Chaotic dynamics of disordered nonlinear lattices

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… and Jacques' indirect contribution (IC)

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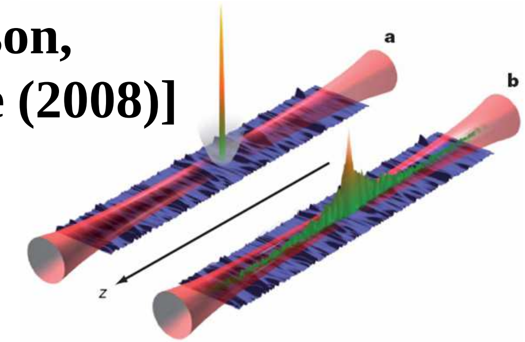
S’ Agaro 1995

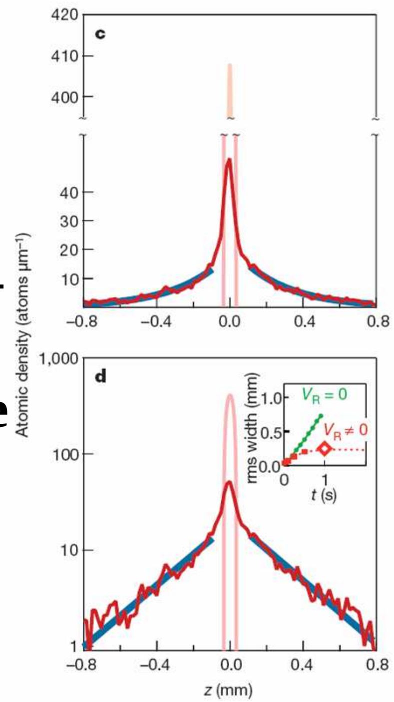
Outline

- **Disordered lattices:**
  - ✓ **The quartic Klein-Gordon (KG) model**
  - ✓ **The disordered nonlinear Schrödinger equation (DNLS)**
  - ✓ **Symplectic Integration of these models (Jacques' IC)**
  - ✓ **Different dynamical behaviors**
- **Chaotic behavior of the KG model**
  - ✓ **Symplectic Integration of variational equations (Jacques' IC)**
  - ✓ **Lyapunov exponents**
  - ✓ **Deviation Vector Distributions**
- **Different integration schemes for DNLS (Jacques' IC)**
- **Summary**

Interplay of disorder and nonlinearity



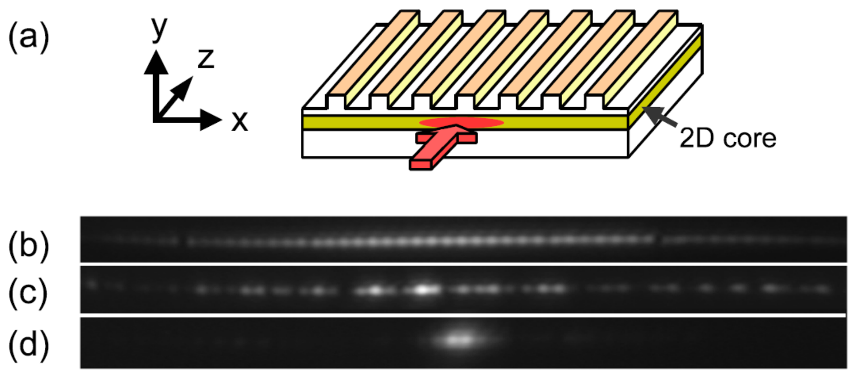
Waves in disordered media – Anderson localization [Anderson, Phys. Rev. (1958)]. Experiments on BEC [Billy et al., Nature (2008)]



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

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 $P=N$.

Symplectic Integrators (SIs)

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

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

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+τ 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.

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

Symplectic Integrator SABA$_2$C

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

$$SABA_2 = e^{c_1 \tau L_A} \; e^{d_1 \tau L_B} \; e^{c_2 \tau L_A} \; e^{d_1 \tau L_B} \; e^{c_1 \tau L_A}$$

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: $SABAC_2 = C \; (SABA_2) \; C$ and its error is of order 4.

The KG model

We apply the SABAC$_2$ integrator scheme to the KG Hamiltonian by using the splitting:

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

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

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

with a corrector term which corresponds to the Hamiltonian function:

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

The DNLS model

A 2nd order SABA Symplectic Integrator with 5 steps, combined with approximate solution for the *B* part (Fourier Transform): SIFT[2]

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

$$H_D = \sum_l \Big(\underbrace{\frac{\varepsilon_l}{2}(q_l^2 + p_l^2) + \frac{\beta}{8}(q_l^2 + p_l^2)^2}_{A} \underbrace{- q_n q_{n+1} - p_n p_{n+1}}_{B} \Big)$$

$$e^{\tau L_A}: \begin{cases} q_l' = q_l \cos(\alpha_l \tau) + p_l \sin(\alpha_l \tau), \\ p_l' = p_l \cos(\alpha_l \tau) - q_l \sin(\alpha_l \tau), \end{cases}$$

$$\alpha_l = \epsilon_l + \beta(q_l^2 + p_l^2)/2$$

$$e^{\tau L_B}: \begin{cases} \varphi_q = \sum_{m=1}^{N} \psi_m e^{2\pi i q(m-1)/N} \\ \varphi_q' = \varphi_q e^{2i\cos(2\pi(q-1)/N)\tau} \\ \psi_l' = \frac{1}{N}\sum_{q=1}^{N} \varphi_q' e^{-2\pi i l(q-1)/N} \end{cases}$$

The DNLS model

Symplectic Integrators produced by Successive Splits (SS)

$$H_D = \sum_l \Big(\underbrace{\frac{\varepsilon_l}{2}\left(q_l^2 + p_l^2\right) + \frac{\beta}{8}\left(q_l^2 + p_l^2\right)^2}_{A} \underbrace{- q_n q_{n+1}}_{B_1} \underbrace{- p_n p_{n+1}}_{B_2} \Big)$$

$B = B_1 + B_2$

$$\begin{cases} q_l' = q_l \cos(\alpha_l \tau) + p_l \sin(\alpha_l \tau), \\ p_l' = p_l \cos(\alpha_l \tau) - q_l \sin(\alpha_l \tau), \end{cases} \quad \begin{cases} q_l' = q_l, \\ p_l' = p_l + (q_{l-1} + q_{l+1})\tau \end{cases} \quad \begin{cases} p_l' = p_l, \\ q_l' = q_l - (p_{l-1} + p_{l+1})\tau \end{cases}$$

Using the SABA$_2$ integrator we get a 2nd order integrator with 13 steps, SS^2:

$$SS^2 = e^{\left[\frac{(3-\sqrt{3})}{6}\tau\right]L_A} e^{\frac{\tau}{2}L_B} e^{\frac{\sqrt{3}\tau}{3}L_A} e^{\frac{\tau}{2}L_B} e^{\left[\frac{(3-\sqrt{3})}{6}\tau\right]L_A}$$

$$\tau' = \tau / 2$$

$$\underbrace{e^{\left[\frac{(3-\sqrt{3})}{6}\tau'\right]L_{B_1}} e^{\frac{\tau'}{2}L_{B_2}} e^{\frac{\sqrt{3}\tau'}{3}L_{B_1}} e^{\frac{\tau'}{2}L_{B_2}} e^{\left[\frac{(3-\sqrt{3})}{6}\tau'\right]L_{B_1}}} \; \underbrace{e^{\left[\frac{(3-\sqrt{3})}{6}\tau'\right]L_{B_1}} e^{\frac{\tau'}{2}L_{B_2}} e^{\frac{\sqrt{3}\tau'}{3}L_{B_1}} e^{\frac{\tau'}{2}L_{B_2}} e^{\left[\frac{(3-\sqrt{3})}{6}\tau'\right]L_{B_1}}}$$

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

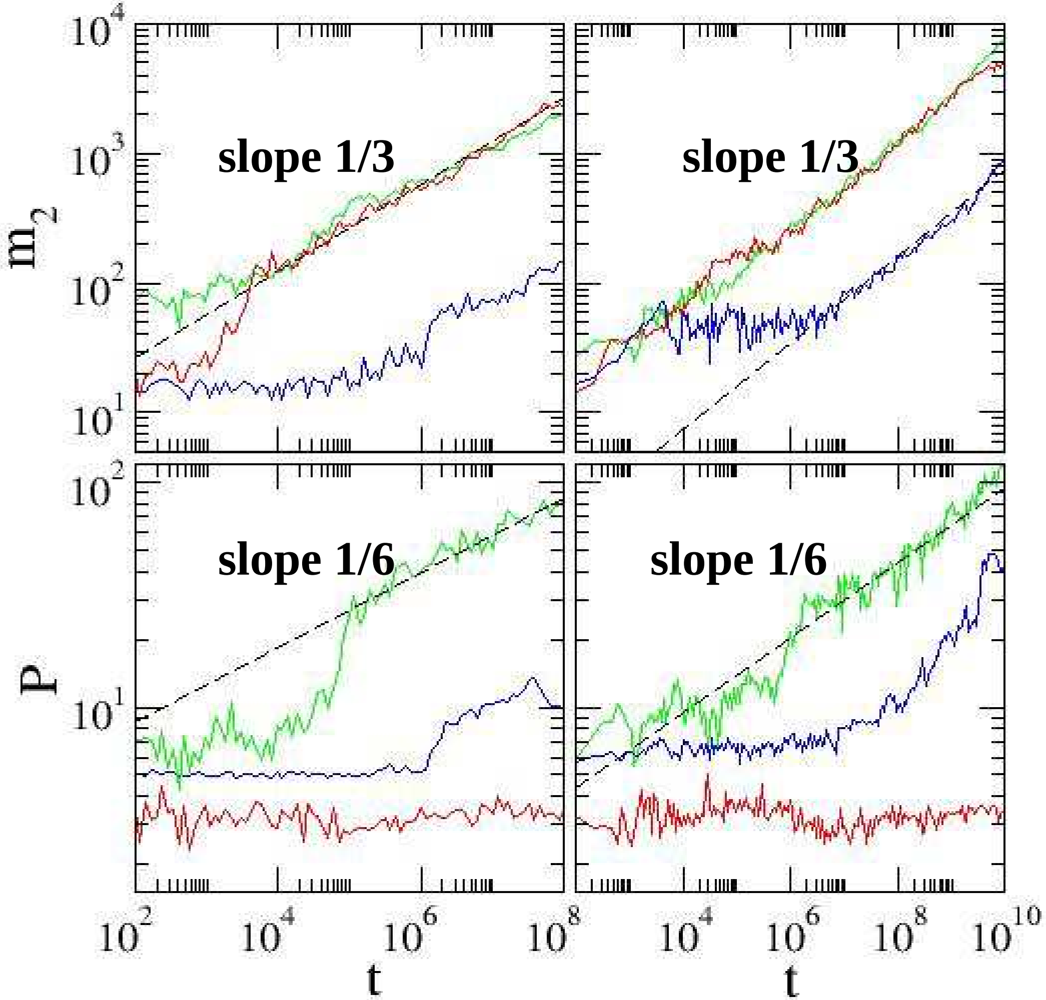
Almost all NMs in the packet are resonantly interacting. Wave packets initially spread faster and eventually enter the weak chaos regime.

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:

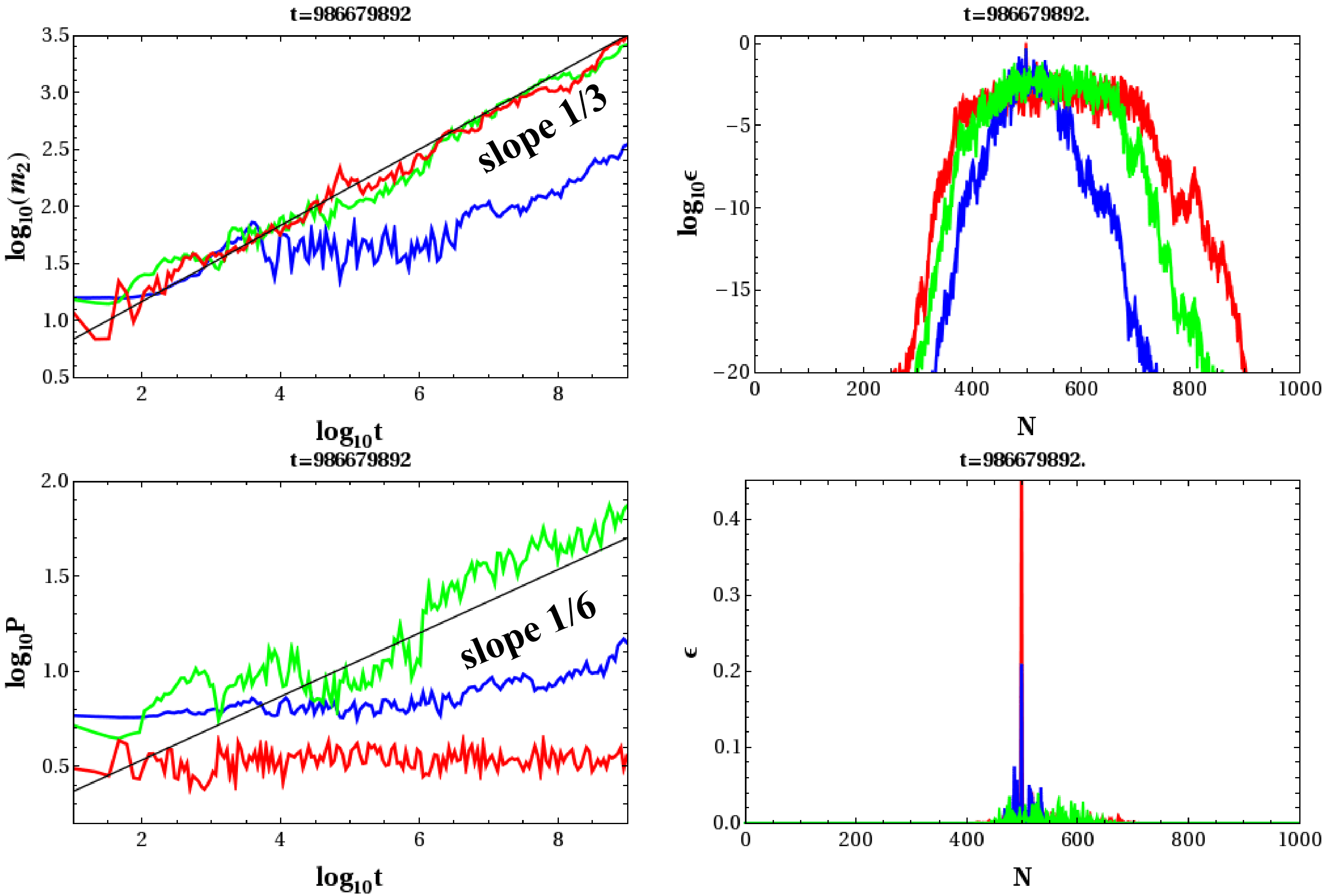
α=0.33±0.05 (KG)

α=0.33±0.02 (DLNS)

Flach et al., PRL (2009)

S. et al., PRE (2009)

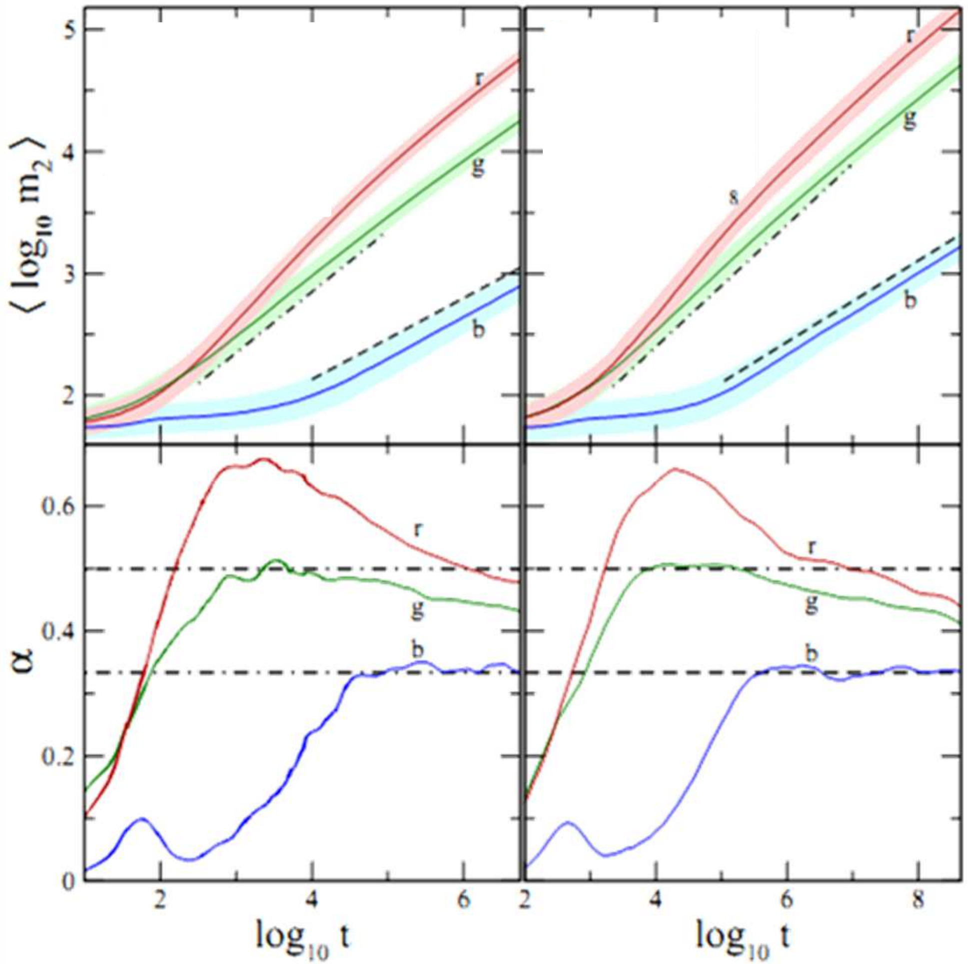
KG: Different spreading regimes



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!

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

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:

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

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

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

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)].**

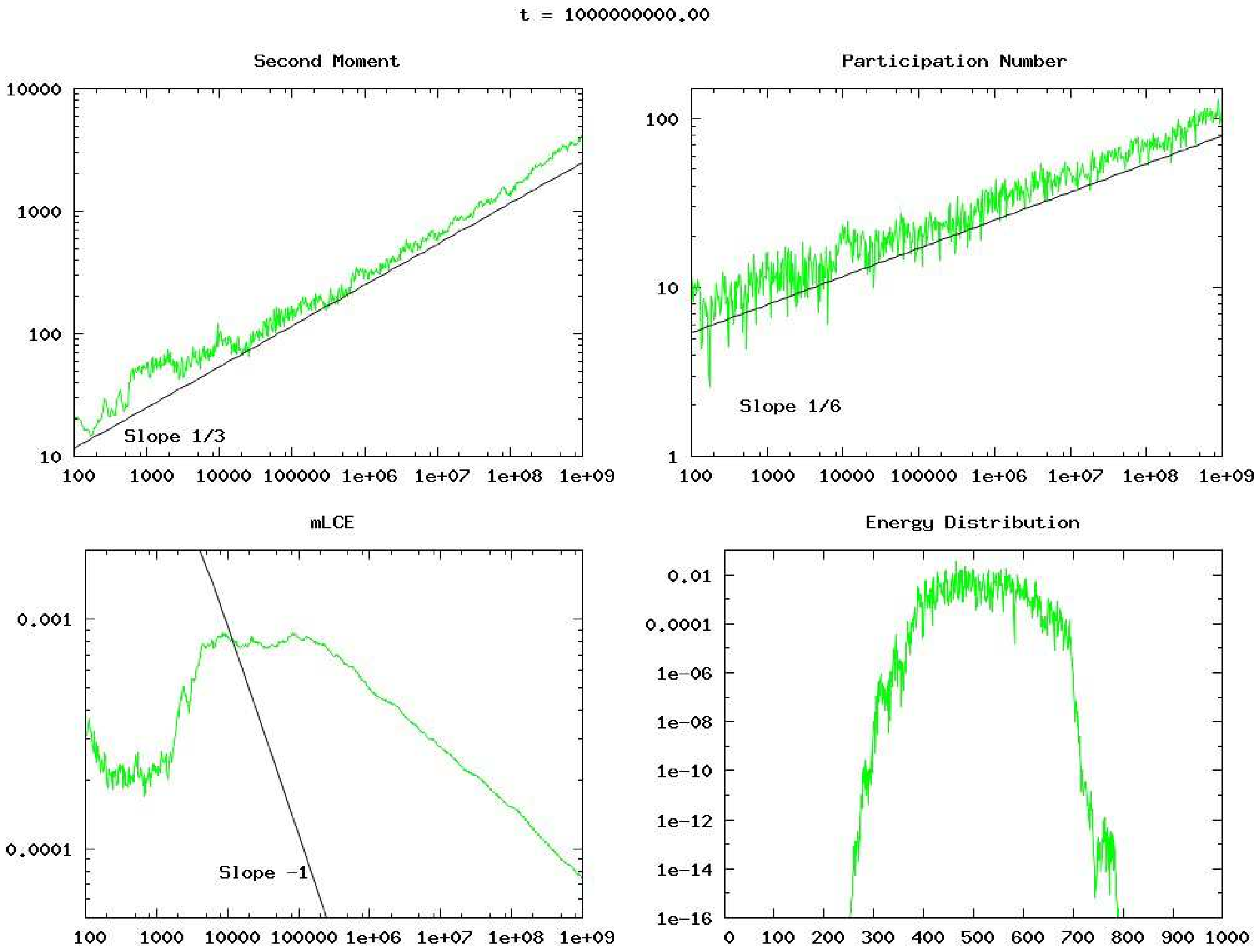
The Hénon-Heiles system can be split as: $A = \frac{1}{2}(p_x^2 + p_y^2) \quad B = \frac{1}{2}(x^2 + y^2) + x^2 y - \frac{1}{3}y^3$

$$\begin{aligned} \dot{x} &= p_x \\ \dot{y} &= p_y \\ \dot{p}_x &= -x - 2xy \\ \dot{p}_y &= y^2 - x^2 - y \\ \dot{\delta x} &= \delta p_x \\ \dot{\delta y} &= \delta p_y \\ \dot{\delta p_x} &= -(1+2y)\delta x - 2x\delta y \\ \dot{\delta p_y} &= -2x\delta x + (-1+2y)\delta y \end{aligned}$$

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

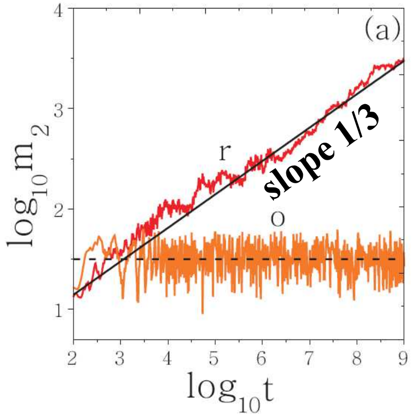
$$\xrightarrow{B(\vec{q})} \quad \left.\begin{aligned} \dot{x} &= 0 \\ \dot{y} &= 0 \\ \dot{p}_x &= -x - 2xy \\ \dot{p}_y &= y^2 - x^2 - y \\ \dot{\delta x} &= 0 \\ \dot{\delta y} &= 0 \\ \dot{\delta p_x} &= -(1+2y)\delta x - 2x\delta y \\ \dot{\delta p_y} &= -2x\delta x + (-1+2y)\delta y \end{aligned}\right\}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

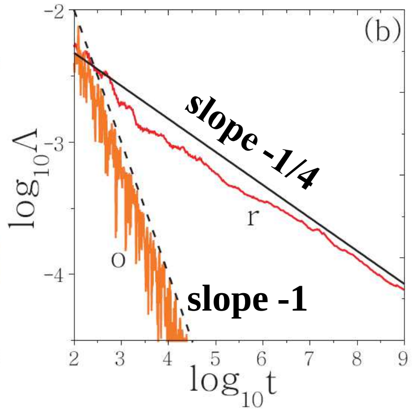
KG: Weak Chaos (E=0.4)

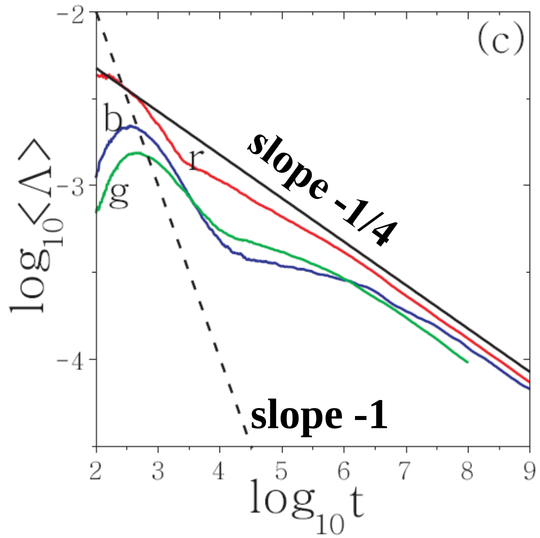


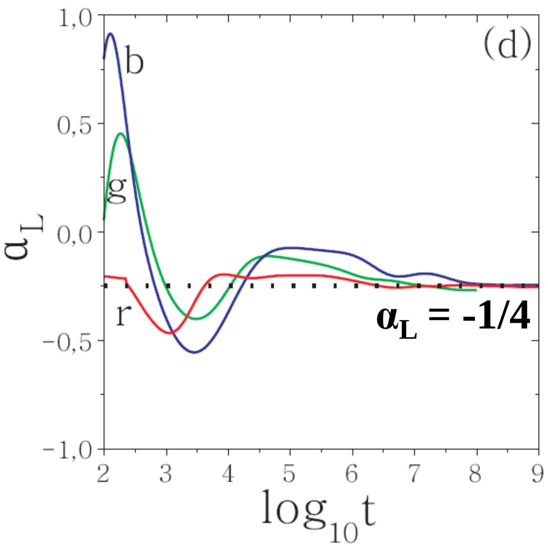
KG: Weak Chaos

Individual runs
Linear case
E=0.4, W=4









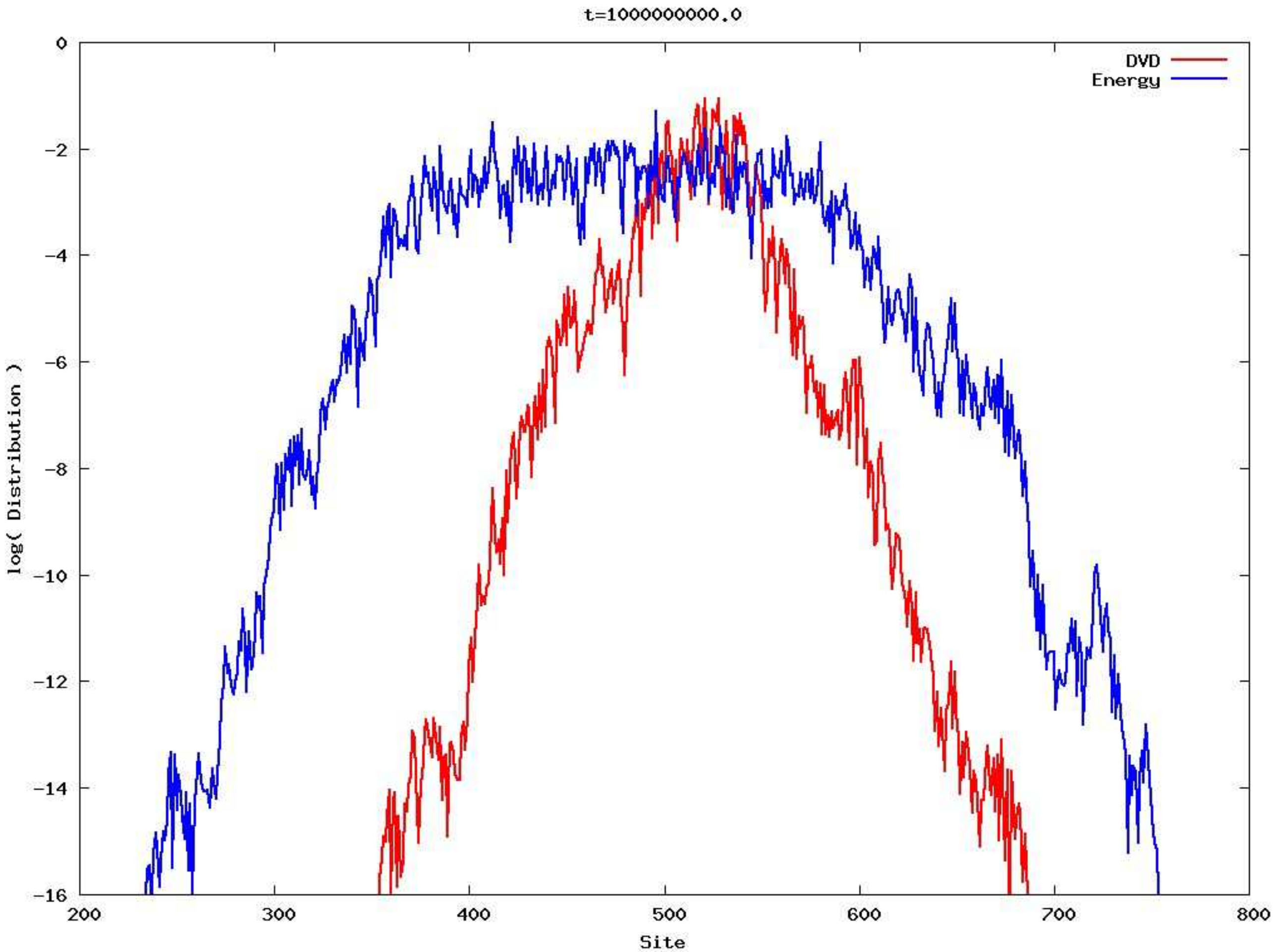
$$\alpha_L = \frac{d\left(\log\langle\Lambda\rangle\right)}{d\log t}$$

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)

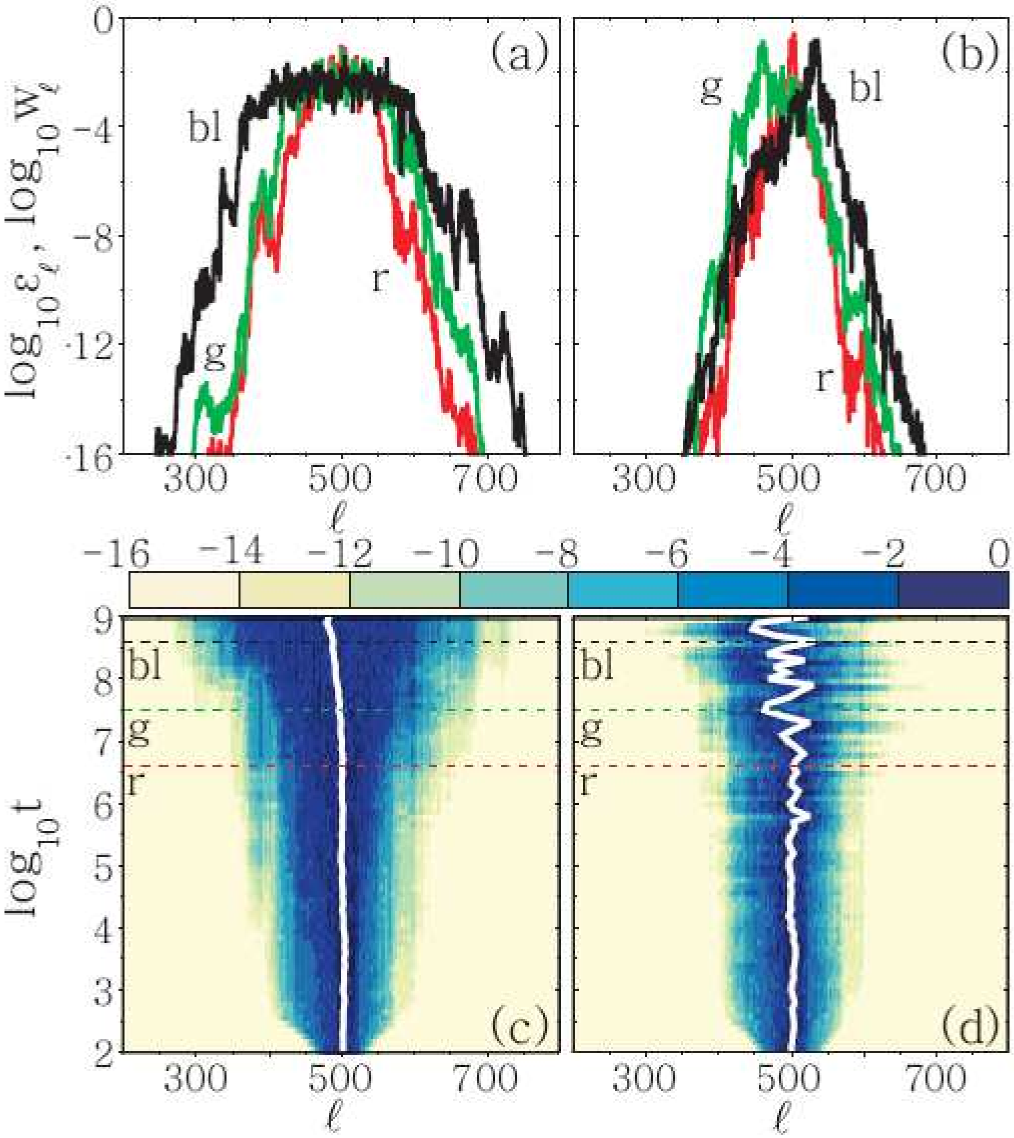


Deviation vector:

v(t)=(δu_1(t), δu_2(t),…, δu_N(t), δp_1(t), δp_2(t),…, δp_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.

Three part split symplectic integrators for the DNLS model

Three part split symplectic integrator of order 2, with 5 steps: ABC^2

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

$$ABC^2 = e^{\frac{\tau}{2}L_A}\, e^{\frac{\tau}{2}L_B}\, e^{\tau L_C}\, e^{\frac{\tau}{2}L_B}\, e^{\frac{\tau}{2}L_A}$$

This low order integrator has already been used by e.g. Chambers, MNRAS (1999) – Goździewski et al., MNRAS (2008).

Composition Methods: 4th order SIs

Starting from any 2nd order symplectic integrator S^{2nd}, we can construct a 4th order integrator S^{4th} using the composition method proposed by Yoshida [Phys. Lett. A (1990)]:

$$S^{4th}(\tau) = S^{2nd}(x_1\tau)\times S^{2nd}(x_0\tau)\times S^{2nd}(x_1\tau), \qquad x_0 = -\frac{2^{1/3}}{2-2^{1/3}}, \qquad x_1 = \frac{1}{2-2^{1/3}}$$

In this way, starting with the 2nd order integrators SS^2, $SIFT^2$ and ABC^2 we construct the 4th order integrators:

SS^4 with 37 steps **$SIFT^4$ with 13 steps** **$ABC^4_{[Y]}$ with 13 steps**

Composition method proposed by Suzuki [Phys. Lett. A (1990)]:

$$S^{4th}(\tau) = S^{2nd}(p_2\tau)\times S^{2nd}(p_2\tau)\times S^{2nd}((1-4p_2)\tau)\times S^{2nd}(p_2\tau)\times S^{2nd}(p_2\tau)$$

$$p_2 = \frac{1}{4-4^{1/3}}, \qquad 1-4p_2 = -\frac{4^{1/3}}{4-4^{1/3}}$$

Starting with the 2nd order integrators ABC^2 we construct the 4th order integrator: $ABC^4_{[S]}$ with 21 steps.

More 4th order SIs

We construct few more integration schemes by considering the 4th order symplectic integrators ABA864, ABA1064, ABAH864 and ABAH1064 introduced by Blanes et al., Appl. Num. Math. (2013) and Farrés et al., Cel. Mech. Dyn. Astr. (2013).

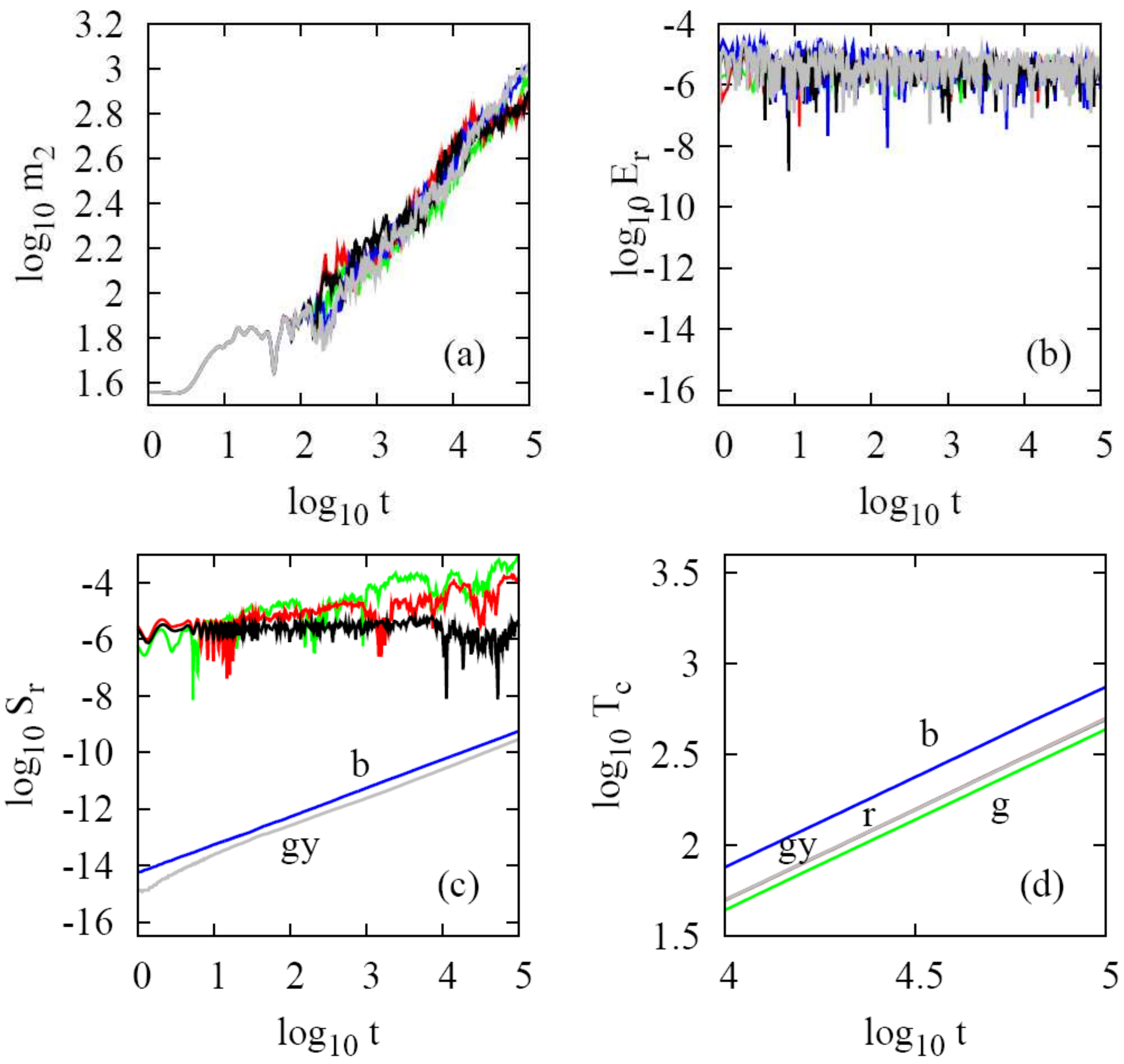
Approximating the solution of the *B* part by a Fourier Transform we construct the 4th order integrators:

$SIFT^4_{864}$ with 43 steps | **$SIFT^4_{1064}$ with 49 steps**

Using successive splits for the *B* part and implementing the $SABA_2$ integrator for its integration, we construct the 4th order integrators (based on ABAH864 and ABAH1064):

SS^4_{864} with 49 steps | **SS^4_{1064} with 55 steps**

4^{th} order integrators: Numerical results (I)



$SIFT^4$ τ=0.125

$SIFT^2$ τ=0.05

$ABC^4_{[S]}$ τ=0.1

SS^4 τ=0.1

$ABC^4_{[Y]}$ τ=0.05

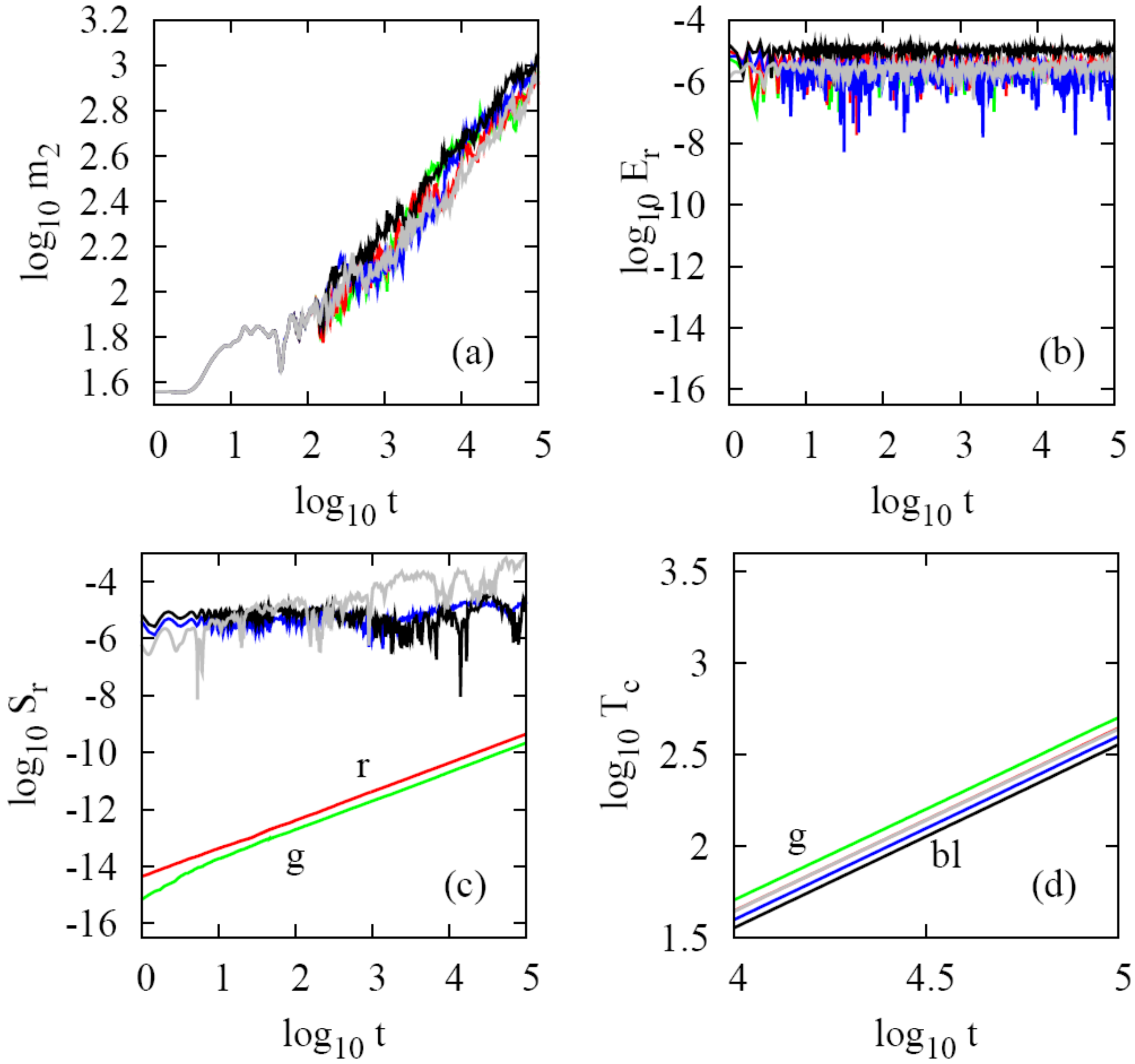
E_r: relative energy error

S_r: relative norm error

T_c: CPU time (sec)

S. et al., Phys. Lett. A (2014)

4^{th} order integrators: Numerical results (II)



$SIFT^4_{1064}$ τ=0.25

$ABC^4_{[Y]}$ τ=0.05

$SIFT^4_{864}$ τ=0.25

SS^4_{1064} τ=0.25

SS^4_{864} τ=0.25

E_r: relative energy error

S_r: relative norm error

T_c: CPU time (sec)

S. et al., Phys. Lett. A (2014)

Summary (I)

- **We presented three different dynamical behaviors for wave packet spreading in 1d nonlinear disordered lattices:**
  - ✓ **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: $\delta>\Delta$**
- **Generality of results:**
  - ✓ **Two different models: KD and DNLS,**
  - ✓ **Predictions made for DNLS are verified for both models.**
- **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.**
- **Our results suggest that Anderson localization is eventually destroyed by nonlinearity, since spreading does not show any sign of slowing down.**

Summary (II)

- We presented several efficient integration methods suitable for the integration of the DNLS model, which are based on symplectic integration techniques.

- The construction of symplectic schemes based on 3 part split of the Hamiltonian was emphasized (ABC methods).
- Algorithms based on the integration of the B part of Hamiltonian via Fourier transforms, i.e. methods $SIFT^2$, $SIFT^4$, $SIFT^4_{864}$ and $SIFT^4_{1064}$ succeeded in keeping the relative norm error S_r very low. Drawback: they require the number of lattice sites to be 2^k, $k \in \mathbb{N}^*$.

- We hope that our results will initiate future research both for the theoretical development of new, improved 3 part split integrators, as well as for their applications to different dynamical systems.

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Thank you for your attention