Symplectic integration methods for multidimensional Hamiltonian systems: Application to the disordered discrete nonlinear Schrödinger (DNLS) equation

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Outline

- **Symplectic Integrators**
- **Disordered lattices**
    - ✓ **The quartic Klein-Gordon (KG) disordered lattice**
    - ✓ **The disordered discrete nonlinear Schrödinger equation (DNLS)**
- **Different integration schemes for DNLS**
- **Conclusions**

Autonomous Hamiltonian systems

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

$$H(\overbrace{q_1,q_2,\ldots,q_N}^{\text{positions}},\ \overbrace{p_1,p_2,\ldots,p_N}^{\text{momenta}})$$

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

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

is governed by the Hamilton's equations of motion

$$\frac{dp_i}{dt} = -\frac{\partial H}{\partial q_i}\ ,\qquad \frac{dq_i}{dt} = \frac{\partial H}{\partial p_i}$$

Symplectic Integration schemes

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_2C

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:

$$C = e^{-\tau^3 \frac{c}{2} L_{\{\{A,B\},B\}}}$$

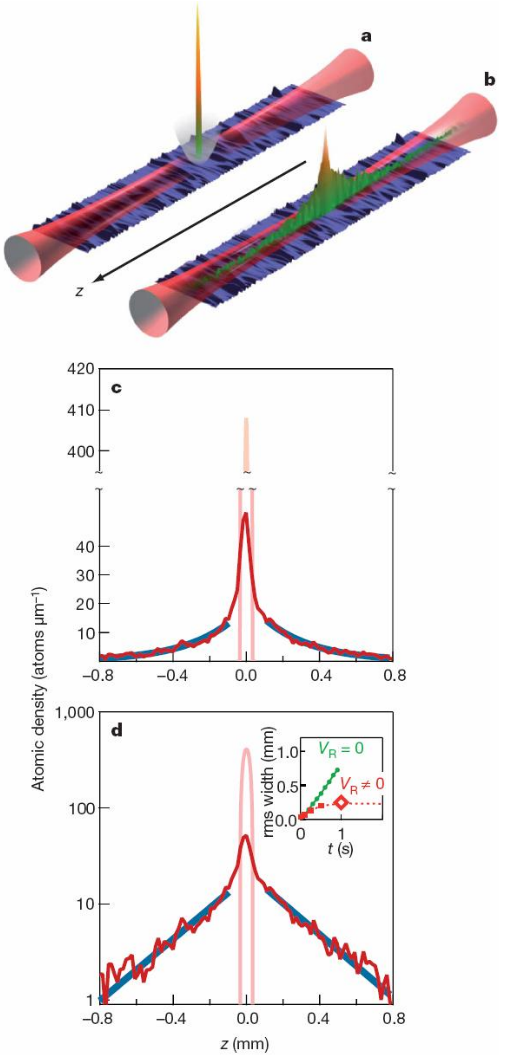
with $c = \frac{2 - \sqrt{3}}{24}.$

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

Interplay of disorder and nonlinearity

Waves in disordered media – Anderson localization

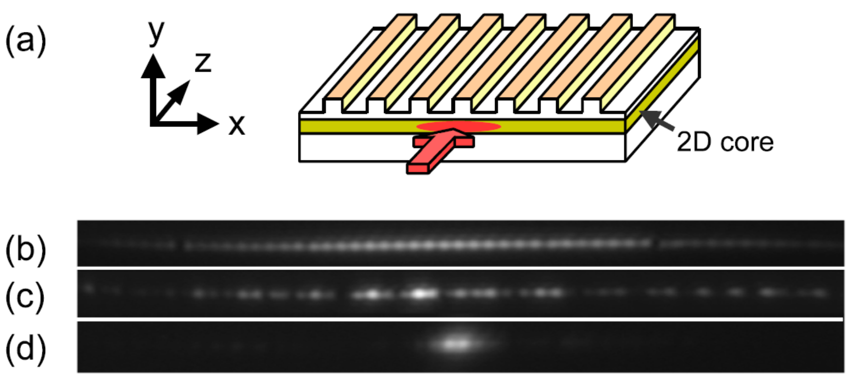
[Anderson, Phys. Rev. (1958)]. Experiments on BEC [Billy et al., Nature (2008)]



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

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

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

The discrete nonlinear Schrödinger (DNLS) equation

We also consider the system:

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

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 $S = \sum_l \left|\psi_l\right|^2$ **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.

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 $P=N$.

The KG model

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

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

A

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:

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

The DNLS model

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

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

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

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

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

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

The DNLS model

Symplectic Integrators produced by Successive Splits (SS)

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

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

B_1:
$$\begin{cases} q_l' = q_l, \\ p_l' = p_l + (q_{l-1} + q_{l+1})\tau \end{cases}$$

B_2:
$$\begin{cases} p_l' = p_l, \\ q_l' = q_l - (p_{l-1} + p_{l+1})\tau \end{cases}$$

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

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

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

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

Different Dynamical Regimes

Three expected evolution regimes [Flach, Chem. Phys (2010) - Ch.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)].

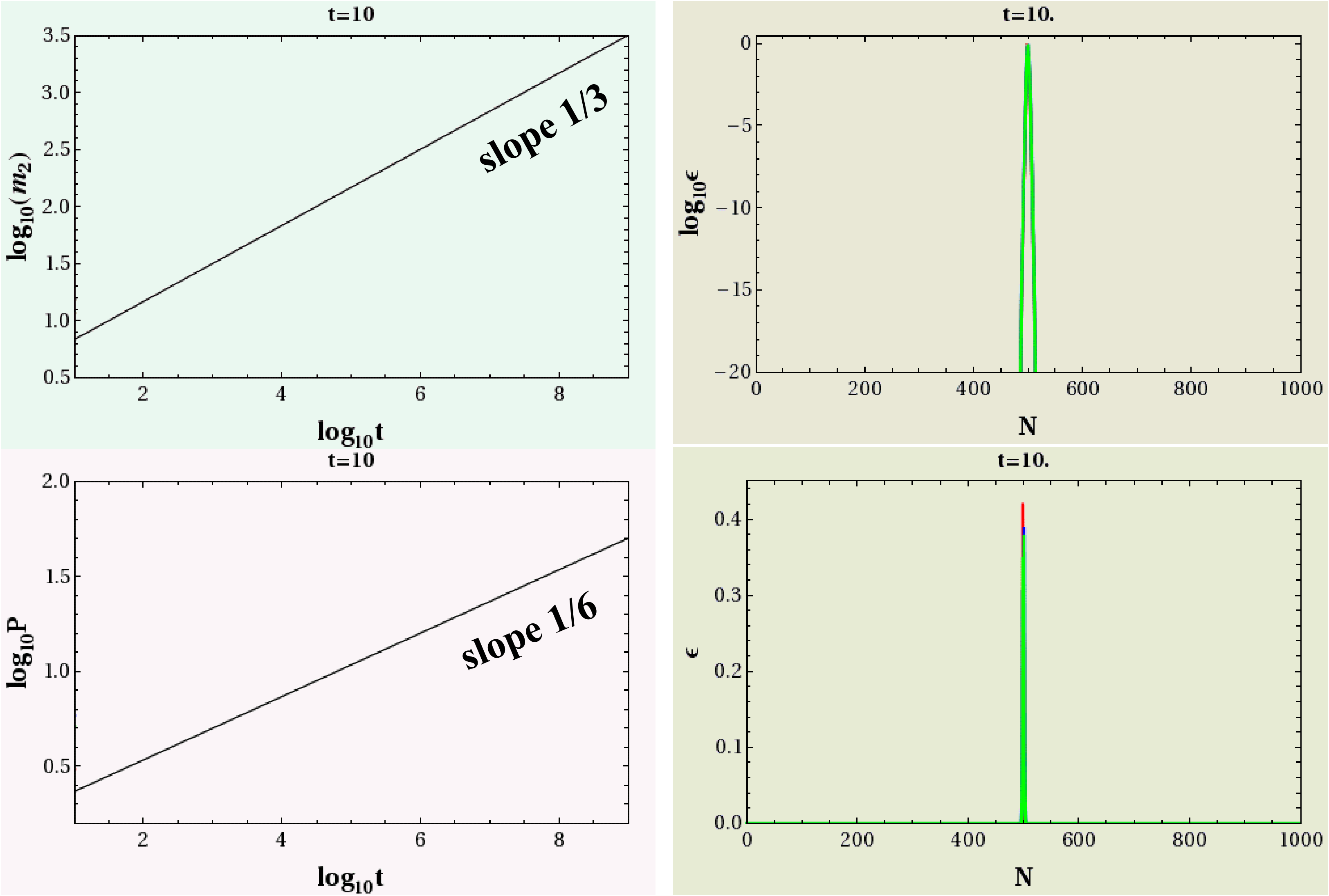
Intermediate Strong Chaos Regime: $d<\delta<\Delta$, $m_2 \sim t^{1/2} \longrightarrow m_2 \sim t^{1/3}$

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

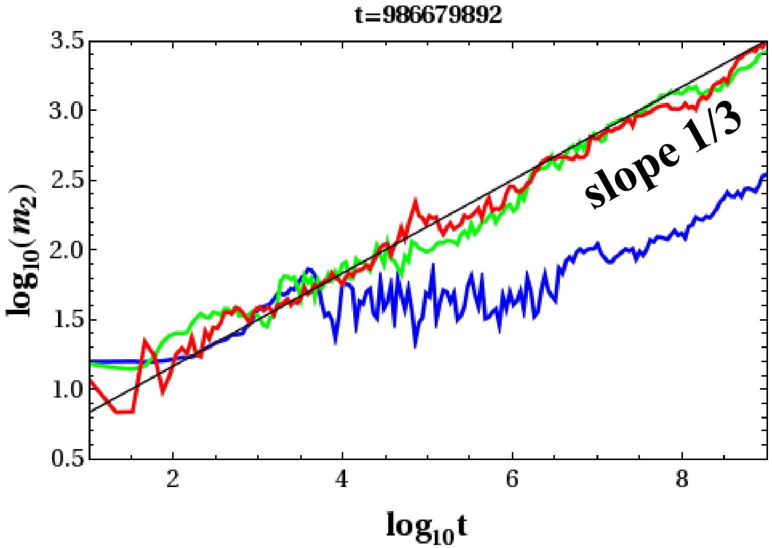
Selftrapping Regime: $\delta>\Delta$

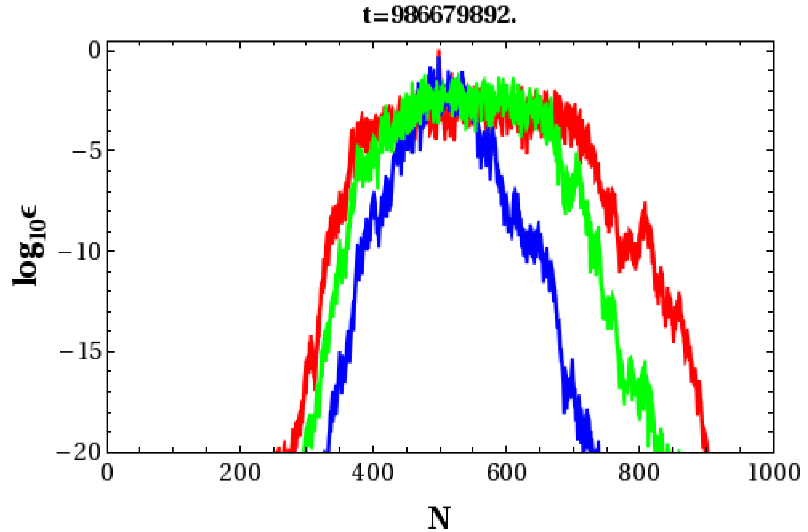
Frequency shift exceeds the spectrum width. Frequencies of excited NMs are tuned out of resonances with the nonexcited ones, leading to selftrapping, while a small part of the wave packet subdiffuses [Kopidakis et al., PRL (2008)].

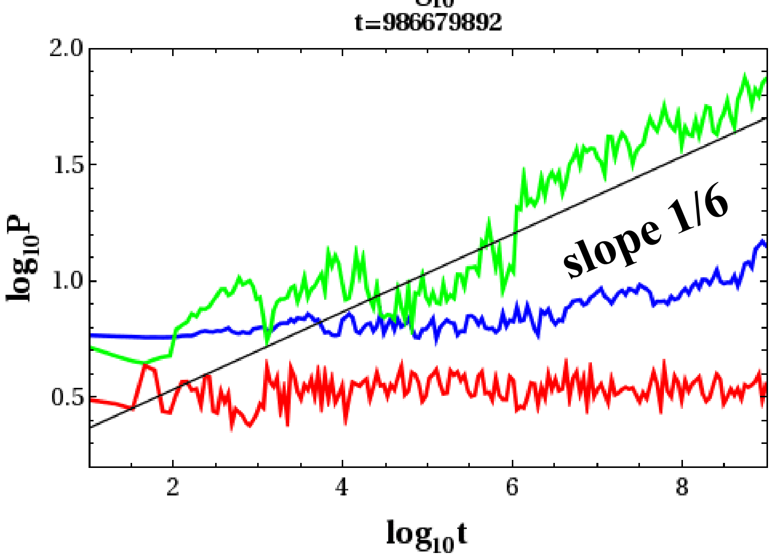
Different spreading regimes

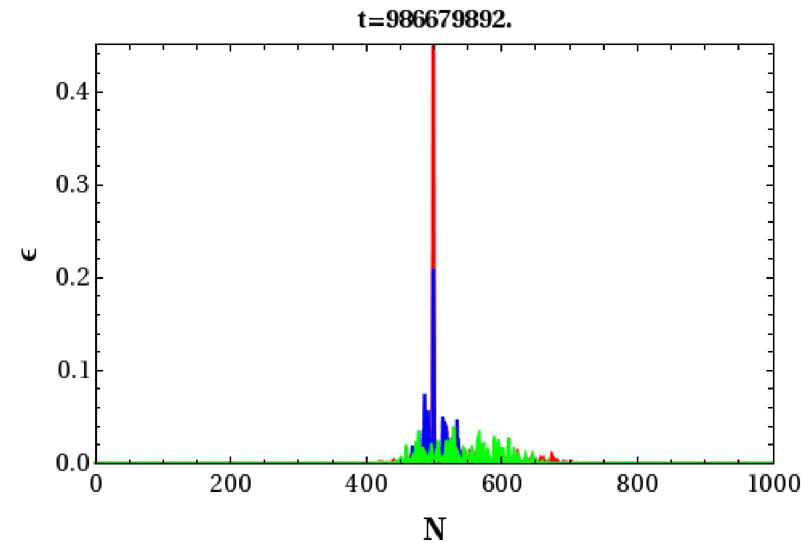


Different spreading regimes



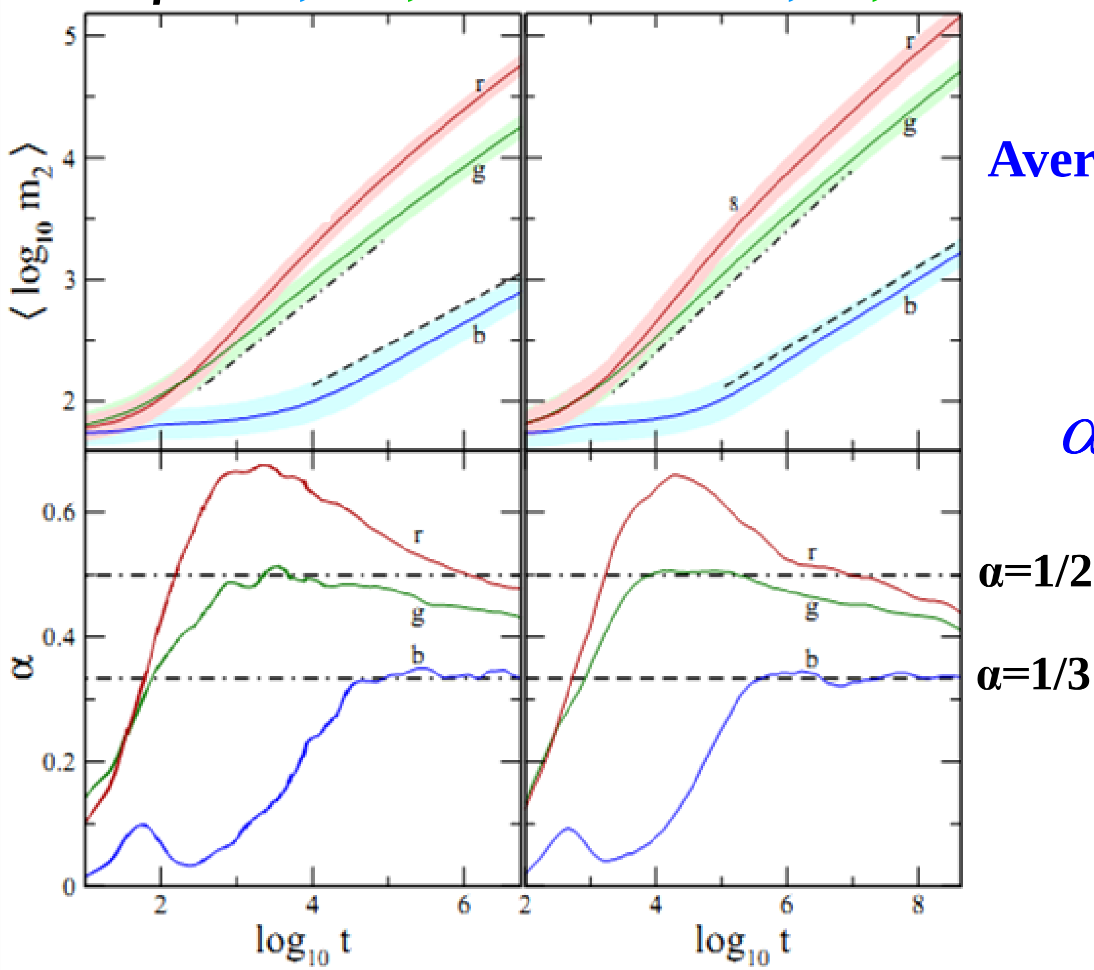






Crossover from strong to weak chaos

DNLS β= 0.04, 0.72, 3.6 KG E= 0.01, 0.2, 0.75



W=4

Average over 1000 realizations!

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

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

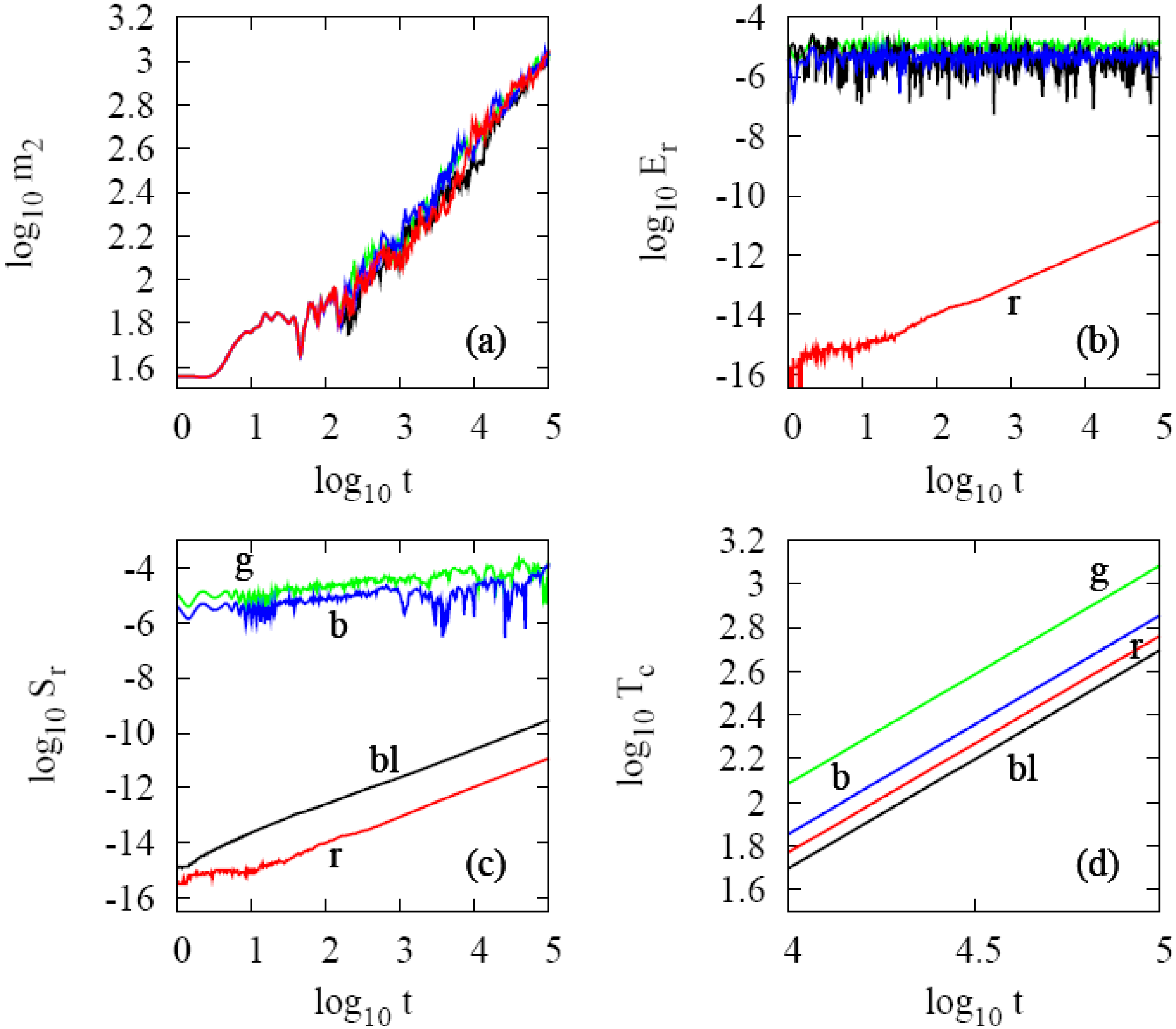
Three part split symplectic integrator of order 2, with 5 steps: ABC^2

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

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

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

2^{nd} order integrators: Numerical results



ABC^2 τ=0.005

SS^2 τ=0.02

$SIFT^2$ τ=0.05

DOP853 $\delta=10^{-16}$

E_r: relative energy error

S_r: relative norm error

4^{th} 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^2 and ABC^2 we construct the 4^{th} order integrators:

- **SS^4 with 37 steps**
- **ABC^4 with 13 steps**

6^{th} order symplectic integrators

As a higher order integrator, we use the 6^{th} order symplectic integrator ABC^6 having 29 steps [Yoshida, Phys. Let. A (1990)]:

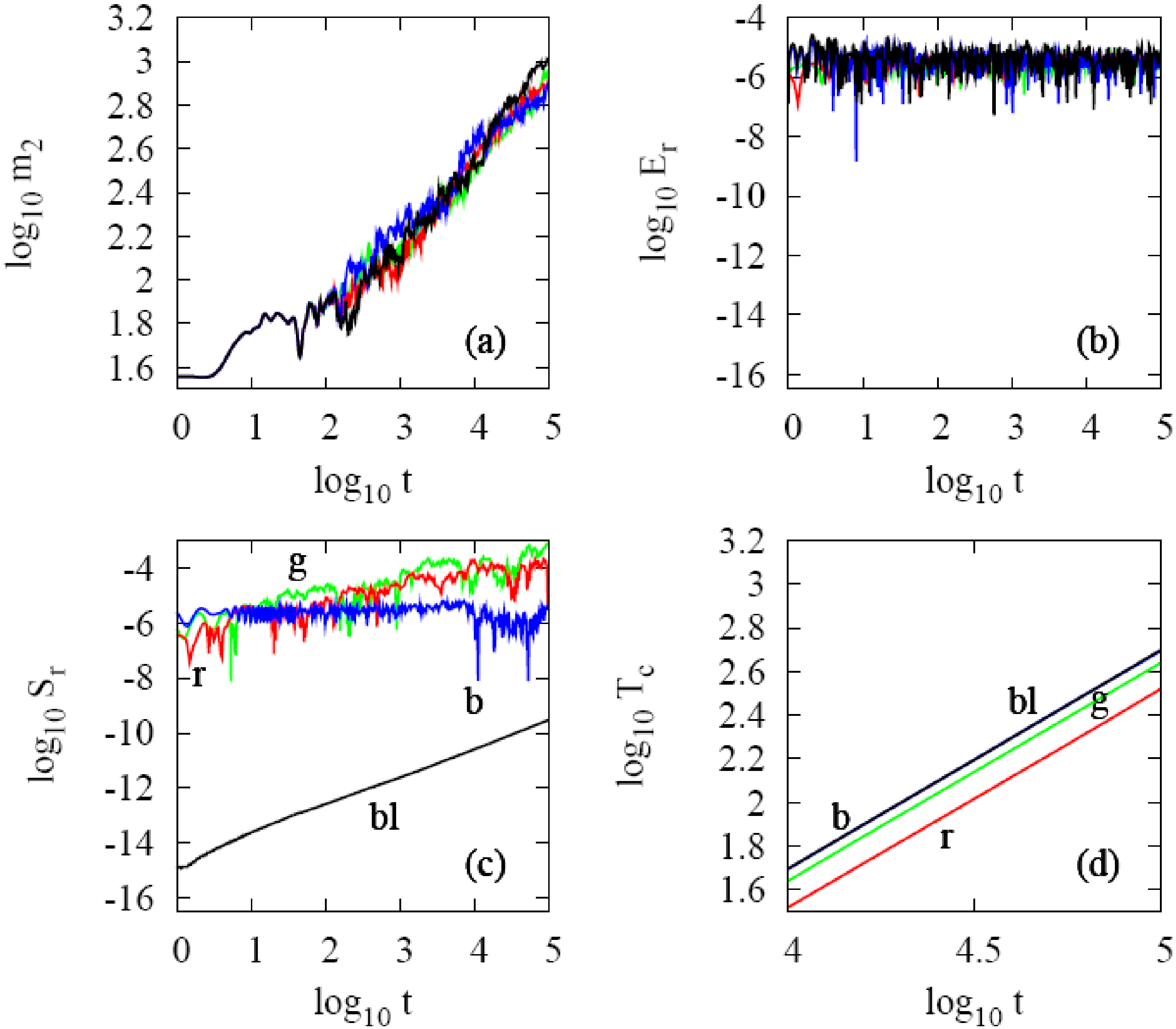
$$ABC^6(\tau) = ABC^2(w_3\tau) \times ABC^2(w_2\tau) \times ABC^2(w_1\tau) \times$$
$$\times ABC^2(w_0\tau) \times ABC^2(w_1\tau) \times ABC^2(w_2\tau) \times ABC^2(w_3\tau)$$

whose coefficients

$$w_1 = -1.17767998417887$$
$$w_2 = 0.235573213359357$$
$$w_3 = 0.784513610477560$$
$$w_0 = 1 - 2(w_1 + w_2 + w_3)$$

cannot be given in analytic form.

High order integrators: Numerical results



SIFT^2 τ=0.05

SS^4 τ=0.1

ABC^4 τ=0.05

ABC^6 τ=0.15

E_r: relative energy error

S_r: relative norm error

Summary

- **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).**
- **A systematic way of constructing high order ABC integrators was presented.**
- **The 4^{th} and 6^{th} order integrators proved to be quite efficient, allowing integration of the DNLS for very long times.**
- **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.**