Chaotic behavior of disordered nonlinear lattices

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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**
- Numerical methods
 - **✓ Symplecic Integrators**
 - **✓ Tangent Map method**
 - **✓ Different integration schemes for DNLS**
- Summary

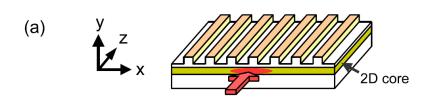
Interplay of disorder and nonlinearity

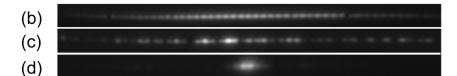
Waves in disordered media – Anderson localization [Anderson, Phys. Rev. (1958)]. Experiments on BEC [Billy et al., Nature (2008)]

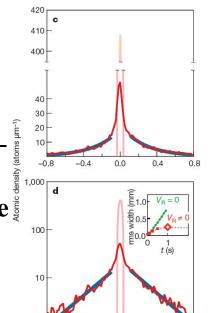
Waves in nonlinear disordered media – localization or delocalization?

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

$$H_{K} = \sum_{l=1}^{N} \frac{p_{l}^{2}}{2} + \frac{\tilde{\varepsilon}_{l}}{2} u_{l}^{2} + \frac{1}{4} u_{l}^{4} + \frac{1}{2W} (u_{l+1} - u_{l})^{2}$$

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) $A_{v,l}$ - Eigenvalue problem:

$$\lambda A_l = \varepsilon_l A_l - (A_{l+1} + A_{l-1})$$
 with $\lambda = W\omega^2 - W - 2$, $\varepsilon_l = W(\tilde{\varepsilon}_l - 1)$

The discrete nonlinear Schrödinger (DNLS) equation

We also consider the system:

$$\boldsymbol{H}_{D} = \sum_{l=1}^{N} \boldsymbol{\varepsilon}_{l} \left| \boldsymbol{\psi}_{l} \right|^{2} + \frac{\boldsymbol{\beta}}{2} \left| \boldsymbol{\psi}_{l} \right|^{4} - \left(\boldsymbol{\psi}_{l+1} \boldsymbol{\psi}_{l}^{*} + \boldsymbol{\psi}_{l+1}^{*} \boldsymbol{\psi}_{l} \right)$$

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

$$z_v \equiv \frac{E_v}{\sum_m E_m}$$
 with $E_v = \frac{1}{2} (\dot{A}_v^2 + \omega_v^2 A_v^2)$, where A_v is the amplitude

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

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

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

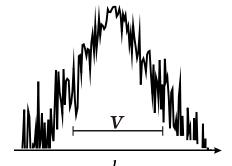
measures the number of stronger excited modes in z_v . Single mode P=1. Equipartition of energy P=N.

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

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

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

$$\Delta_{K} = 1 + \frac{4}{W}$$
Localization volume of an eigenstate:
$$V \sim \frac{1}{\sum_{l=1}^{N} A_{v,l}^{4}}$$



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

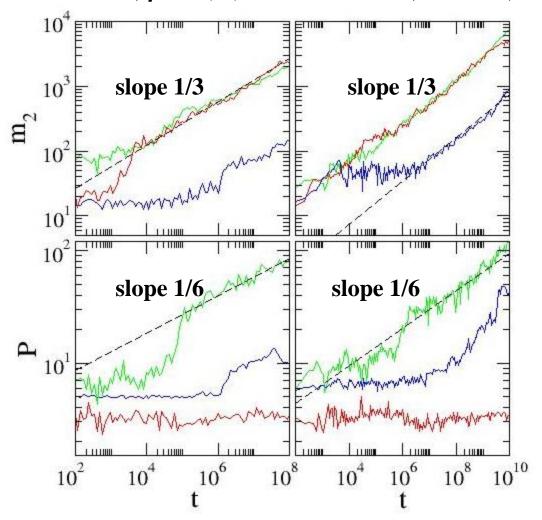
Almost all NMs in the packet are resonantly interacting. Wave packets initially spread faster and eventually enter the weak chaos regime.

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



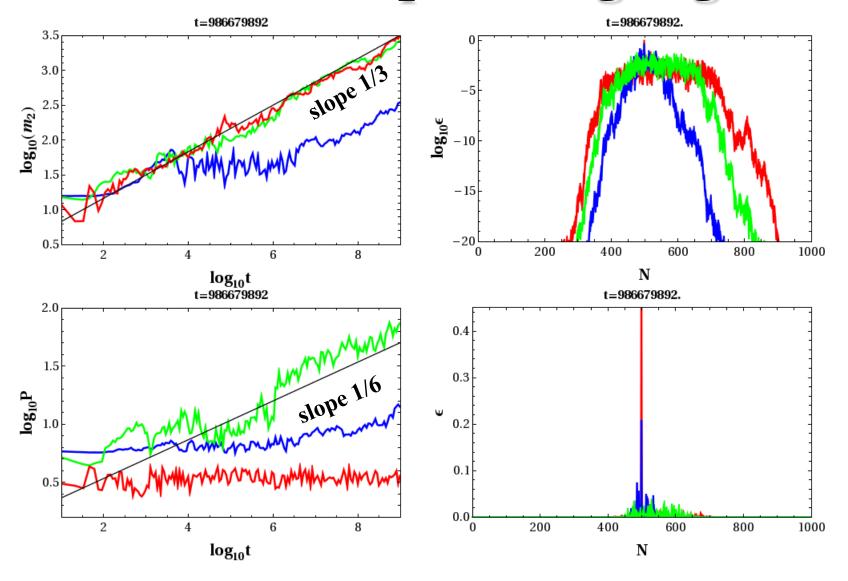
No strong chaos regime

In weak chaos regime we averaged the measured exponent α (m₂~t $^{\alpha}$) over 20 realizations:

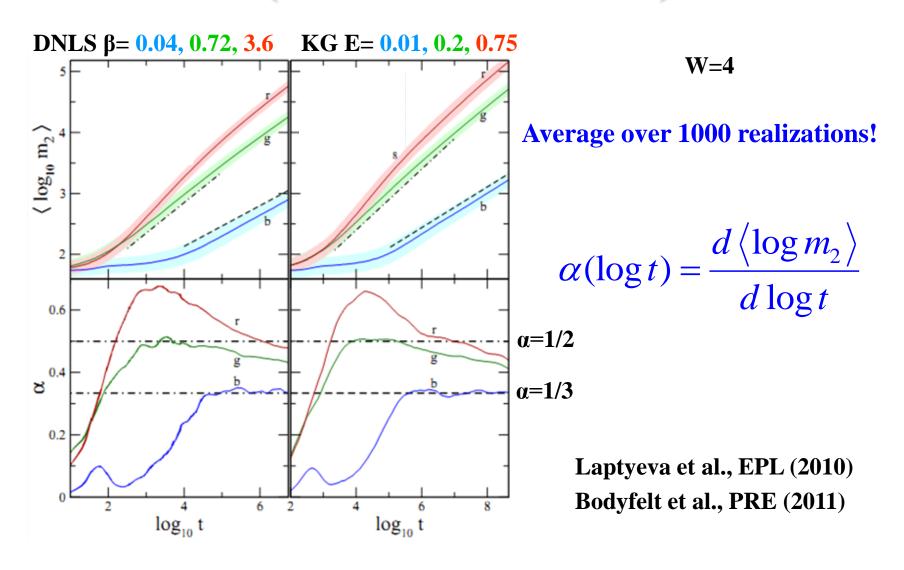
 α =0.33±0.05 (KG) α =0.33±0.02 (DLNS)

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

KG: Different spreading regimes



Crossover from strong to weak chaos (block excitations)



Lyapunov Exponents (LEs)

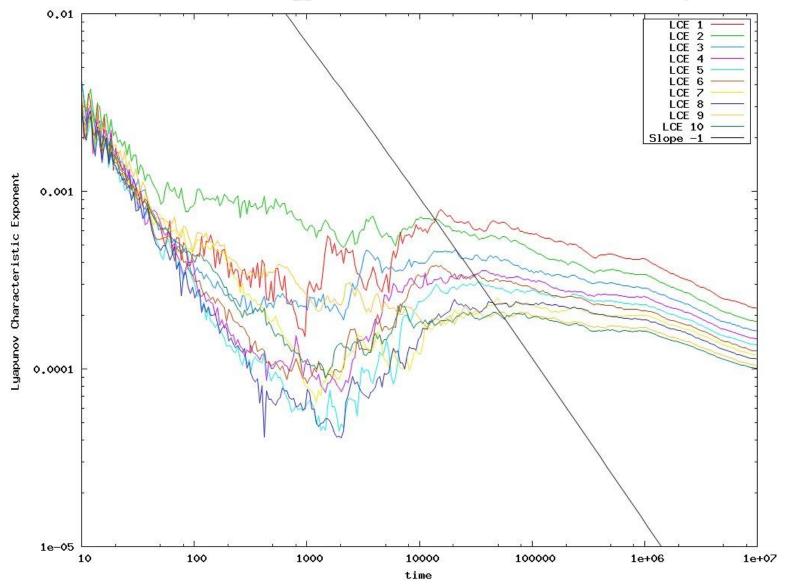
Roughly speaking, the Lyapunov exponents of a given orbit characterize the mean exponential rate of divergence of trajectories surrounding it.

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

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

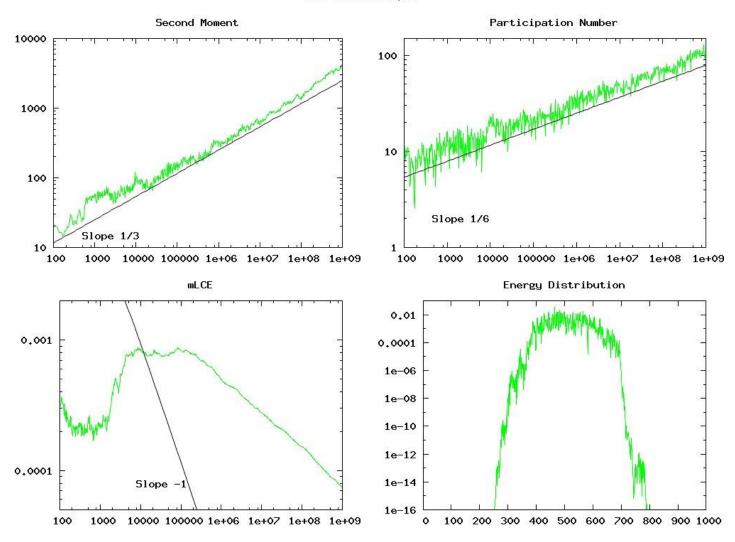
 λ_1 =0 → Regular motion ∞ (t⁻¹) λ_1 ≠0 → Chaotic motion

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



KG: Weak Chaos (E=0.4)

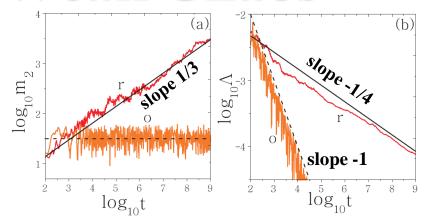
t = 1000000000.00

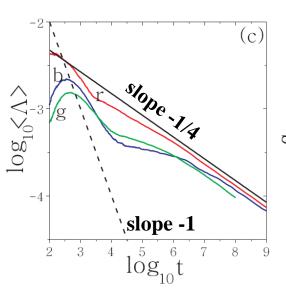


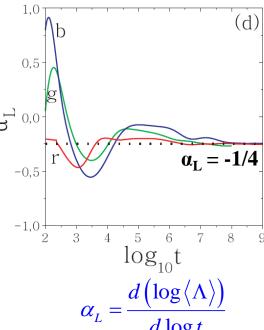
KG: Weak Chaos

Individual runs

Linear case E=0.4, W=4







Average over 50 realizations

Single site excitation E=0.4, W=4

Block excitation (21 sites)

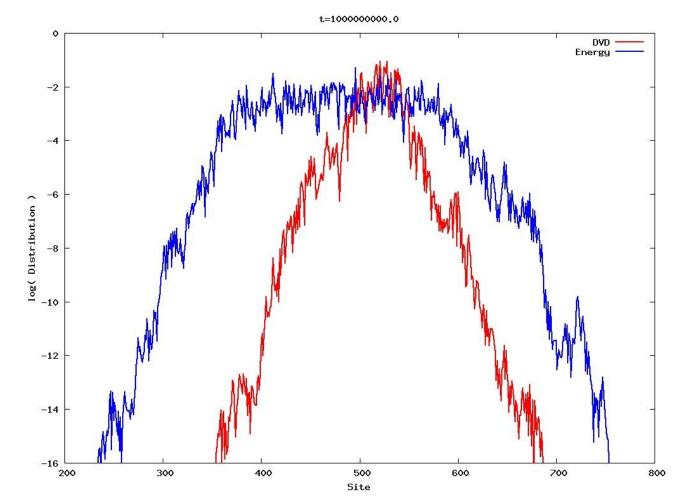
E=0.21, W=4

Block excitation (37 sites)

E=0.37, W=3

S. et al. PRL (2013)

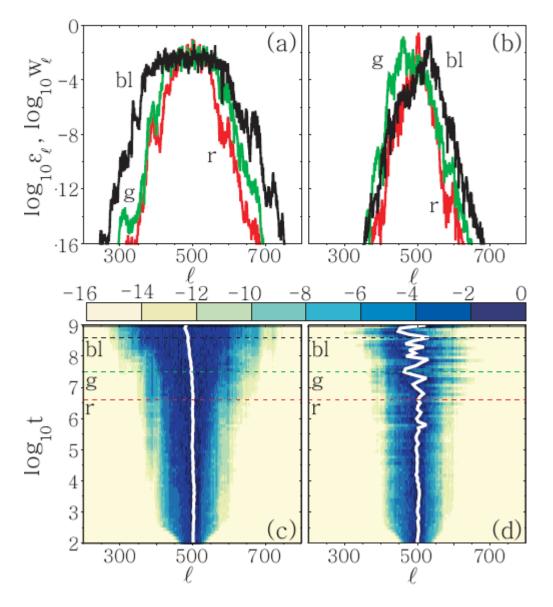
Deviation Vector Distributions (DVDs)



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

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

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.

Integration scheme

Consider an N degree of freedom autonomous Hamiltonian system having a Hamiltonian function of the form:

$$H(q_1,q_2,...,q_N, p_1,p_2,...,p_N)$$

The time evolution of an orbit (trajectory) with initial condition

$$P(0)=(q_1(0), q_2(0),...,q_N(0), p_1(0), p_2(0),...,p_N(0))$$

is governed by the Hamilton's equations of motion

$$\frac{d\mathbf{p_i}}{dt} = -\frac{\partial \mathbf{H}}{\partial \mathbf{q_i}} , \frac{d\mathbf{q_i}}{dt} = \frac{\partial \mathbf{H}}{\partial \mathbf{p_i}}$$

Autonomous Hamiltonian systems

Let us consider an N degree of freedom autonomous Hamiltonian systems of the $H(\vec{q},\vec{p}) = \frac{1}{2} \sum_{i=1}^N p_i^2 + V(\vec{q})$ form:

$$H(\vec{q}, \vec{p}) = \frac{1}{2} \sum_{i=1}^{N} p_i^2 + V(\vec{q})$$

As an example, we consider the Hénon-Heiles system:

$$H_2 = \frac{1}{2}(p_x^2 + p_y^2) + \frac{1}{2}(x^2 + y^2) + x^2y - \frac{1}{3}y^3$$

Hamilton equations of motion:
$$\begin{cases} \dot{x} &= p_x \\ \dot{y} &= p_y \\ \dot{p}_x &= -x - 2xy \\ \dot{p}_y &= y^2 - x^2 - y \end{cases}$$

Variational equations:

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

Symplectic Integrators (SIs)

Formally the solution of the Hamilton equations of motion can be written as: $\frac{1}{\sqrt{n}}$

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

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 $t+\tau$ consists of approximating the operator $e^{\tau L_H}$ by

$$\mathbf{e}^{\tau \mathbf{L}_{\mathbf{H}}} = \mathbf{e}^{\tau (\mathbf{L}_{\mathbf{A}} + \mathbf{L}_{\mathbf{B}})} = \prod_{i=1}^{J} \mathbf{e}^{\mathbf{c}_{i} \tau \mathbf{L}_{\mathbf{A}}} \mathbf{e}^{\mathbf{d}_{i} \tau \mathbf{L}_{\mathbf{B}}} + O(\boldsymbol{\tau}^{\mathbf{n}+1})$$

for appropriate values of constants c_i, d_i. This is an integrator of order n.

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

Symplectic Integrator SABA₂C

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 $c_{1} = \frac{1}{2} \cdot \frac{\sqrt{3}}{6}$, $c_{2} = \frac{\sqrt{3}}{3}$, $d_{1} = \frac{1}{2}$.

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.

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: $A = \frac{1}{2}(p_x^2 + p_y^2)$ $B = \frac{1}{2}(x^2 + y^2) + x^2y - \frac{1}{2}y^3$

$$\dot{x} = p_{x}
\dot{y} = p_{y}
\dot{p}_{x} = -x - 2xy
\dot{p}_{y} = y^{2} - x^{2} - y$$

$$\dot{x} = p_{x}
\dot{y} = p_{y}
\dot{p}_{x} = 0
\dot{p}_{y} = 0
\dot{\delta x} = \delta p_{x}
\dot{\delta y} = \delta p_{y}
\dot{\delta p}_{x} = 0
\dot{\delta p}_{y} = 0$$

$$\dot{x} = p_{x}
\dot{y} = p_{y}
\dot{p}_{x} = 0
\dot{\delta x} = \delta p_{x}
\dot{\delta p}_{x} = 0
\dot{\delta p}_{y} = 0$$

$$\dot{p}_{y} = 0
\dot{p}_{y} = 0
\dot{p}_{y} = 0
\dot{p}_{y} = 0$$

$$\dot{p}_{y} = 0
\dot{p}_{y} = 0
\dot{p}_{y} = 0$$

$$\dot{p}_{y} = 0
\dot{p}_{y} = 0
\dot{p}_{y} = 0$$

$$\begin{pmatrix}
\vec{x} &= 0 \\
\dot{y} &= 0 \\
\dot{p}_{x} &= -x - 2xy \\
\dot{p}_{y} &= y^{2} - x^{2} - y \\
\delta \dot{x} &= 0 \\
\delta \dot{y} &= 0
\end{pmatrix}$$

$$\begin{vmatrix}
\vec{x} &= 0 \\
\dot{p}_{x} &= -x - 2xy \\
\dot{p}_{y} &= y^{2} - x^{2} - y
\end{vmatrix}$$

$$\begin{vmatrix}
\vec{x} &= x \\
y' &= y \\
p'_{x} &= p_{x} - x(1 + 2y)\tau \\
p'_{y} &= p_{y} + (y^{2} - x^{2} - y)\tau \\
\delta x' &= \delta x \\
\delta y' &= \delta y \\
\delta y' &= \delta y \\
\delta p'_{x} &= \delta p_{x} - [(1 + 2y)\delta x + 2x\delta y]\tau \\
\delta p'_{y} &= \delta p_{y} + [-2x\delta x + (-1 + 2y)\delta y]\tau
\end{vmatrix}$$

 $\delta p_y = -2x\delta x + (-1+2y)\delta y$

$$\frac{d\vec{u}}{dt} = L_{BV}\vec{u} \implies e^{\tau L_{BV}} : \begin{cases}
y' = y \\
p'_x = p_x - x(1 + y) \\
p'_y = p_y + (y^2 - y) \\
\delta x' = \delta x \\
\delta y' = \delta y \\
\delta p'_x = \delta p_x - [(1 + y) + y]
\end{cases}$$

The KG model

We apply the SABAC₂ integrator scheme to the KG Hamiltonian by using the splitting:

$$H_{K} = \sum_{l=1}^{N} \left(\frac{p_{l}^{2}}{2} + \frac{\tilde{\varepsilon}_{l}}{2} u_{l}^{2} + \frac{1}{4} u_{l}^{4} + \frac{1}{2W} (u_{l+1} - u_{l})^{2} \right)$$

$$B$$

$$e^{\tau L_{A}}: \begin{cases} u'_{l} = p_{l}\tau + u_{l} \\ p'_{l} = p_{l}, \end{cases}$$

$$e^{\tau L_{B}}: \begin{cases} u'_{l} = u_{l} \\ p'_{l} = \left[-u_{l}(\tilde{\epsilon}_{l} + u_{l}^{2}) + \frac{1}{W}(u_{l-1} + u_{l+1} - 2u_{l}) \right] \tau + p_{l}, \end{cases}$$

with a corrector term which corresponds to the Hamiltonian function:

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

The DNLS model

A 2nd order SABA Symplectic Integrator with 5 steps, combined with approximate solution for the *B* part (Fourier Transform): SIFT²

$$\begin{split} \boldsymbol{H}_{D} &= \sum_{l} \boldsymbol{\varepsilon}_{l} \left| \boldsymbol{\psi}_{l} \right|^{2} + \frac{\beta}{2} \left| \boldsymbol{\psi}_{l} \right|^{4} - \left(\boldsymbol{\psi}_{l+1} \boldsymbol{\psi}_{l}^{*} + \boldsymbol{\psi}_{l+1}^{*} \boldsymbol{\psi}_{l} \right), \quad \boldsymbol{\psi}_{l} = \frac{1}{\sqrt{2}} \left(\boldsymbol{q}_{l} + i \boldsymbol{p}_{l} \right) \\ \boldsymbol{H}_{D} &= \sum_{l} \left(\frac{\boldsymbol{\varepsilon}_{l}}{2} \left(\boldsymbol{q}_{l}^{2} + \boldsymbol{p}_{l}^{2} \right) + \frac{\beta}{8} \left(\boldsymbol{q}_{l}^{2} + \boldsymbol{p}_{l}^{2} \right)^{2} - \boldsymbol{q}_{n} \boldsymbol{q}_{n+1} - \boldsymbol{p}_{n} \boldsymbol{p}_{n+1} \right) \\ \boldsymbol{B} \\ \boldsymbol{e}^{\tau L_{A}} : \begin{cases} q'_{l} &= q_{l} \cos(\alpha_{l} \tau) + p_{l} \sin(\alpha_{l} \tau), \\ p'_{l} &= p_{l} \cos(\alpha_{l} \tau) - q_{l} \sin(\alpha_{l} \tau), \\ \boldsymbol{\phi}_{l} &= e_{l} + \beta(q_{l}^{2} + p_{l}^{2})/2 \end{cases} \\ \boldsymbol{e}^{\tau L_{B}} : \begin{cases} \boldsymbol{\varphi}_{q} &= \sum_{m=1}^{N} \psi_{m} e^{2\pi i q(m-1)/N} \\ \boldsymbol{\varphi}_{q}' &= \boldsymbol{\varphi}_{q} e^{2i \cos(2\pi (q-1)/N)\tau} \\ \boldsymbol{\psi}_{l}' &= \frac{1}{N} \sum_{q=1}^{N} \boldsymbol{\varphi}_{q}' e^{-2\pi i l(q-1)/N} \end{cases} \end{split}$$

The DNLS model

Symplectic Integrators produced by Successive Splits (SS)

$$H_{D} = \sum_{l} \left(\frac{\varepsilon_{l}}{2} \left(q_{l}^{2} + p_{l}^{2} \right) + \frac{\beta}{8} \left(q_{l}^{2} + p_{l}^{2} \right)^{2} - q_{n} q_{n+1} - p_{n} p_{n+1} \right)$$

$$\begin{cases} q'_{l} = q_{l} \cos(\alpha_{l} \tau) + p_{l} \sin(\alpha_{l} \tau), & p'_{l} = q_{l}, \\ p'_{l} = p_{l} \cos(\alpha_{l} \tau) - q_{l} \sin(\alpha_{l} \tau), & p'_{l} = p_{l} + (q_{l-1} + q_{l+1})\tau \end{cases}$$

$$\begin{cases} p'_{l} = p_{l}, & p'_{l} = p_{l}, \\ p'_{l} = p_{l} - (p_{l-1} + p_{l+1})\tau \end{cases}$$

Using the SABA₂ integrator we get a 2nd order integrator with 13

steps, SS²:
$$SS^{2} = e^{\left[\frac{(3-\sqrt{3})}{6}\tau\right]L_{A}} e^{\frac{\tau}{2}L_{B}} e^{\frac{\sqrt{3}\tau}{3}L_{A}} \left[e^{\frac{\tau}{2}L_{B}}\right] e^{\left[\frac{(3-\sqrt{3})}{6}\tau\right]L_{A}}$$

$$\tau' = \tau/2 e^{\left[\frac{(3-\sqrt{3})}{6}\tau'\right]L_{B_{1}}} e^{\frac{\tau'}{2}L_{B_{2}}} e^{\frac{\sqrt{3}\tau'}{3}L_{B_{1}}} e^{\frac{\tau'}{2}L_{B_{2}}} e^{\left[\frac{(3-\sqrt{3})}{6}\tau'\right]L_{B_{1}}} e^{\frac{\tau'}{2}L_{B_{2}}} e^{\left[\frac{(3-\sqrt{3})}{6}\tau'\right]L_{B_{1}}} e^{\frac{\tau'}{2}L_{B_{2}}} e^{\frac{(3-\sqrt{3})}{6}\tau'} L_{B_{1}}$$

Non-symplectic methods for the DNLS model

In our study we also use the DOP853 integrator which is an explicit non-symplectic Runge-Kutta integration scheme of order 8.

DOP853: Hairer et al. 1993,

http://www.unige.ch/~hairer/software.html

Three part split symplectic integrators for the DNLS model

Three part split symplectic integrator of order 2, with 5 steps: ABC²

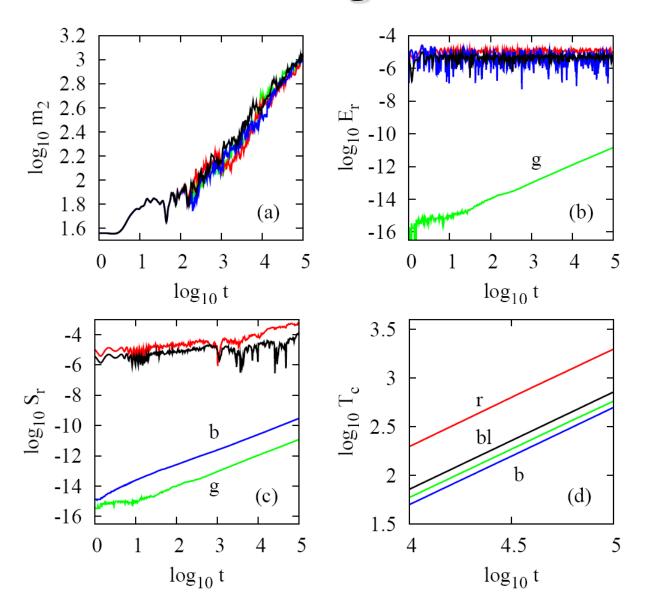
$$H_{D} = \sum_{l} \left(\frac{\varepsilon_{l}}{2} \left(q_{l}^{2} + p_{l}^{2} \right) + \frac{\beta}{8} \left(q_{l}^{2} + p_{l}^{2} \right)^{2} - q_{n} q_{n+1} p_{n} p_{n+1} \right)$$

$$A \qquad B \qquad C$$

$$ABC^{2} = e^{\frac{\tau}{2} L_{A}} e^{\frac{\tau}{2} L_{B}} e^{\tau L_{C}} e^{\frac{\tau}{2} L_{B}} e^{\frac{\tau}{2} L_{A}}$$

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

2nd order integrators: Numerical results



ABC² τ =0.005 SS² τ =0.02 DOP853 δ =10⁻¹⁶ SIFT² 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)

Composition Methods: 4th order SIs

Starting from any 2^{nd} order symplectic integrator S^{2nd} , we can construct a 4^{th} 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 SS², SIFT² and ABC² we construct the 4th order integrators:

SS⁴ with 37 steps

SIFT⁴ with 13 steps

ABC⁴_[Y] with 13 steps

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

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

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

Starting with the 2nd order integrators ABC² we construct the 4th order integrator: ABC⁴[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 4^{th} order integrators:

SIFT⁴₈₆₄ with 43 steps

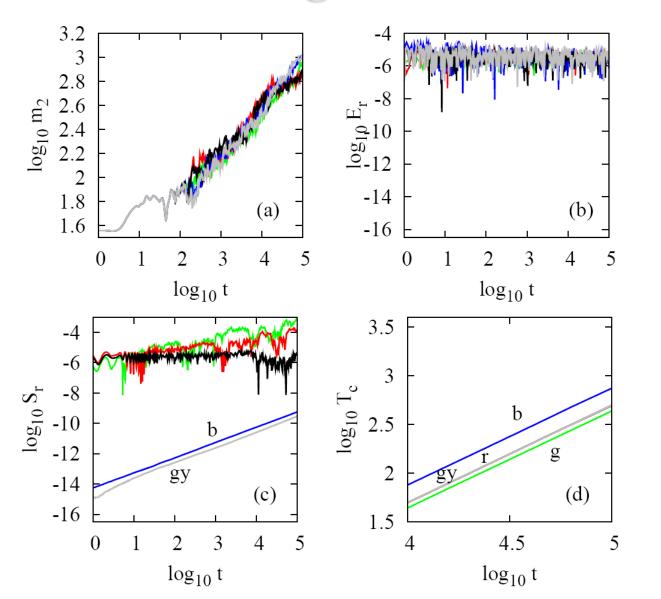
SIFT⁴₁₀₆₄ with 49 steps

Using successive splits for the B part and implementing the SABA₂ integrator for its integartion, we construct the 4^{th} order integrators:

SS⁴₈₆₄ with 49 steps

 SS^4_{1064} with 55 steps

4th order integrators: Numerical results (I)



SIFT⁴ τ =0.125 SIFT² τ =0.05 ABC⁴_[S] τ =0.1 SS⁴ τ =0.1 ABC⁴_[Y] τ =0.05

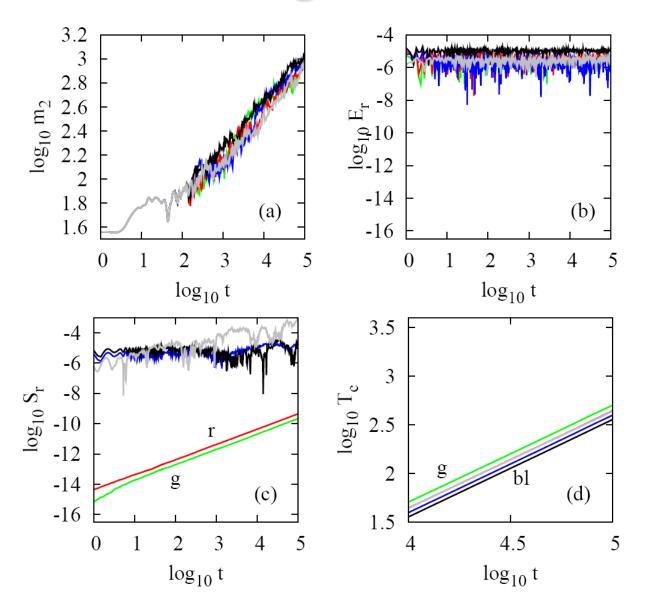
E_r: relative energy error

S_r: relative norm error

T_c: CPU time (sec)

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

4th order integrators: Numerical results (II)



SIFT⁴₁₀₆₄
$$\tau$$
=0.25
ABC⁴_[Y] τ =0.05
SIFT⁴₈₆₄ τ =0.25
SS⁴₁₀₆₄ τ =0.25
SS⁴₈₆₄ 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)

High order composition methods (I)

Using a composition technique introduced by Yoshida [Phys. Let. A (1990)] we construct the 6^{th} order symplectic integrator $ABC_{[Y]}^6$ having 29 steps:

$$\mathbf{ABC}^{6}(\tau) = \mathbf{ABC}^{2}(\mathbf{w}_{3}\tau) \times \mathbf{ABC}^{2}(\mathbf{w}_{2}\tau) \times \mathbf{ABC}^{2}(\mathbf{w}_{1}\tau) \times \mathbf{ABC}^{2}(\mathbf{w}_{1}\tau) \times \mathbf{ABC}^{2}(\mathbf{w}_{1}\tau) \times \mathbf{ABC}^{2}(\mathbf{w}_{2}\tau) \times \mathbf{ABC}^{2}(\mathbf{w}_{3}\tau)$$

whose coefficients

$$\mathbf{w}_1 = -1.17767998417887$$

$$\mathbf{w}_2 = \mathbf{0.235573213359357}$$

$$w_3 = 0.784513610477560$$

$$w_0 = 1 - 2(w_1 + w_2 + w_3)$$

cannot be given in analytic form.

High order composition methods (II)

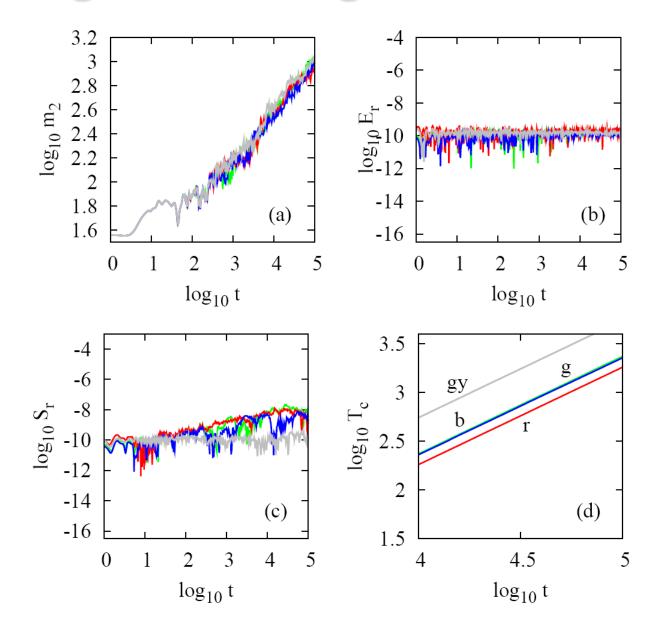
In addition, following the works of Kahan & Li, Math Comput. (1997), and Sofroniou & Spaletta, Optim. Methods Softw. (2005) we implement some efficient high order composition methods, considering as the basic block the 2nd order ABC² integrator.

ABC⁶_[KL] with 37 steps ABC⁶_[SS] with 45 steps

ABC⁸_[Y] with 61 steps ABC⁸_[KL] with 69 steps ABC⁸_[SS] with 77 steps

 $ABC^{10}_{[SS]}$ with 125 steps

High order integrators: Numerical results (I)



 $SS^4_{864} \tau = 0.015625$ $ABC^6_{[Y]} \tau = 0.03$ $ABC^6_{[KL]} \tau = 0.04$ $ABC^6_{[SS]} \tau = 0.125$

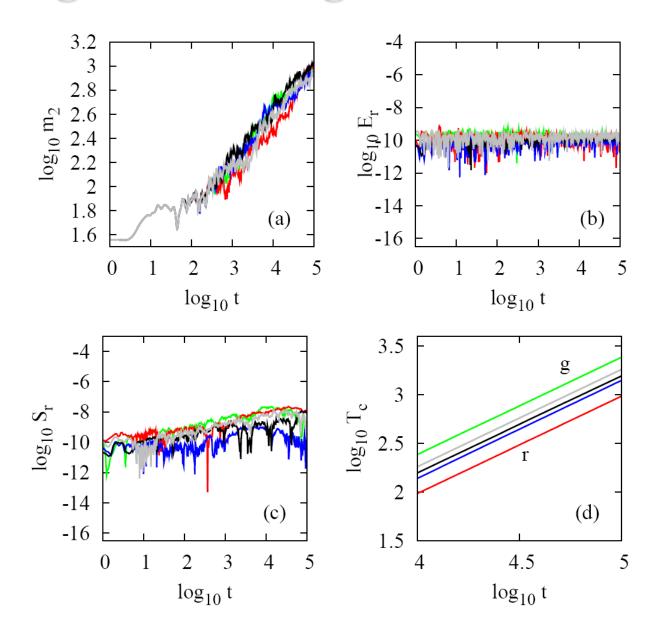
E_r: relative energy error

S_r: relative norm error

T_c: CPU time (sec)

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

High order integrators: Numerical results (II)



ABC $^{8}_{[Y]}$ τ =0.0625 ABC $^{6}_{[SS]}$ τ =0.125 ABC $^{10}_{[SS]}$ τ =0.2 ABC $^{8}_{[KL]}$ τ =0.125 ABC $^{8}_{[SS]}$ τ =0.2

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 SIFT², SIFT⁴, SIFT⁴₈₆₄ and SIFT⁴₁₀₆₄ 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