Chaos in disordered nonlinear Hamiltonian systems

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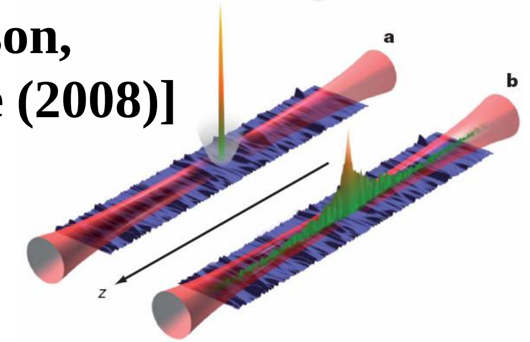
Outline

- Disordered 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
  - ✓ q-Gaussian distributions
- Chaotic behavior of granular chains
- DNA model [Malcolm Hillebrand, Saturday 17 June]
- Summary

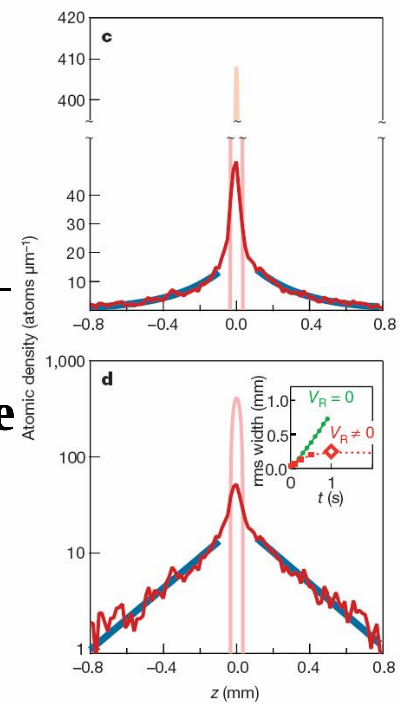
Interplay of disorder and nonlinearity



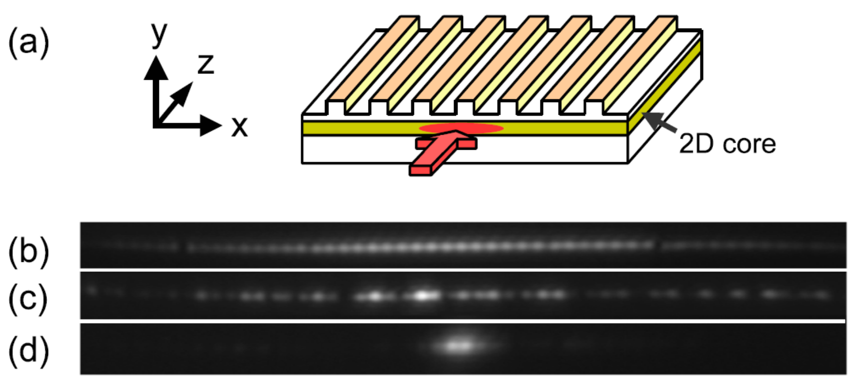
Waves in disordered media – Anderson localization [Anderson, Phys. Rev. (1958)]. Experiments on BEC [Billy et al., Nature (2008)]

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 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:

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

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

Distribution characterization

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

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

, where A_ν is the amplitude of the νth NM (KG) or norm distributions (DNLS).

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

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

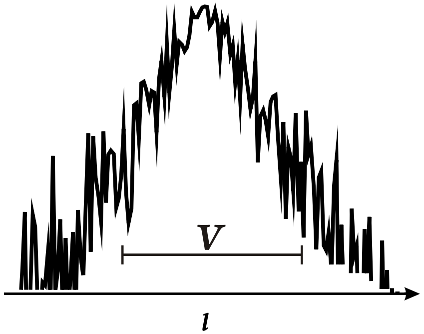
Linear case: $\omega_\nu^2 \in \left[\frac{1}{2}, \frac{3}{2} + \frac{4}{W}\right]$**, width of the squared frequency spectrum:**

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

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

Localization volume of an eigenstate:

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



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

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

The relation of the two scales $d_K \le \Delta_K$ 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) - 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: $d<\delta<\Delta$, $m_2 \sim t^{1/2} \longrightarrow m_2 \sim t^{1/3}$

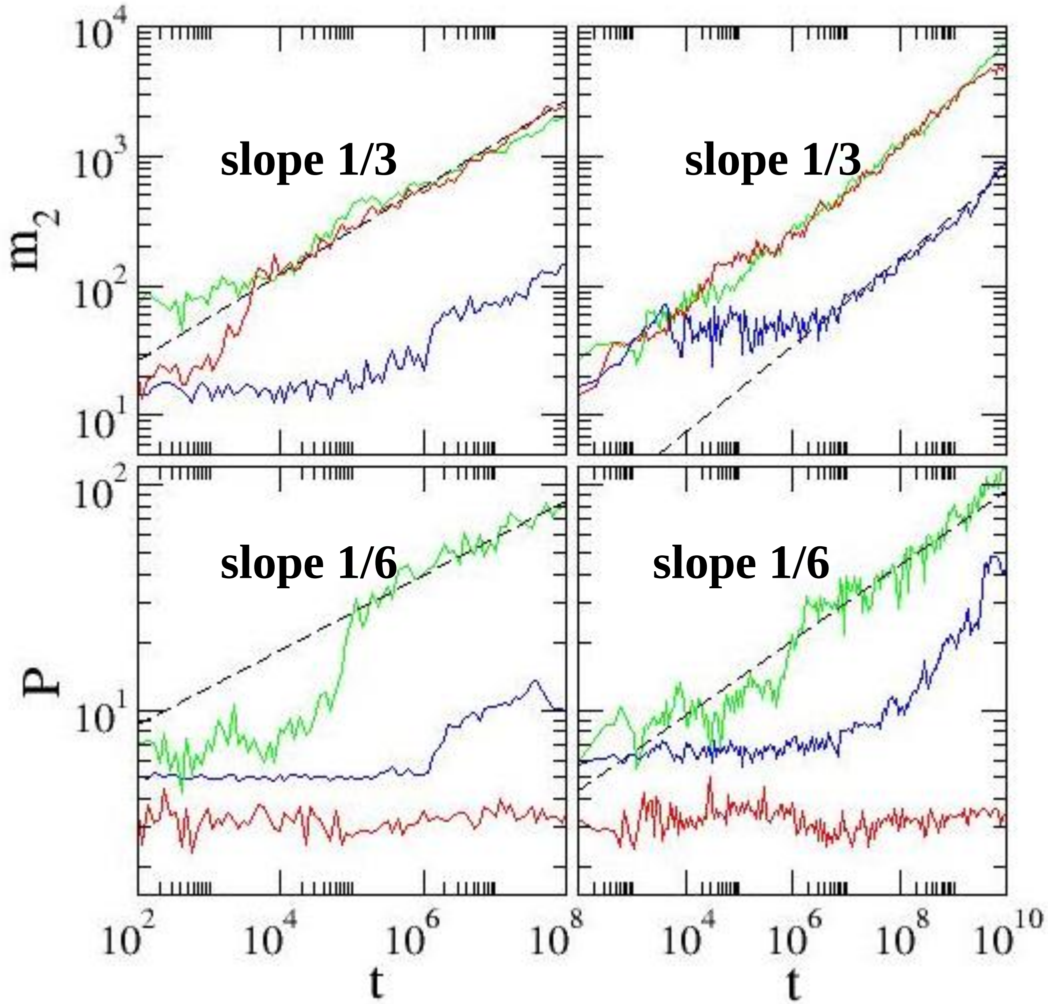
Almost all NMs in the packet are resonantly interacting. Wave packets initially spread faster and eventually enter the weak chaos regime.

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~t^α) over 20 realizations:

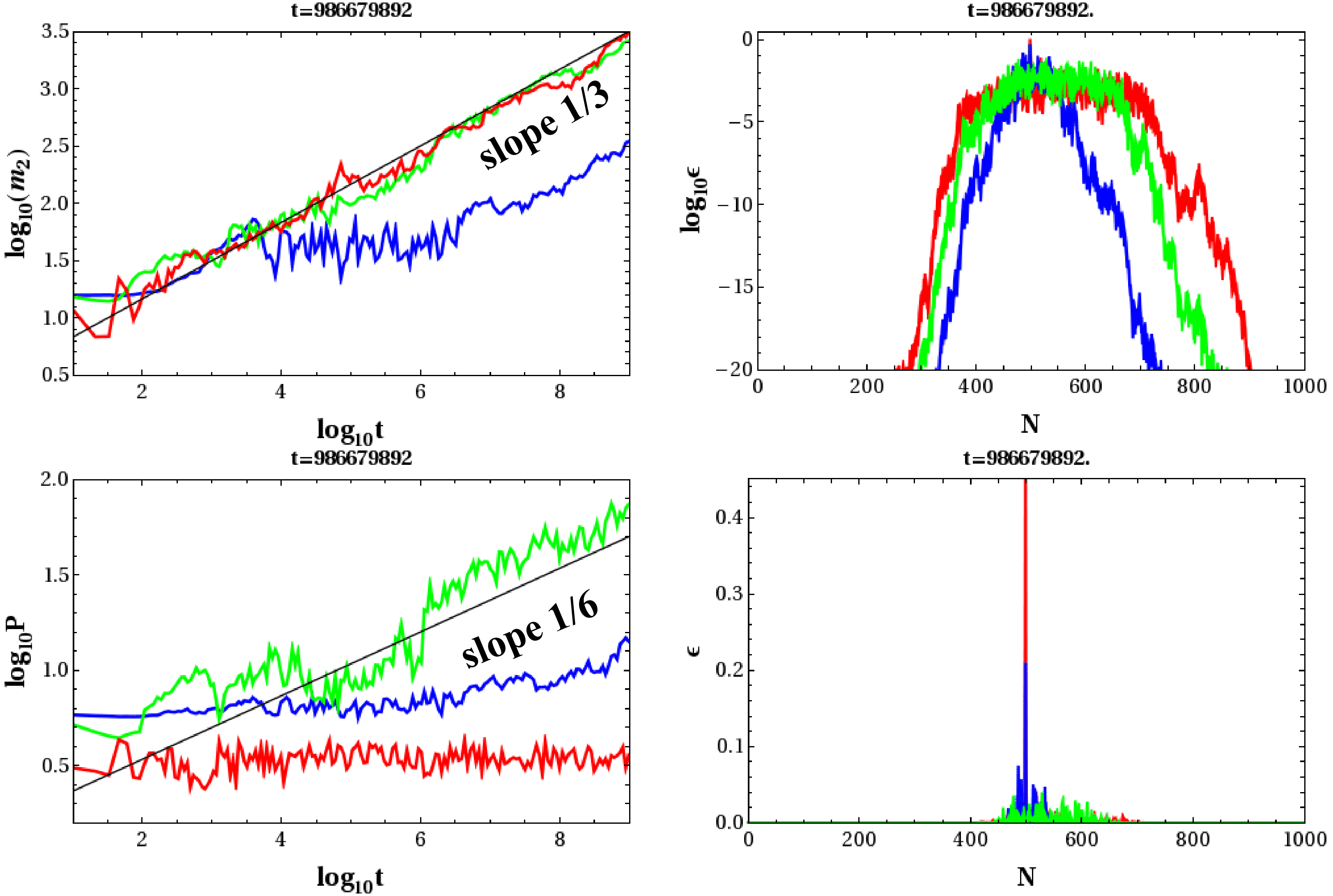
α=0.33±0.05 (KG)

α=0.33±0.02 (DLNS)

Flach et al., PRL (2009)

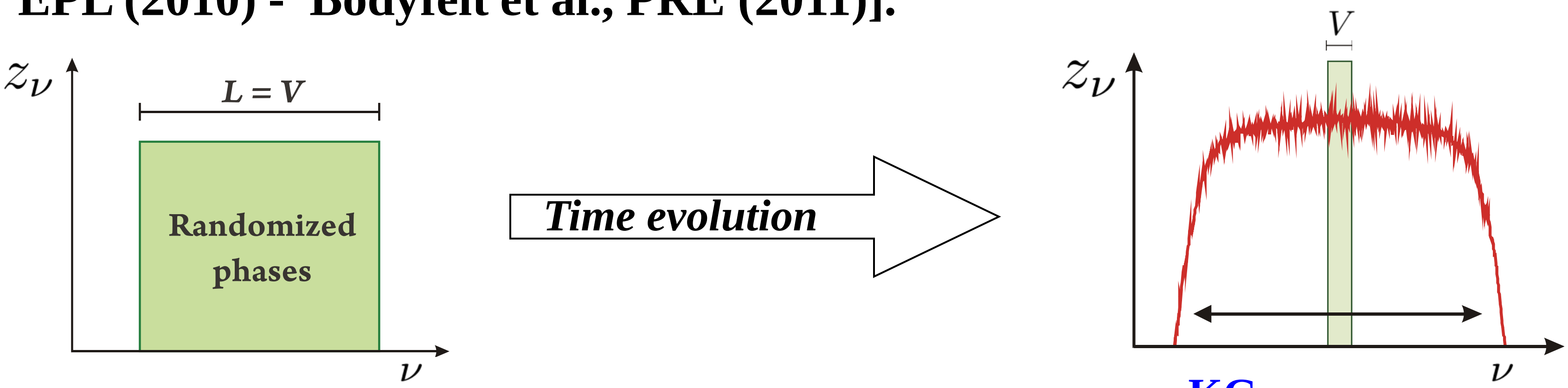
S. et al., PRE (2009)

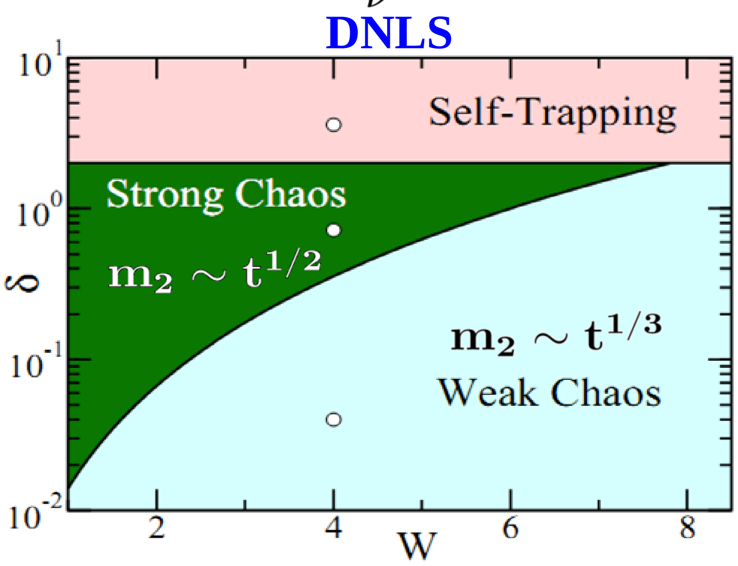
KG: Different spreading regimes

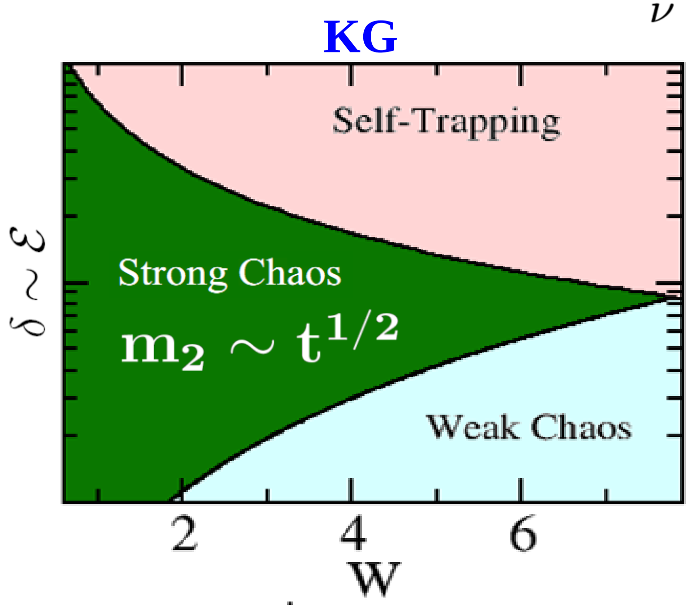


Crossover from strong to weak chaos

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

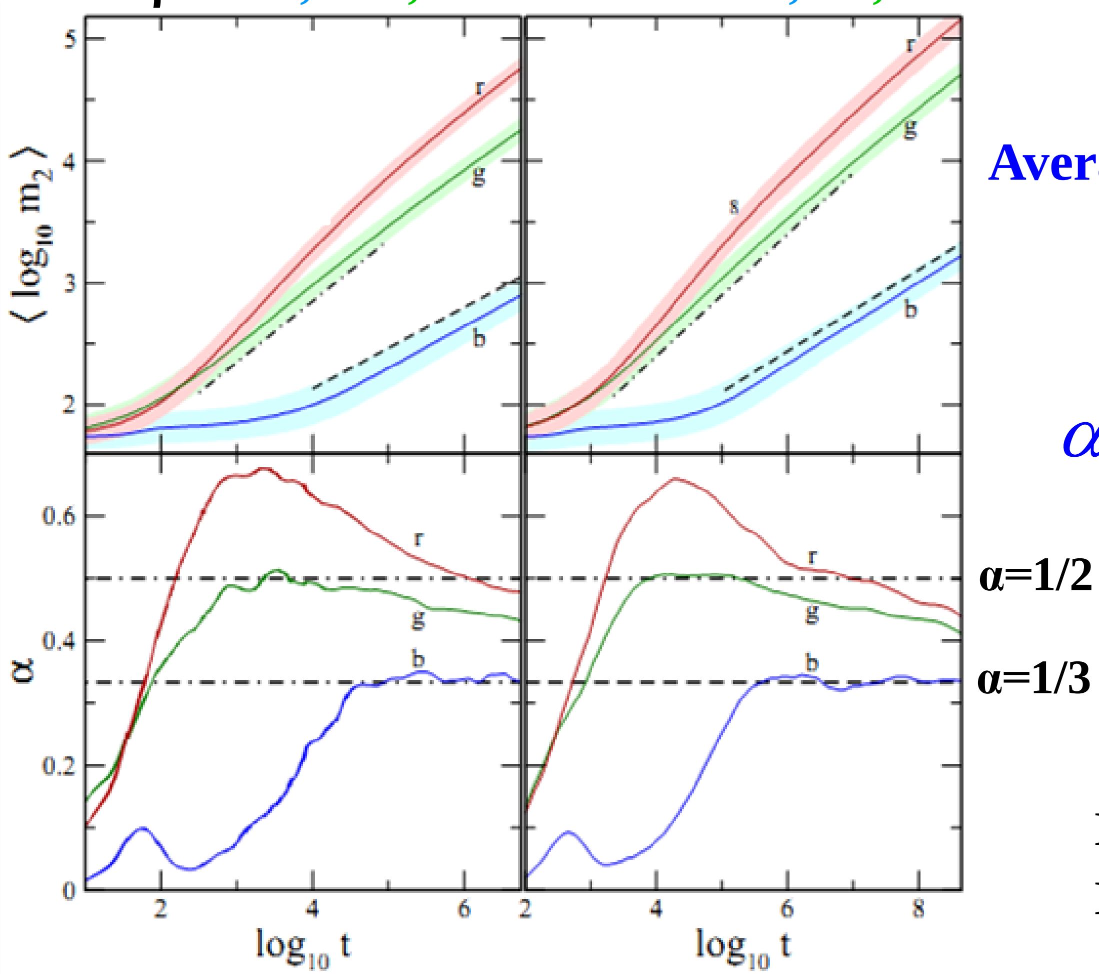






Crossover from strong to weak chaos (block excitations)

DNLS 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)

Lyapunov Exponents (LEs)

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

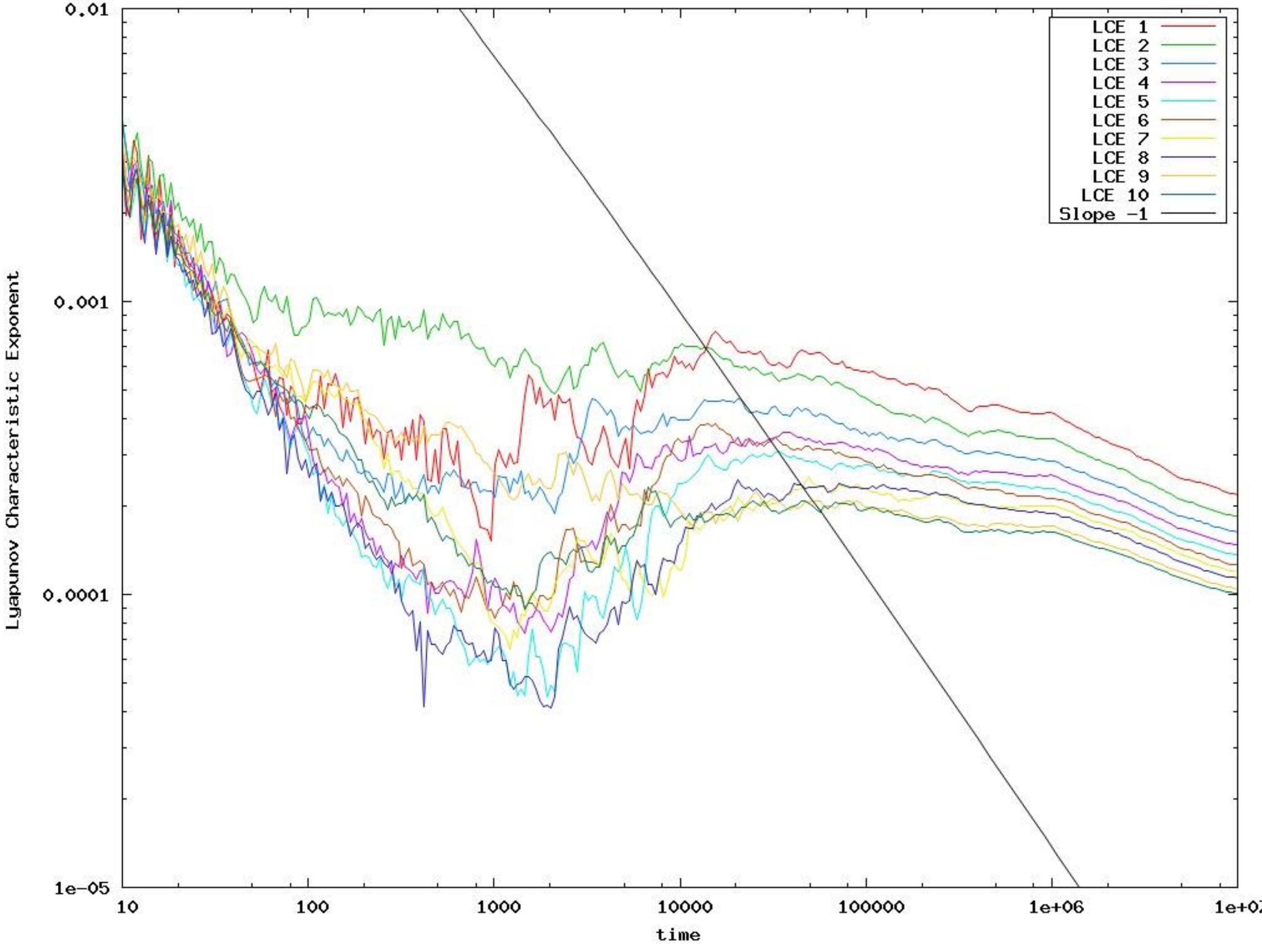
Consider an orbit in the 2N-dimensional phase space with initial condition x(0) and an initial deviation vector from it v(0). Then the mean exponential rate of divergence is:

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

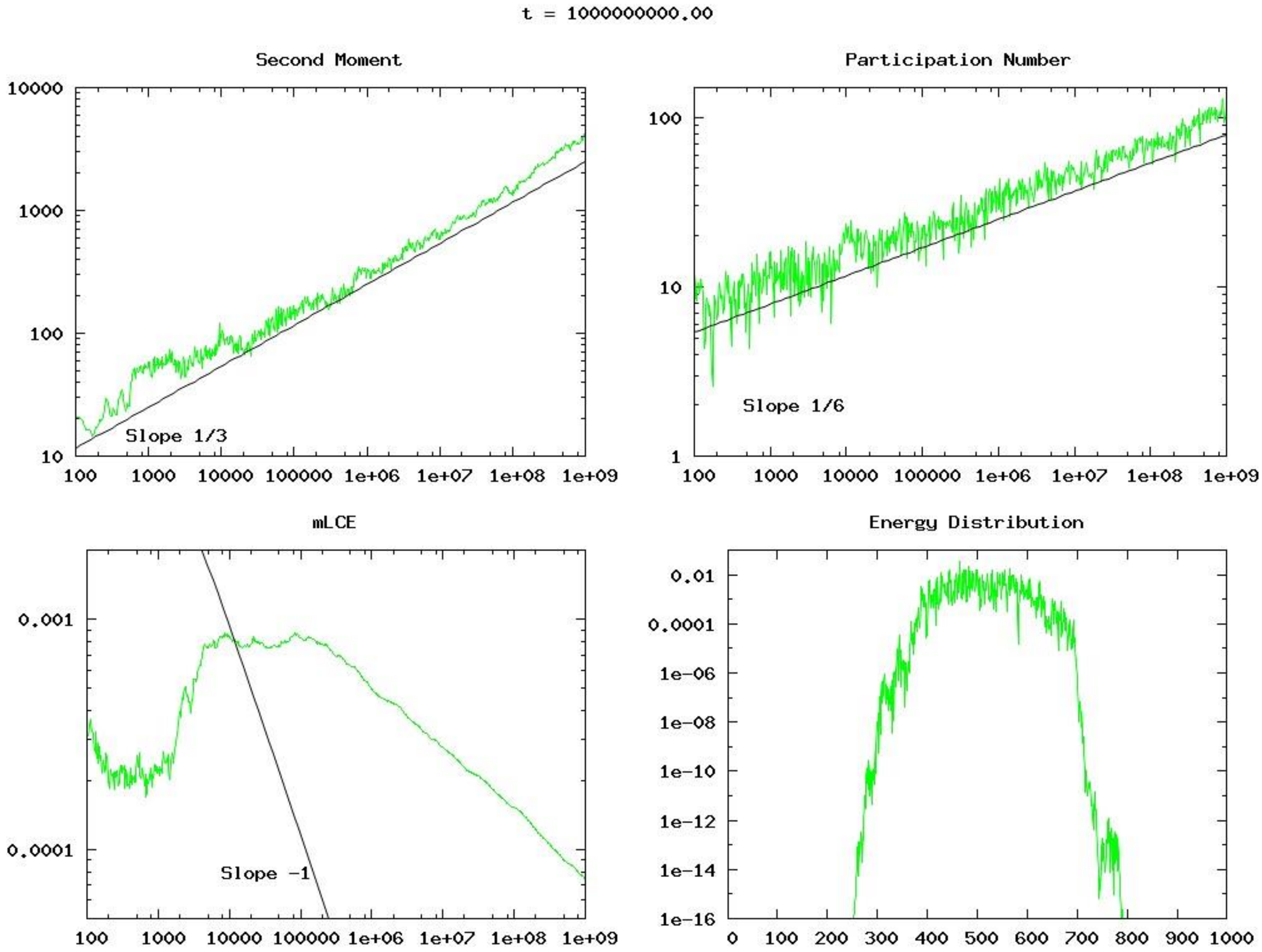
$\lambda_1 = 0 \rightarrow$ **Regular motion** $\propto (t^{-1})$

$\lambda_1 \neq 0 \rightarrow$ **Chaotic motion**

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



KG: Weak Chaos (E=0.4)

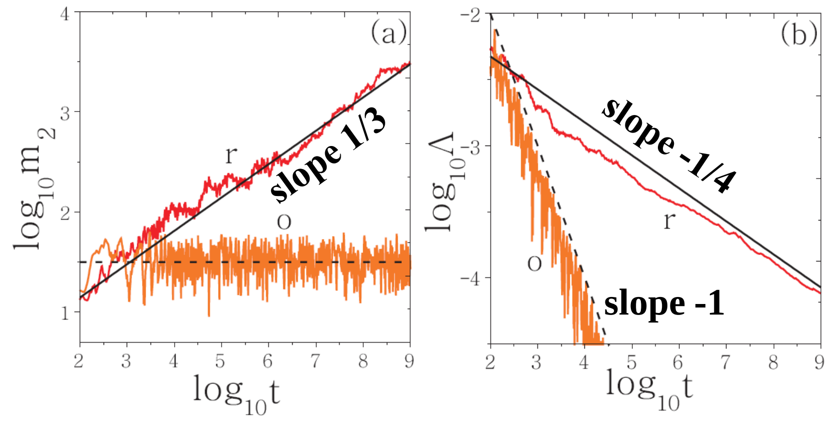


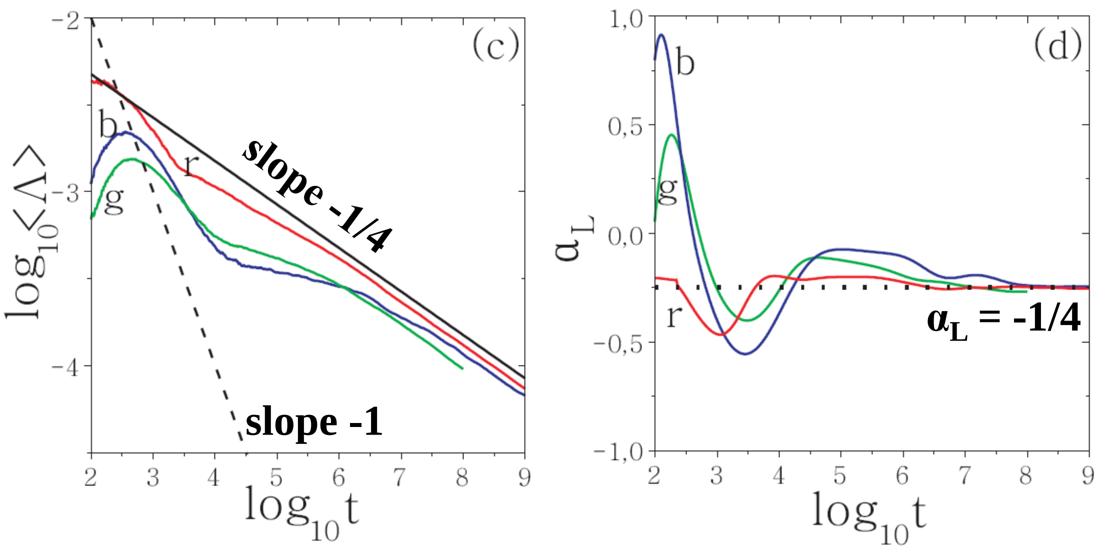
KG: Weak Chaos

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

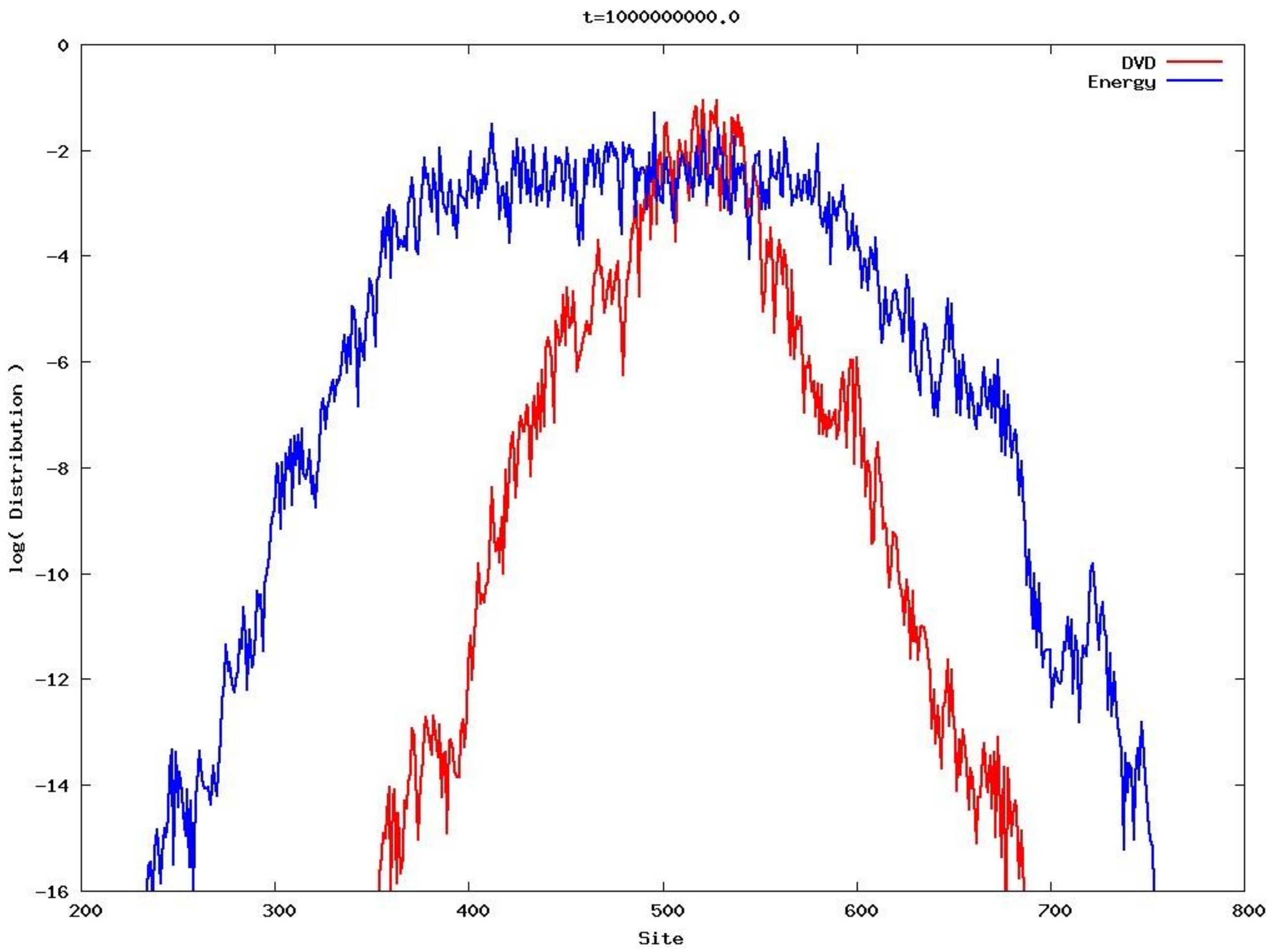
Single site excitation E=0.4, W=4

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

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

S. et al. PRL (2013)

Deviation Vector Distributions (DVDs)

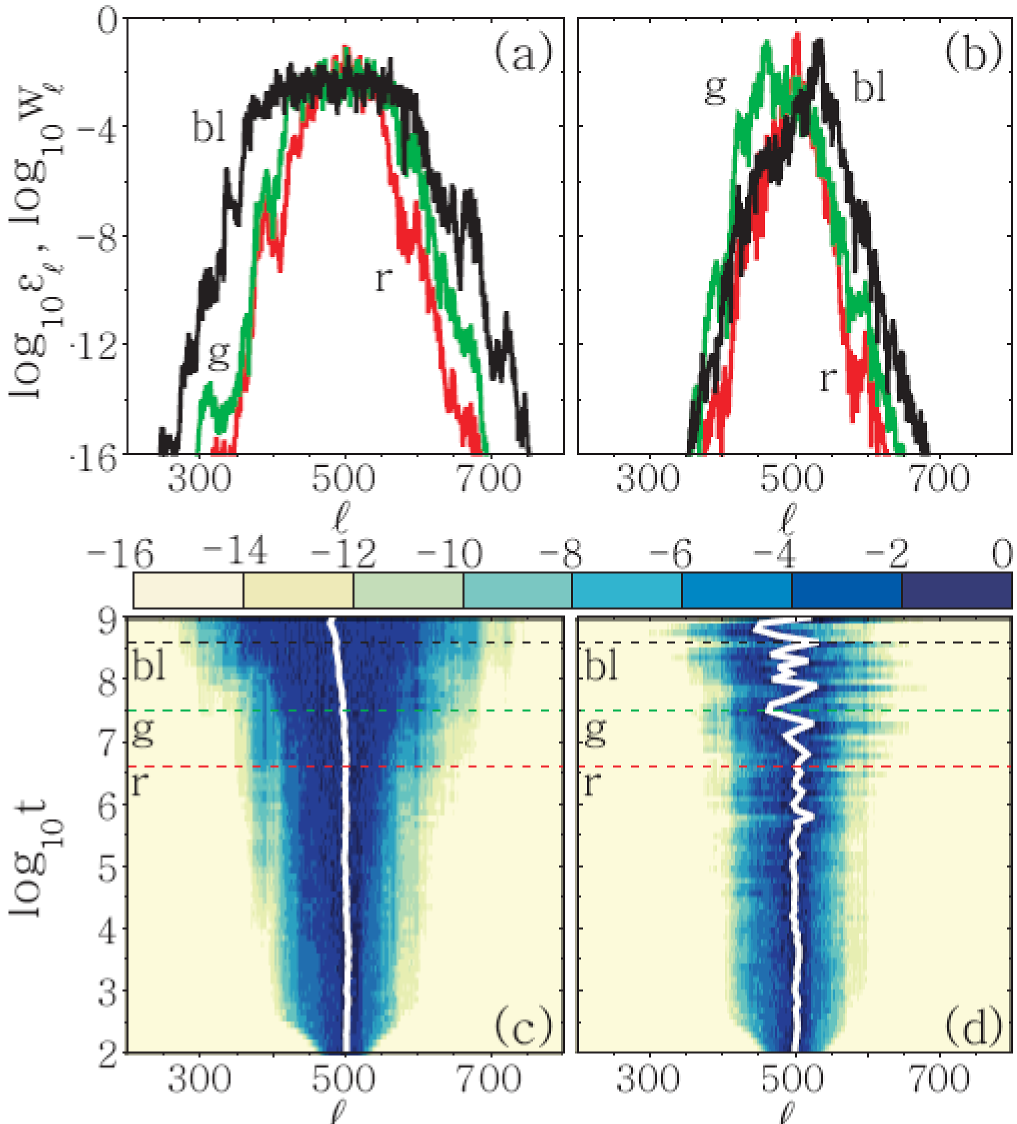


Deviation vector:

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

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

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.

q-Gaussian distributions

We construct probability distribution functions (pdfs) of rescaled sums of M values of an observable η(t_i), which depends linearly on positions u.

$$S_M^{(j)} = \sum_{i=1}^{M} \eta_i^{(j)}$$

We rescale them by their standard deviation

$$s_M^{(j)} \equiv \frac{1}{\sigma_M}\left(S_M^{(j)} - \langle S_M^{(j)} \rangle\right) \qquad \sigma_M^2 = \frac{1}{N_{\mathrm{ic}}}\sum_{j=1}^{N_{\mathrm{ic}}}\left(S_M^{(j)} - \langle S_M^{(j)} \rangle\right)^2$$

and compare the resulting numerically computed pdfs with a q-Gaussian [Tsallis, Springer (2009)]

$$\mathrm{P}(s_M^{(j)}) = a \exp_q(-\beta s_M^{(j)2}) \equiv a\left[1 - (1-q)\beta s_M^{(j)2}\right]^{\frac{1}{1-q}}$$

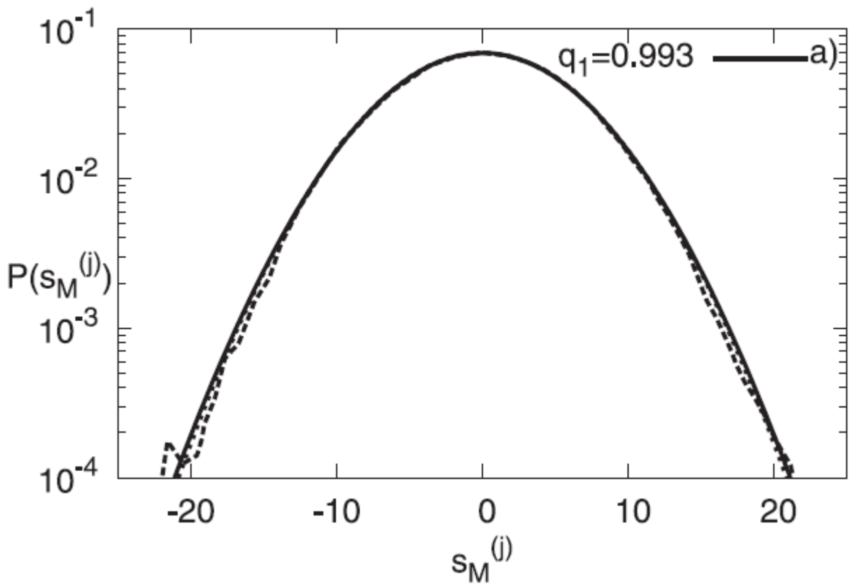
q (entropic index)

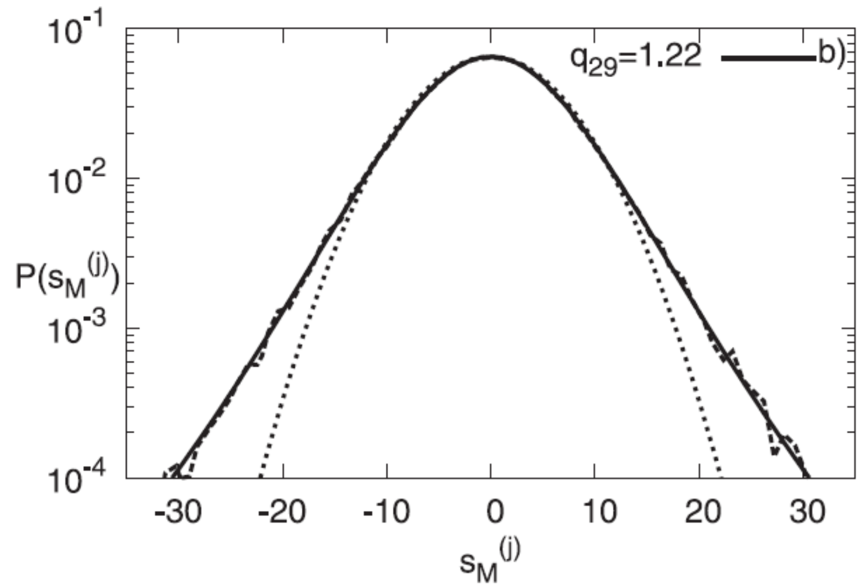
q=1: Gaussian pdf

q ≠ 1: system is at the so-called 'edge of chaos' regime, characterized by the non-additive and generally non-extensive Tsallis entropy.

q-Gaussian distributions

Weak chaos case: E=0.4, W=4. Dotted curves: Gaussian pdf (q=1)





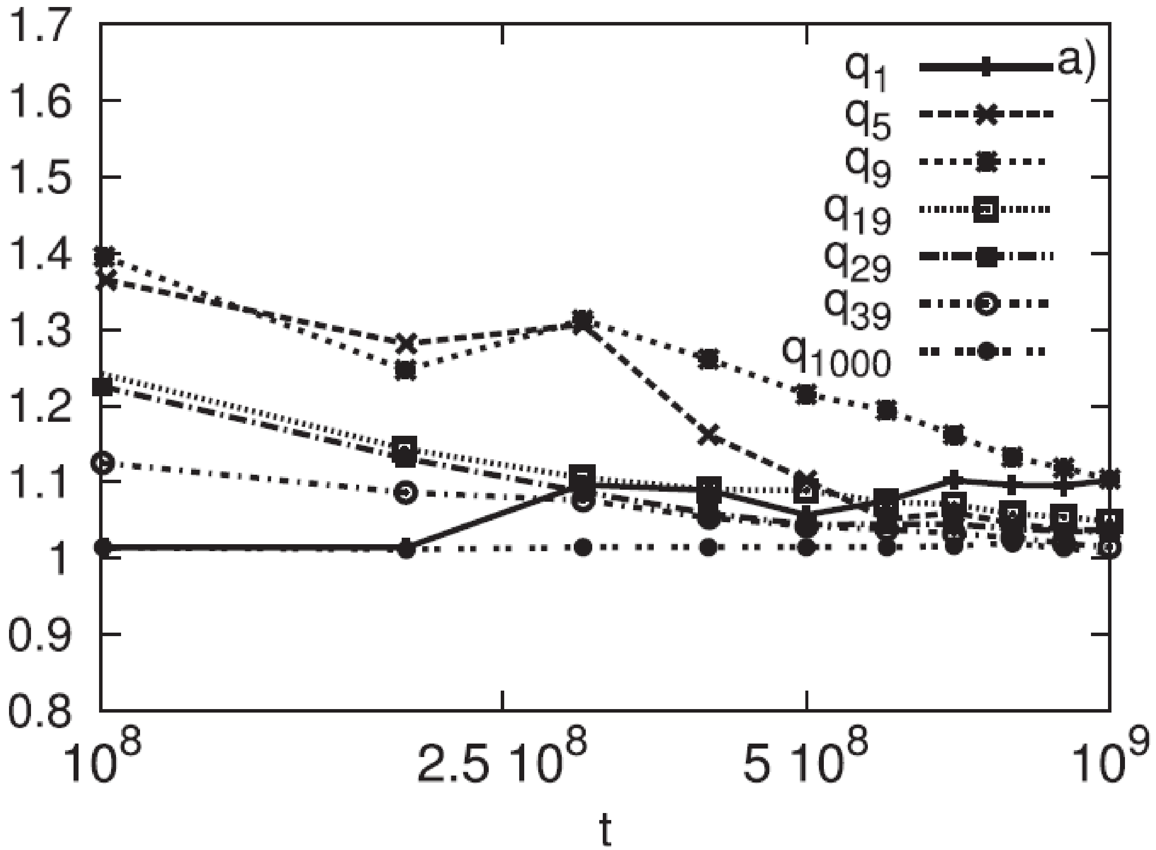
$\eta_1 = u_1$
Well defined chaos

$\eta_{29} = u_{486} + u_{487} + \ldots + u_{513} + u_{514}$
(29 central particles)
$q \neq 1$ 'edge of chaos'

Antonopoulos et al. Chaos (2014)

q-Gaussian distributions

Weak chaos case: E=0.4, W=4.



Antonopoulos et al. Chaos (2014)

Numerical Integration methods

We use Symplecic Integrators for solving numerically

- **the equations of motion, and**
- **the variational equations (Tangent Map method)**

How do LEs and DVDs behave for the other dynamical regimes?

For more information attend the presentation:

‘Chaotic dynamics of the disordered Klein-Gordon lattice’

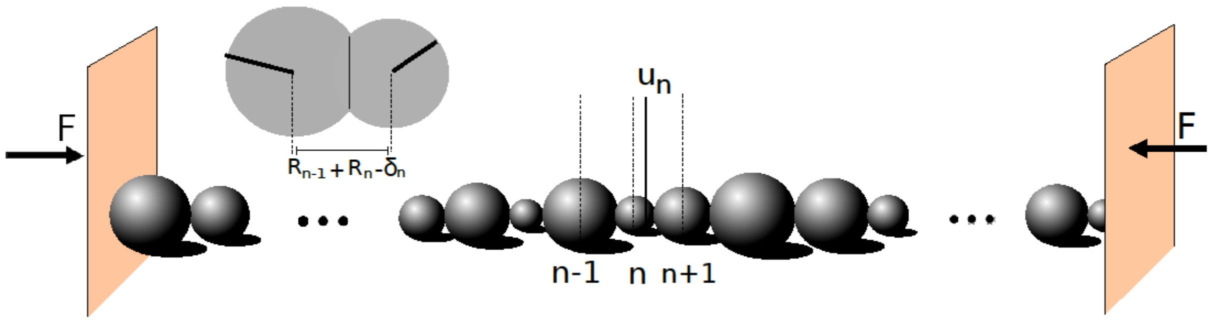
by Bob Senyange on Saturday 17 June

Granular media

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

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

Hamiltonian model



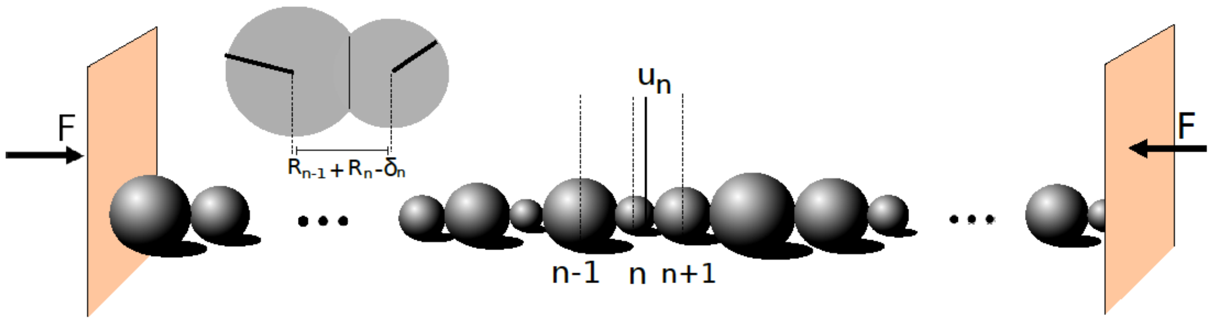
$$H=\sum_{n=1}^{N}\left(\frac{p_n^2}{2m_n}+\frac{2}{5}A_n[\delta_n+u_{n-1}-u_n]_+^{5/2}-\frac{2}{5}A_n\delta_n^{5/2}-A_n\delta_n^{3/2}(u_{n-1}-u_n)\right)$$

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

$[x]_+$=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



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

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

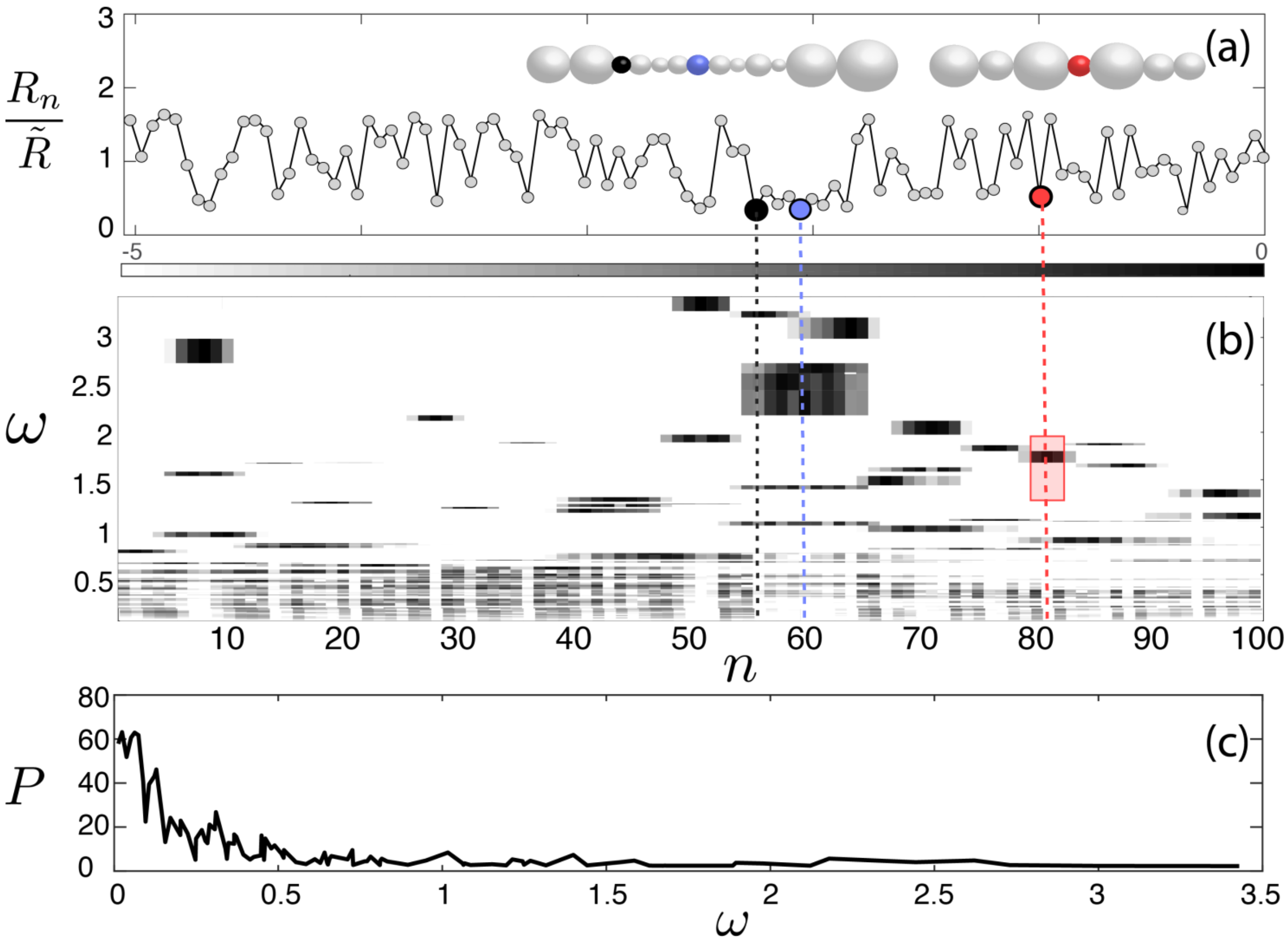
$[x]_+=0$ if $x<0$: formation of a gap. ν: Poisson's ratio, $\mathcal{E}$: Elastic modulus.

Hertzian forces between spherical beads. Fixed boundary conditions.

Disorder both in couplings and masses

$R_n \in [R, \alpha R]$ with $\alpha \geq 1$

Eigenmodes and single site excitations



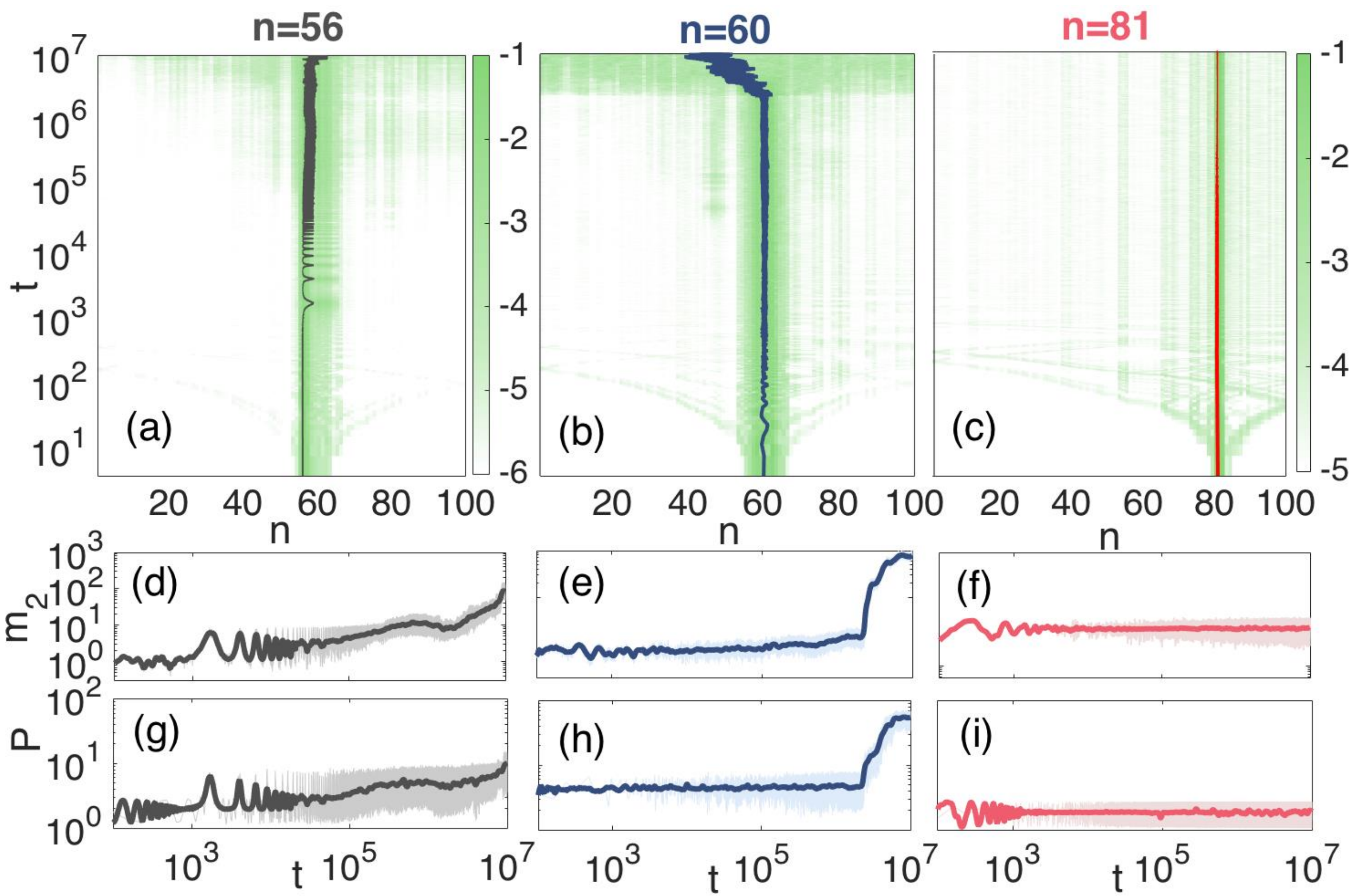
Disorder realization with N=100 beads

Displacement excitation of bead n

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

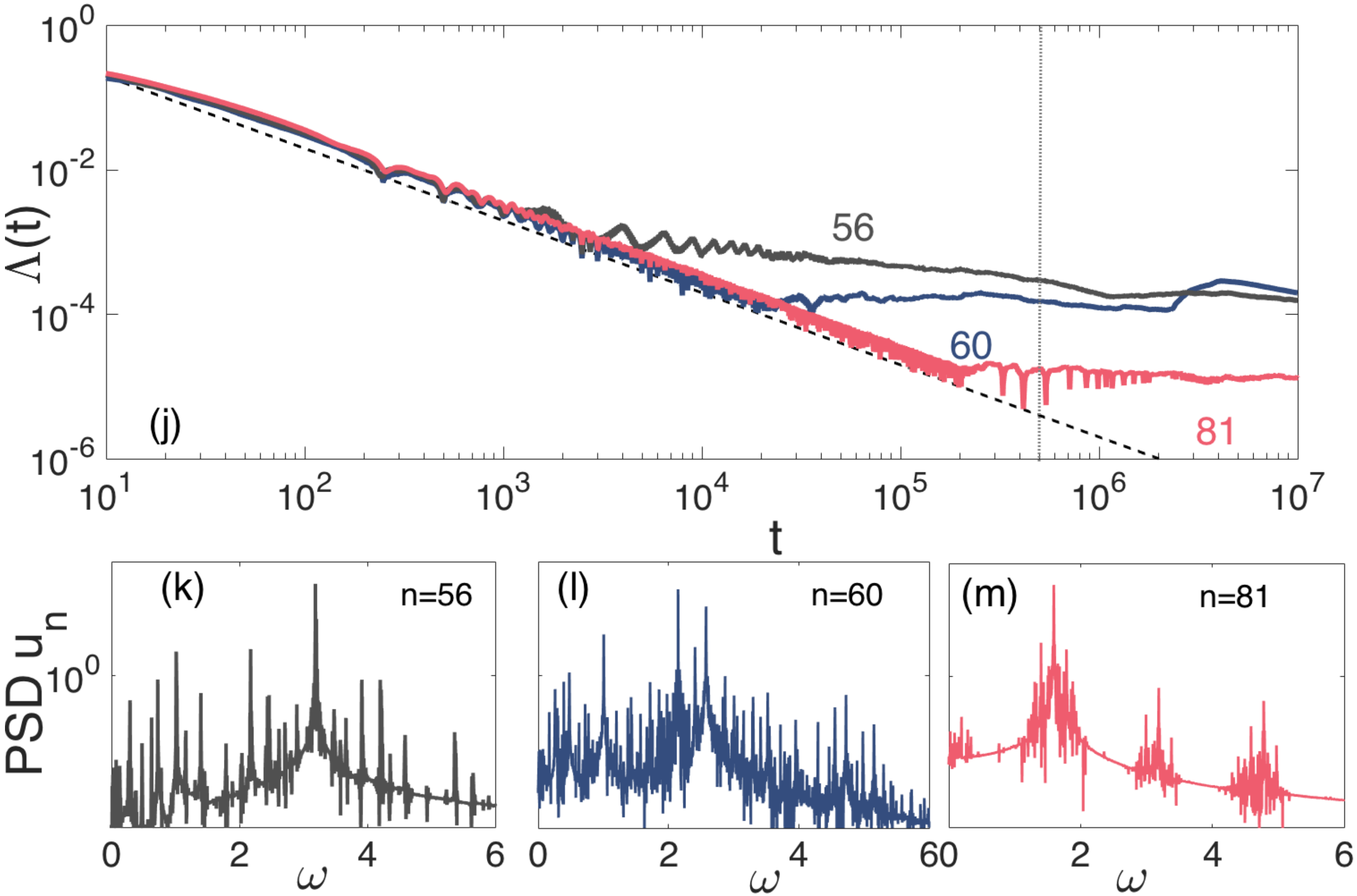
Achilleos et al. (2017) in preparation

Weak nonlinearity: Long time evolution



Delocalization **Delocalization** **Localization**

Weak nonlinearity: Chaoticity



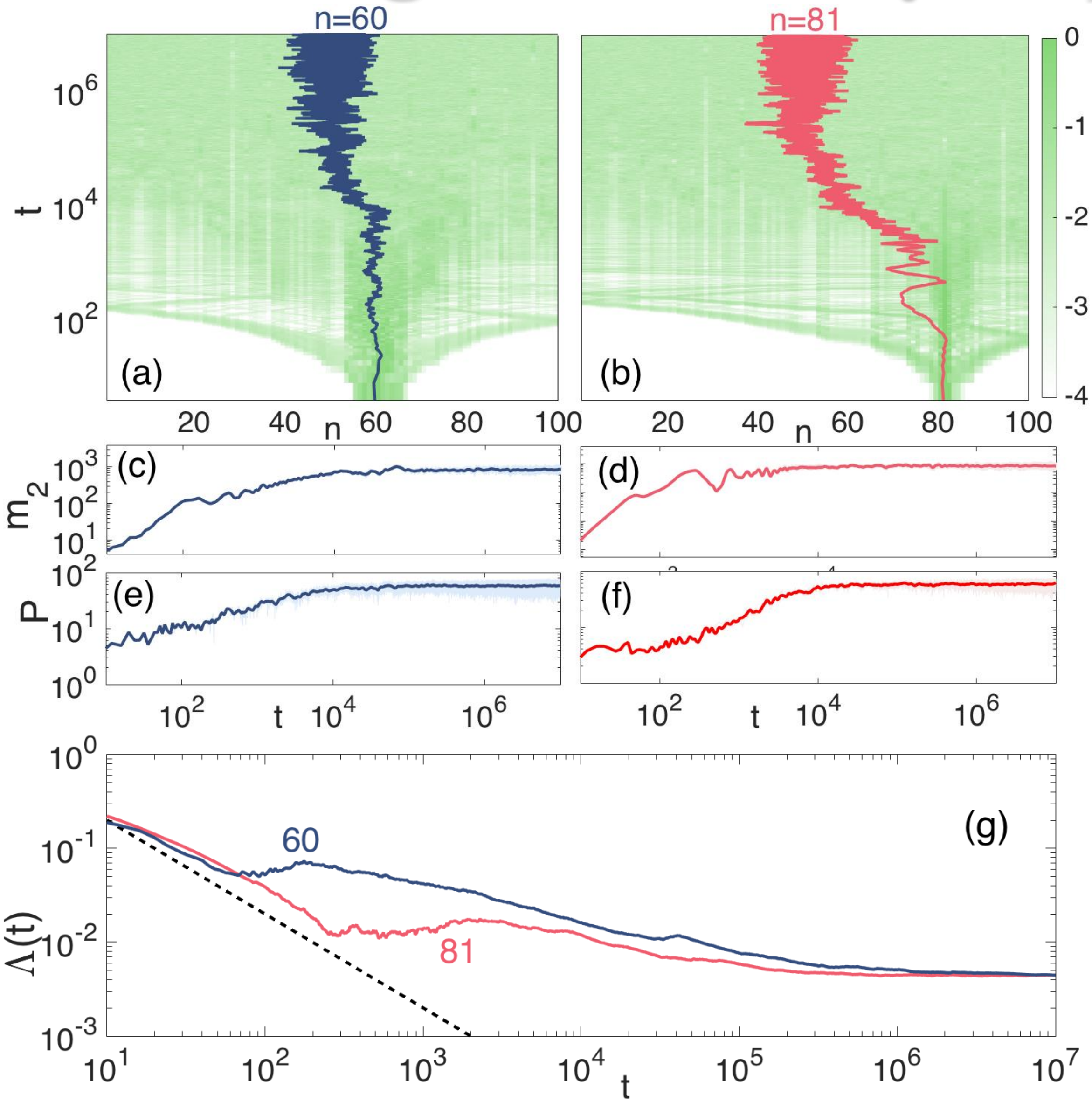
mLCE

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.

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: $d<\delta<\Delta$, $m_2 \sim t^{1/2} \longrightarrow m_2 \sim t^{1/3}$**
  - ✓ **Selftrapping Regime: $\delta>\Delta$**
- **Lyapunov exponent computations show that:**
  - ✓ **Chaos not only exists, but also persists.**
  - ✓ **Slowing down of chaos does not cross over to regular dynamics.**
  - ✓ **Chaotic hot spots meander through the system, supporting a homogeneity of chaos inside the wave packet.**
- **Statistical computations of q-Gaussian distributions show that the system's motion remains chaotic in the long time limit.**
- **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.**

References

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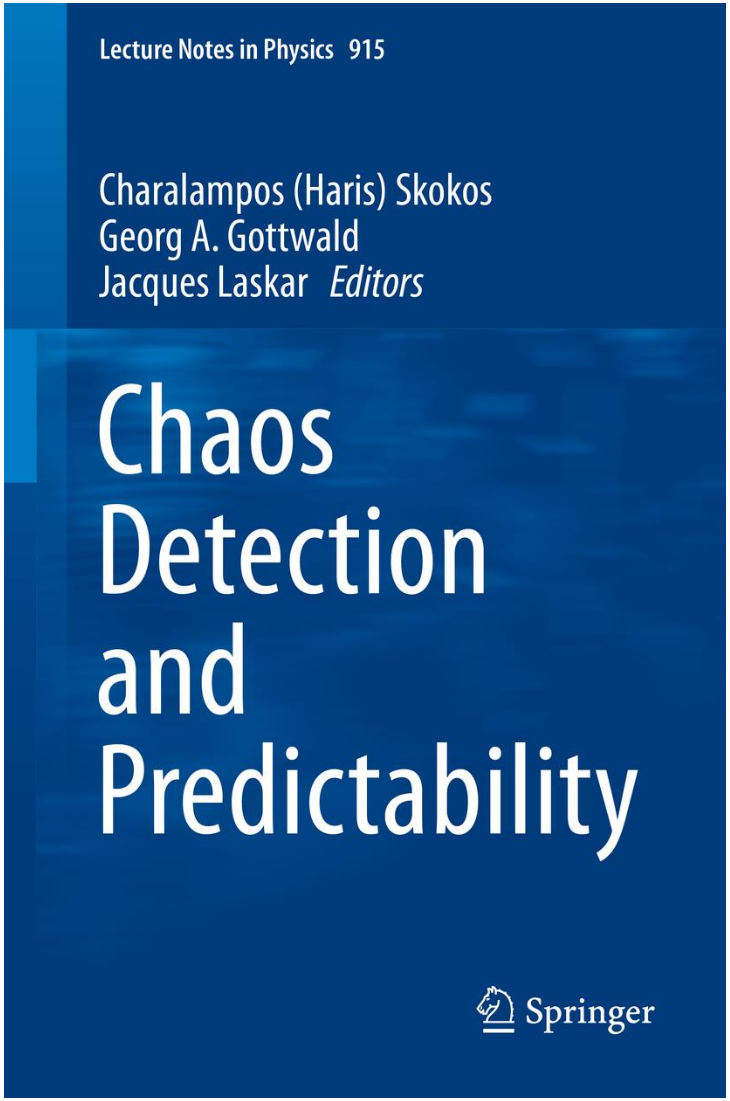
- **Antonopoulos, S., Bountis, Flach (2017) nlin.CD/1705.06127**

- **Achilleos , Theocharis, S. (2016) PRE, 93, 022903**
- **Achilleos , Theocharis, S. (2017) in preparation**

Thank you for your attention

A …shameless promotion



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Contents