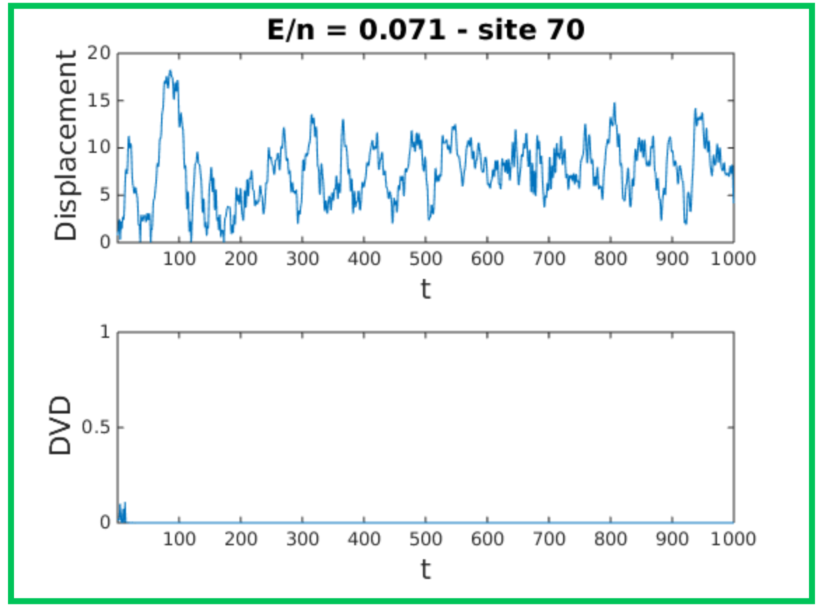
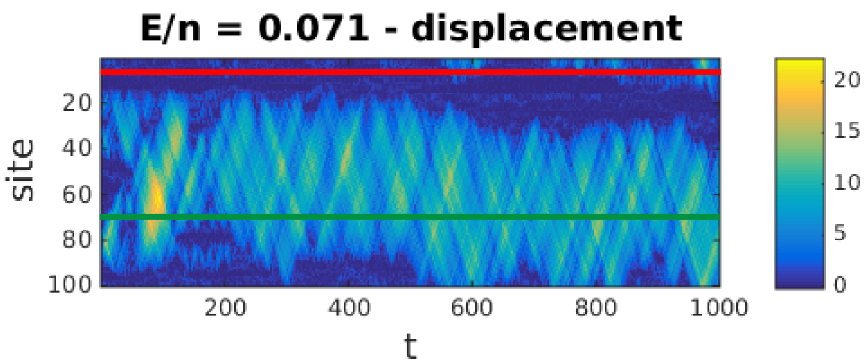


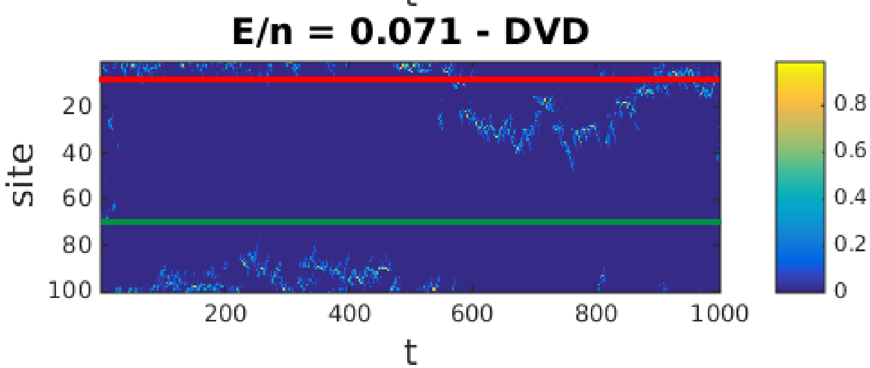


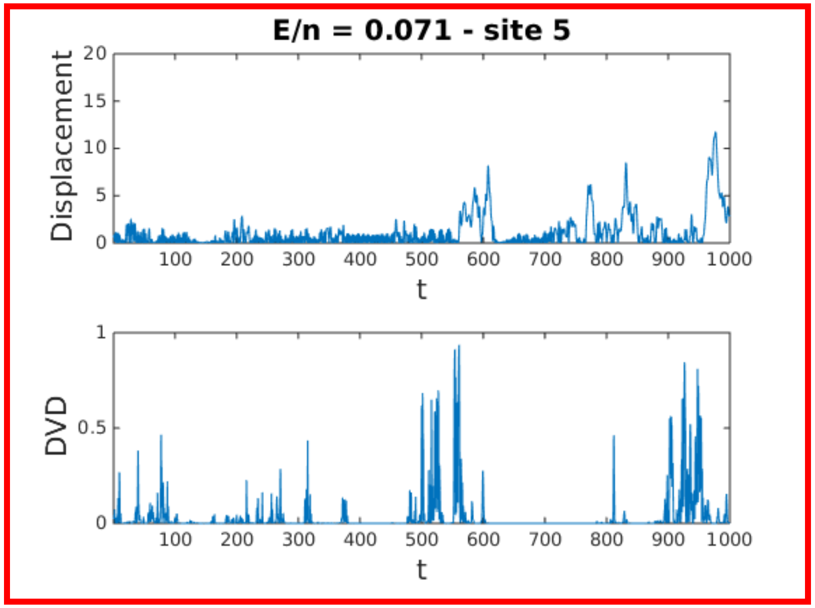


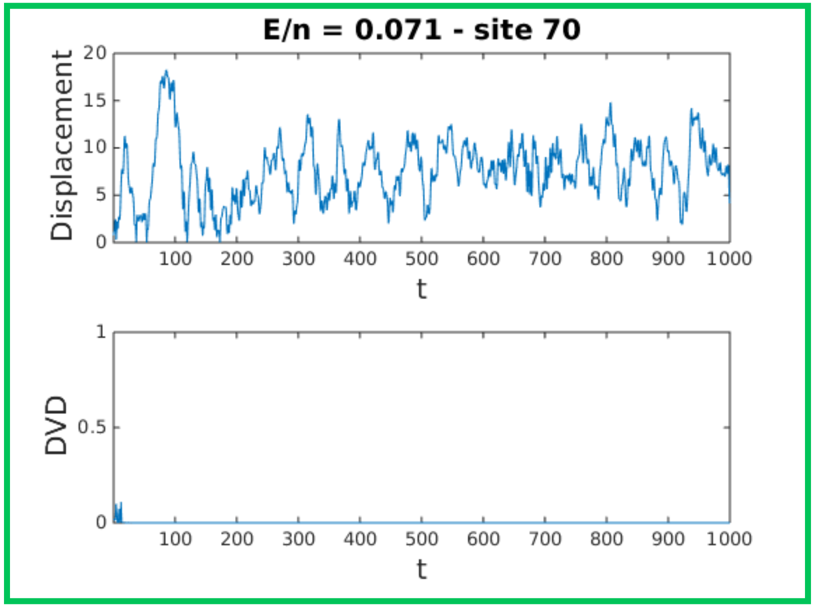
DVD and the formation of bubbles

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



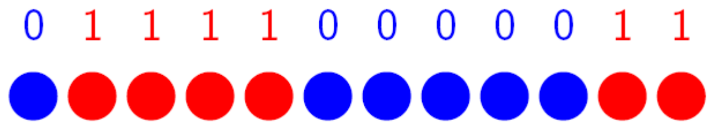






Mixing of the DNA chain

Mixing parameter α = Number of alternations in the chain (AT and GC).



$\alpha = 4$

$$(1)\bar{0}111\bar{1}0000\bar{0}1\bar{1}(0)$$

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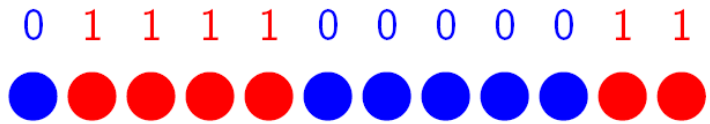
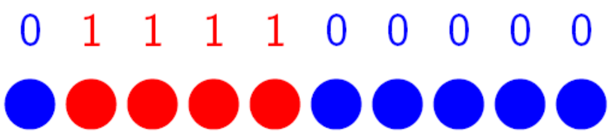


α=4

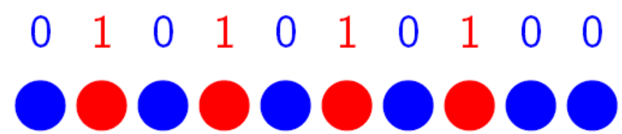
$$(1)\bar{0}111\bar{1}0000\bar{0}1\bar{1}(0)$$

Example case: N=10, N_{AT}=4, N_{GC}=6.

Extreme cases: α=2 and α=8



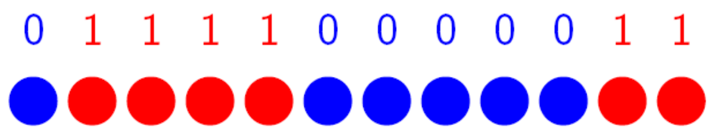
$\alpha = 2$



$\alpha = 8$

Mixing of the DNA chain

Mixing parameter α = Number of alternations in the chain (AT and GC).

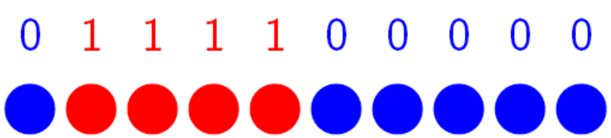


α=4

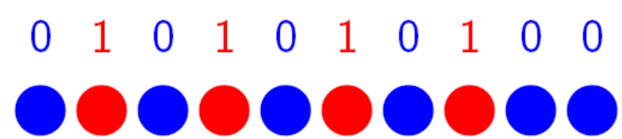
$$(1)\bar{0}111\bar{1}0000\bar{0}1\bar{1}(0)$$

Example case: N=10, N_{AT}=4, N_{GC}=6.

Extreme cases: α=2 and α=8



$\alpha = 2$

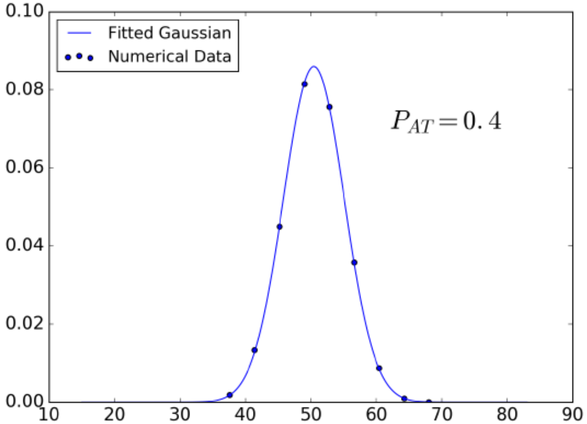


$\alpha = 8$

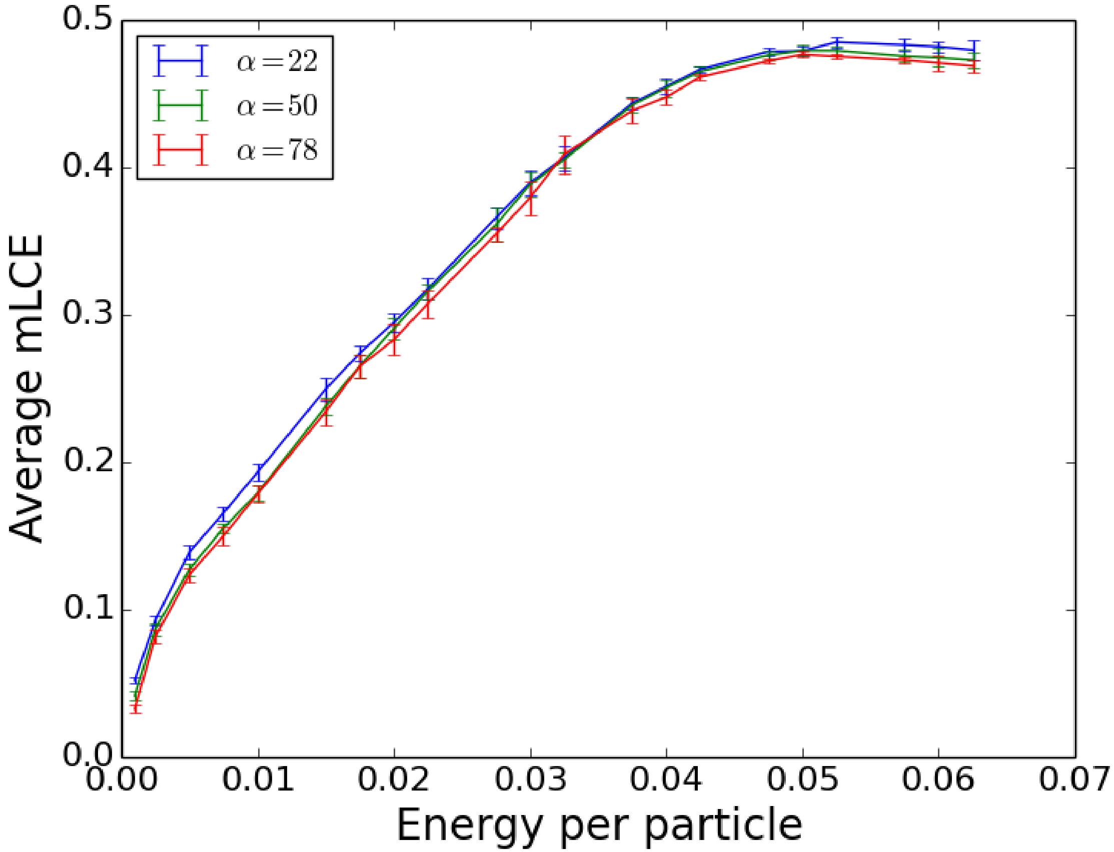
$$2 \leq \alpha \leq \min\{2N_{AT}, 2N_{GC}\}, \quad \alpha \text{ even}$$

Effect of mixing

Probability distribution function P(α)



α



The more heterogeneous chains are slightly less chaotic

Summary

- **Granular chain model**
  - ✓ **Moderate nonlinearities: although the overall system behaves chaotically, it can exhibit long lasting energy localization for particular single particle excitations.**
  - ✓ **Sufficiently strong nonlinearities: the granular chain reaches energy equipartition and an equilibrium chaotic state, independent of the initial position excitation.**
- **DNA model**
  - ✓ **Heterogeneity influences the behavior of the mLE and the system's chaotic behavior.**
  - ✓ **There seems to be a relation between the concentration of the DVD at a site and the formation of a bubble.**
  - ✓ **Mixing does not influence significantly the system's chaoticity.**
  - ✓ **The behavior of DVDs can provide important information about the chaotic behavior of a dynamical system.**