# Symplectic integration methods for multidimensional disordered nonlinear lattices

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### **Outline**

- Symplectic Integrators: Application to disordered nonlinear lattices
  - **✓** Models
    - The quartic Klein-Gordon (KG) disordered lattice
    - The disordered discrete nonlinear Schrödinger equation (DNLS)
  - **✓** Symplectic integration of KG and DNLS models
  - **✓ Numerical results: different dynamical behaviors**
- Symplectic integration of variational equations: The Tangent Map (TM) method
  - **✓ Chaos indicators** 
    - Lyapunov exponents
    - Generalized Alignment Index (GALI)
  - ✓ Chaotic behavior of the KG model
- High order three part split symplectic integrators for the DNLS model
- Outlook

### Autonomous Hamiltonian systems

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

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

# Symplectic Integration schemes

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

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

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<sub>i</sub>, d<sub>i</sub>. This is an integrator of order n.

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

# Symplectic Integrator SABA<sub>2</sub>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  $c_{1} = \frac{1}{2} \cdot \frac{\sqrt{3}}{6}$ ,  $c_{2} = \frac{\sqrt{3}}{3}$ ,  $d_{1} = \frac{1}{2}$ .

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 
$$c = \frac{2 - \sqrt{3}}{24}$$
.

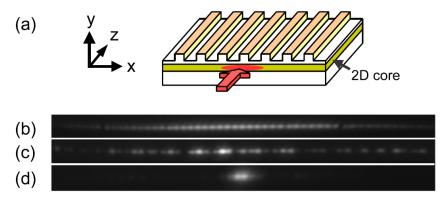
Thus the full integrator scheme becomes:  $SABAC_2 = C (SABA_2) C$  and its error is of order 4.

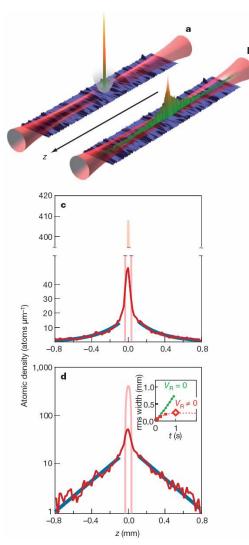
### Interplay of disorder and nonlinearity

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)] 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  $\left[\frac{1}{2}, \frac{3}{2}\right]$ .

### The discrete nonlinear Schrödinger (DNLS) equation

We also consider the system:

$$H_{D} = \sum_{l=1}^{N} \varepsilon_{l} |\psi_{l}|^{2} + \frac{\beta}{2} |\psi_{l}|^{4} - (\psi_{l+1} \psi_{l}^{*} + \psi_{l+1}^{*} \psi_{l})$$

where  $\varepsilon_l$  chosen uniformly from  $\left[-\frac{W}{2}, \frac{W}{2}\right]$  and  $\beta$  is the

nonlinear parameter.

Conserved quantities: The energy and the norm 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.

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

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

### The KG model

We apply the SABAC<sub>2</sub> 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 2<sup>nd</sup> order SABA Symplectic Integrator with 5 steps, combined with approximate solution for the B part (Fourier Transform): SIFT<sub>2</sub>

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

### The DNLS model

Symplectic Integrators produced by Successive Splits (SS)

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

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

Using the SABA<sub>2</sub> integrator we get a 2<sup>nd</sup> order integrator with 13

$$\begin{aligned} &\text{steps, SS(SABA}_2)_2 : \\ &\text{SS(SABA}_2)_2 = e^{\left[\frac{(3-\sqrt{3})}{6}\tau\right]L_A} e^{\frac{\tau}{2}L_B} e^{\frac{\sqrt{3}\tau}{3}L_A} \left(e^{\frac{\tau}{2}L_B}\right) e^{\left[\frac{(3-\sqrt{3})}{6}\tau\right]L_A} \\ &\tau' = \tau/2 \quad e^{\left[\frac{(3-\sqrt{3})}{6}\tau'\right]L_{B_1}} e^{\frac{\tau'}{2}L_{B_2}} e^{\frac{\sqrt{3}\tau'}{3}L_{B_1}} e^{\frac{\tau'}{2}L_{B_2}} e^{\left[\frac{(3-\sqrt{3})}{6}\tau'\right]L_{B_1}} e^{\left[\frac{(3-\sqrt{3})}{6}\tau'\right]L_{B_1}} e^{\frac{\tau'}{2}L_{B_2}} e^{\frac{(3-\sqrt{3})}{6}\tau'} L_{B_1} e^{\frac{\tau'}{2}L_{B_2}} e^{\frac{(3-\sqrt{3})}{6}\tau'} L_{B_2} e^{\frac{(3$$

# Different Dynamical Regimes

Three expected evolution regimes [Flach, Chem. Phys (2010) - Ch.S. & Flach, PRE (2010) - Laptyeva et al., EPL (2010) - Bodyfelt et al., PRE (2011)]

 $\Delta$ : width of the frequency spectrum, d: average spacing of interacting modes,  $\delta$ : 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)].

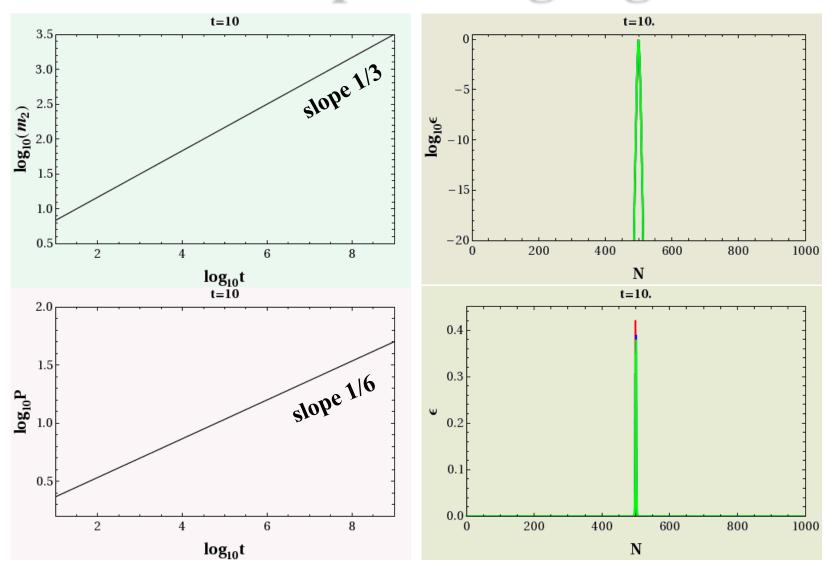
Intermediate Strong Chaos Regime:  $d<\delta<\Delta$ ,  $m_2\sim t^{1/2} \longrightarrow m_2\sim t^{1/3}$ 

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

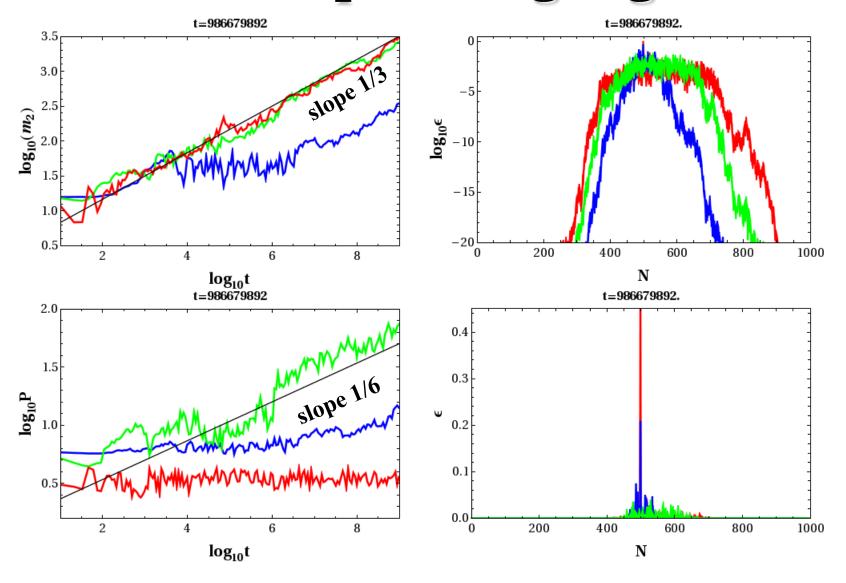
### Selftrapping Regime: $\delta > \Delta$

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)].

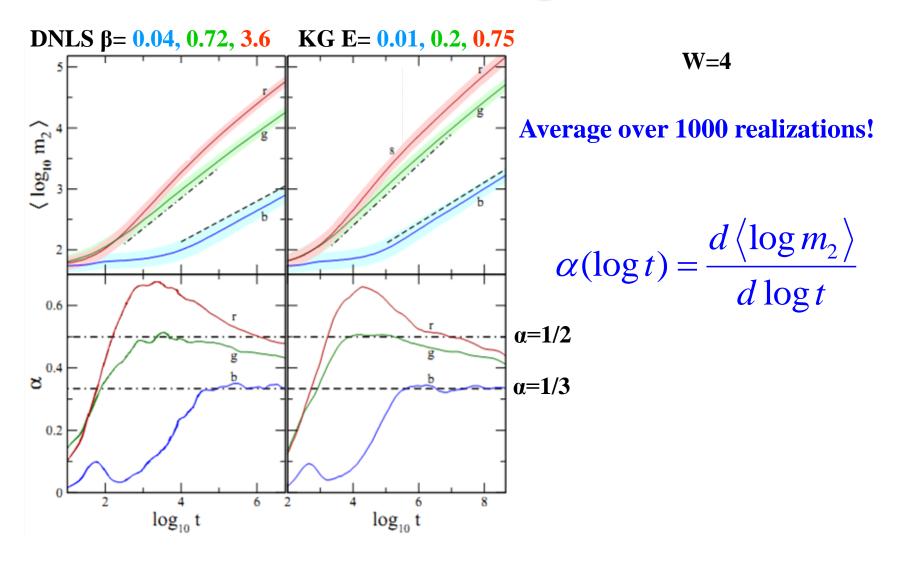
# Different spreading regimes



### Different spreading regimes



### Crossover from strong to weak chaos



# Symplectic integration of variational equations

### Autonomous Hamiltonian systems

We study 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:

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

### Chaos detection methods

The maximum Lyapunov exponent of a given orbit characterizes the mean exponential rate of divergence of trajectories surrounding this orbit.

$$\mathbf{mLCE} = \lambda_1 = \lim_{t \to \infty} \frac{1}{t} \ln \frac{\|\vec{\mathbf{w}}(t)\|}{\|\vec{\mathbf{w}}(0)\|} \qquad \begin{array}{c} \lambda_1 = 0 \to \text{Regular motion } (\infty \ t^{-1}) \\ \lambda_1 \neq 0 \to \text{Chaotic motion} \end{array}$$

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

Following the evolution of k deviation vectors with  $2 \le k \le 2N$ , we define (Ch.S. et al., 2007) the Generalized Alignment Index (GALI) of order k:

$$GALI_{k}(t) = ||\hat{\mathbf{w}}_{1}(t) \wedge \hat{\mathbf{w}}_{2}(t) \wedge ... \wedge \hat{\mathbf{w}}_{k}(t)||$$

$$\begin{array}{lll} \textbf{Chaotic motion:} & \textbf{GALI}_k(t) \propto e^{-[(\lambda_1-\lambda_2)+(\lambda_1-\lambda_3)+...+(\lambda_1-\lambda_k)]t} \\ \textbf{Regular motion on an} & \textbf{s-dimensional torus with s} \leq \textbf{N}: & \textbf{GALI}_k(t) \propto \begin{cases} \textbf{constant} & \textbf{if} & 2 \leq k \leq s \\ \frac{1}{t^{k-s}} & \textbf{if} & s < k \leq 2N-s \\ \frac{1}{t^{2(k-N)}} & \textbf{if} & 2N-s < k \leq 2N \end{cases} \\ \textbf{Solution on an solution on an solution of the solution of$$

### Tangent Map (TM) Method

Use symplectic integration schemes for the whole set of equations [Ch.S. & Gerlach, PRE (2010) - Gerlach & Ch.S., Discr. Cont. Dyn. Sys. Supp. (2011) – Gerlach et al., Int. J. Bif. Chaos (2012)]

We apply the SABAC<sub>2</sub> integrator scheme to the Hénon-Heiles system by using the splitting:

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

with a corrector term which corresponds to the Hamiltonian function:

$$C = \{\{A, B\}, B\} = (x + 2xy)^2 + (x^2 - y^2 + y)^2$$

We approximate the dynamics by the act of Hamiltonians A, B and C, which correspond to the symplectic maps:

$$e^{\tau L_{A}} : \begin{cases} x' = x + p_{x}\tau \\ y' = y + p_{y}\tau \\ p'_{x} = p_{x} \\ p'_{y} = p_{y} \end{cases}, \\ e^{\tau L_{B}} : \begin{cases} x' = x \\ p'_{x} = y \\ y' = y \\ p'_{x} = p_{x} - x(1 + 2y)\tau \\ p'_{y} = p_{y} + (y^{2} - x^{2} - y)\tau \end{cases}, e^{\tau L_{C}} : \begin{cases} x' = x \\ y' = y \\ p'_{x} = p_{x} - 2x(1 + 2x^{2} + 6y + 2y^{2})\tau \\ p'_{y} = p_{y} - 2(y - 3y^{2} + 2y^{3} + 3x^{2} + 2x^{2}y)\tau \end{cases}.$$

### Tangent Map (TM) Method

symplectic integration scheme used for solving the Hamilton equations of motion, which involves the act of Hamiltonians A, B and C, can be extended in order to integrate simultaneously the variational equations.

equations.
$$e^{\tau L_{A}} : \begin{cases} x' = x + p_{x}\tau \\ y' = y + p_{y}\tau \\ y' = y + p_{y}\tau \\ y' = p_{x} \\ p'_{y} = p_{y} \end{cases} : \begin{cases} x' = x + p_{x}\tau \\ y' = y + p_{y}\tau \\ px' = p_{x} \\ \delta x' = \delta x + \delta p_{x}\tau \\ \delta y' = \delta y + \delta p_{y}\tau \\ \delta p'_{y} = \delta p_{y} \end{cases} : \begin{cases} x' = x \\ y' = y \\ p'_{x} = p_{x} - x(1 + 2y)\tau \\ \delta x' = \delta x \\ \delta y' = \delta y \end{cases} : \begin{cases} x' = x \\ y' = y \\ p'_{x} = p_{x} - x(1 + 2y)\tau \\ \delta x' = \delta x \\ \delta y' = \delta y \\ \delta p'_{x} = \delta p_{x} - [(1 + 2y)\delta x + 2x\delta y]\tau \\ \delta p'_{y} = p_{y} + (y^{2} - x^{2} - y)\tau \end{cases}$$

$$e^{\tau L_C} : \begin{cases} x' = x \\ y' = y \\ p'_x = p_x - 2x(1 + 2x^2 + 6y + 2y^2)\tau \\ p'_y = p_y - 2(y - 3y^2 + 2y^3 + 3x^2 + 2x^2y)\tau \end{cases} \qquad e^{\tau L_{CV}} : \begin{cases} x' = x \\ y' = y \\ p'_x = p_x - 2x(1 + 2x^2 + 6y + 2y^2)\tau \\ \delta x' = \delta x \\ \delta y' = \delta y \\ \delta p'_x = \delta p_x - 2\left[(1 + 6x^2 + 2y^2 + 6y)\delta x + +2x(3 + 2y)\delta y\right]\tau \\ \delta p'_y = \delta p_y - 2\left[2x(3 + 2y)\delta y\right]\tau \\ \delta p'_y = \delta p_y - 2\left[2x(3 + 2y)\delta x + +(1 + 2x^2 + 6y^2 - 6y)\delta y\right]\tau \end{cases}$$

$$\begin{cases} x' &= x \\ y' &= y \\ p'_x &= p_x - 2x(1 + 2x^2 + 6y + 2y^2)\tau \\ p'_y &= p_y - 2(y - 3y^2 + 2y^3 + 3x^2 + 2x^2y)\tau \\ \delta x' &= \delta x \\ \delta y' &= \delta y \\ \delta p'_x &= \delta p_x - 2\left[ (1 + 6x^2 + 2y^2 + 6y)\delta x + +2x(3 + 2y)\delta y \right]\tau \\ \delta p'_y &= \delta p_y - 2\left[ 2x(3 + 2y)\delta x + +(1 + 2x^2 + 6y^2 - 6y)\delta y \right]\tau \end{cases}$$

# Chaotic behavior of the KG model

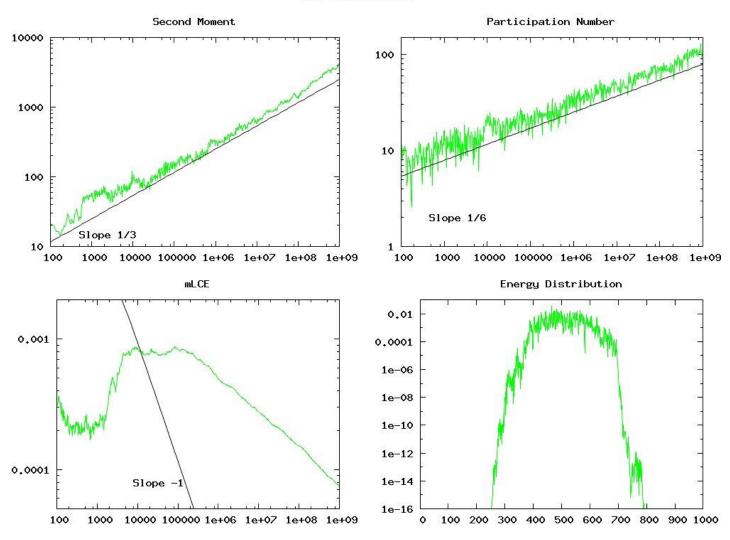
Ch.S., I. Gkolias & S. Flach, 2012 (in preparation)

# KG: Weak Chaos (E=0.4)

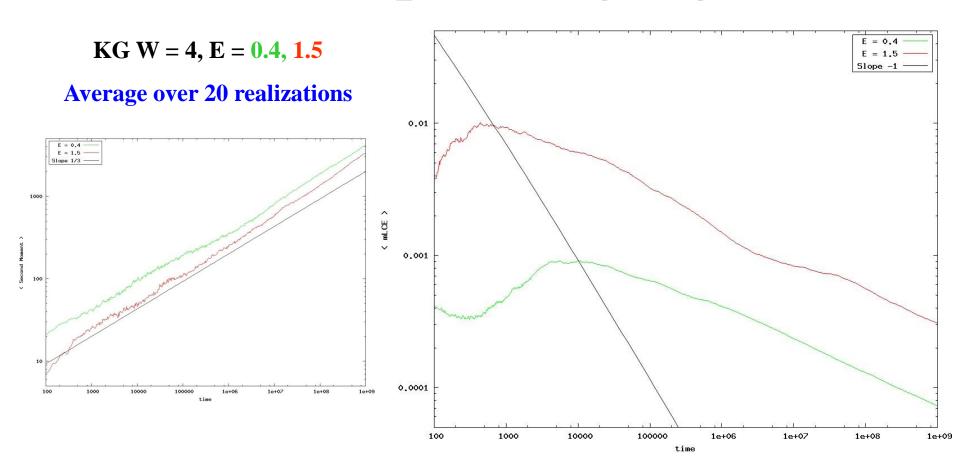


### KG: Weak Chaos (E=0.4)

t = 1000000000.00



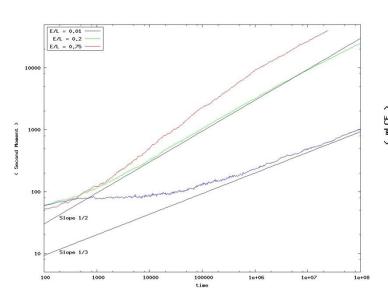
# Single site excitations: Different spreading regimes

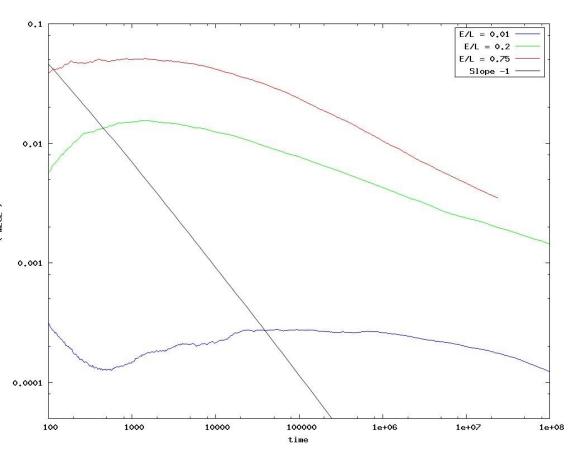


# Block excitations: Different spreading regimes

W = 4, E/L = 0.01, 0.2, 0.75

**Average over 20 realizations** 





# High order three part split symplectic integrators for the DNLS model

Ch.S., E. Gerlach, J. Bodyfelt, G. Papamikos & S. Eggl, 2012 (in preparation)

# Three part split symplectic integrators for the DNLS model

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

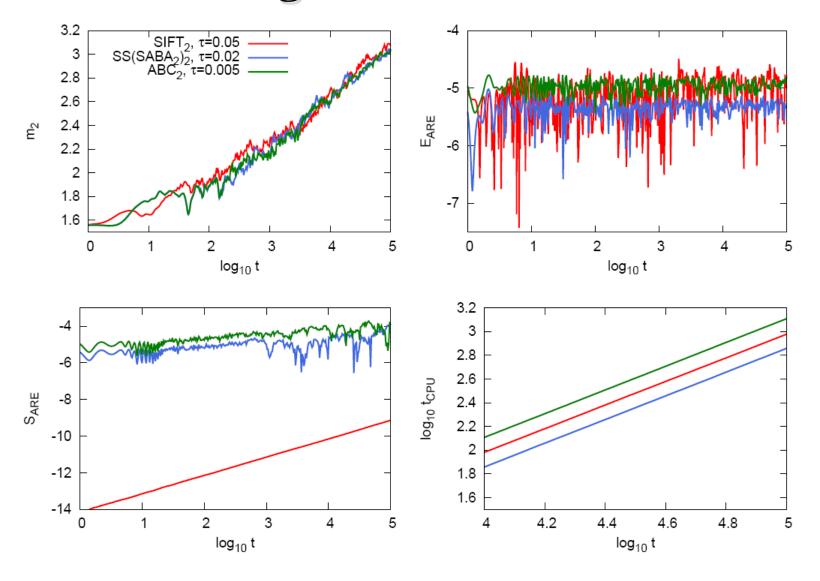
$$H_{D} = \sum_{l} \left( \frac{\varepsilon_{l}}{2} \left( q_{l}^{2} + p_{l}^{2} \right) + \frac{\beta}{8} \left( q_{l}^{2} + p_{l}^{2} \right)^{2} - q_{n} q_{n+1} p_{n} p_{n+1} \right)$$

$$A \qquad B \qquad C$$

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

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

### 2<sup>nd</sup> order integrators: Numerical results



### 4<sup>th</sup> order symplectic integrators

Starting from any  $2^{nd}$  order symplectic integrator  $S_{2nd}$ , we can construct a  $4^{th}$  order integrator  $S_{4th}$  using a composition method [Yoshida, Phys. Let. A (1990)]:

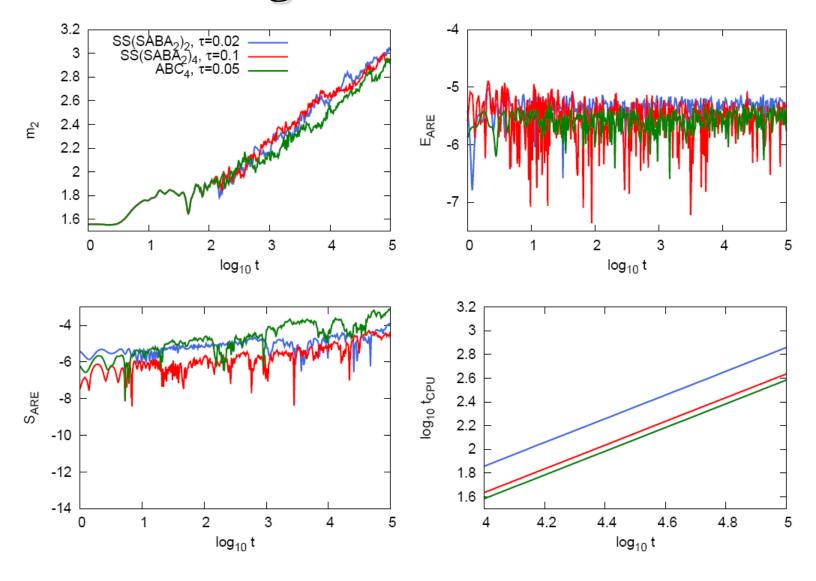
$$S_{4th}(\tau) = S_{2nd}(x_1\tau) \times S_{2nd}(x_0\tau) \times S_{2nd}(x_1\tau)$$

$$x_0 = -\frac{2^{1/3}}{2 - 2^{1/3}}, \qquad x_1 = \frac{1}{2 - 2^{1/3}}$$

Starting with the  $2^{nd}$  order integrators  $SS(SABA_2)_2$  and  $ABC_2$  we construct the  $4^{th}$  order integrators:

•SS(SABA<sub>2</sub>)<sub>4</sub> with 37 steps •ABC<sub>4</sub> with 13 steps

### 4<sup>th</sup> order integrators: Numerical results



### **Outlook**

#### Disordered nonlinear lattices:

- ✓ Quantify the chaotic behavior of energy spreading: Find theoretical or empirical laws for the evolution of Lyapunov exponents.
- ✓ Use covariant Lyapunov vectors and frequency map analysis in order to study the chaotic nature of energy spreading: Do 'chaotic hot spots' exist?
- **✓** Determine the limiting states of wave packets.
- **✓** Identification of the selftrapped and spreading parts of wave packets.
- ✓ Extension to higher spatial dimensions, and interactions beyond nearest neighbors.

### Three part split symplectic integrators

- **✓** Computation of chaos indicators for the DNLS model.
- **✓** Different techniques for constructing high order integrators.
- **✓** Investigate the possible use of corrector terms.
- ✓ Applications to other dynamical systems (e.g. models studied at UCT).

### Chaos detection techniques

- **✓** Behavior of GALI<sub>k</sub> indices for time dependent Hamiltonians, dissipative systems, and time series.
- **✓** Computation of the spectrum of LCEs using the compound matrix theory.
- **✓** Review paper: Comparative study of the various existing methods.

### Main references

#### Disordered systems

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- ✓ Ch.S., D.O. Krimer, S. Komineas, S. Flach (2009) PRE, 79, 056211
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#### TM method

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### • Three part split symplectic integrators

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### **Summary**

- Multidimensional disordered nonlinear lattices :
  - ✓ The use of symplectic schemes allow us to follow their evolution for very long time intervals.
  - We predicted theoretically and verified numerically the existence of different dynamical behaviors: a) Weak Chaos Regime:  $\delta < d$ ,  $m_2 \sim t^{1/3}$ , b) Intermediate Strong Chaos Regime:  $d < \delta < \Delta$ ,  $m_2 \sim t^{1/2} \longrightarrow m_2 \sim t^{1/3}$ , c) Selftrapping Regime:  $\delta > \Delta$
  - ✓ Generality of results: a) Two different models: KG and DNLS, b) Predictions made for DNLS are verified for both models.
- Numerical schemes based on symplectic integrators can be used for the efficient integration of the variational equations of multidimensional Hamiltonian systems.
  - ✓ Our results suggest that Anderson localization is eventually destroyed by the slightest amount of nonlinearity, since spreading does not show any sign of slowing down.
  - ✓ Energy spreading is a chaotic phenomenon, as Lyapunov exponent estimators decrease following an evolution different than in the case of regular motion.
- Three part split symplectic integrators
  - ✓ Proved to be efficient integration methods suitable for the integration of the DNLS model.
  - ✓ The 4<sup>th</sup> order integrator allows integration of the DNLS model for very long times.
  - ✓ A systematic way of constructing high order three part split symplectic integrators was introduced.