Symplectic longtime integration of the disordered discrete nonlinear Schrödinger equation

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Outline

- **Symplectic Integrators – Tangent Map Method**
- **Disordered lattices and their dynamical behavior**
- **Different 2-part and 3-part spilt symplectic integrators for the disordered discrete nonlinear Schrödinger equation (DNLS)**
- **Summary**

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.

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

Symplectic Integrator $\mathrm{SABA_2C}$

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.

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 [Ch.S. & Gerlach, PRE (2010) – Gerlach & Ch.S., Discr. Cont. Dyn. Sys. (2011) – Gerlach et al., IJBC (2012)].

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

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

$$\xrightarrow{A(\vec{p})}$$

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

$$B(\vec{q})$$

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

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

<u>Linear case</u> (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:

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

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

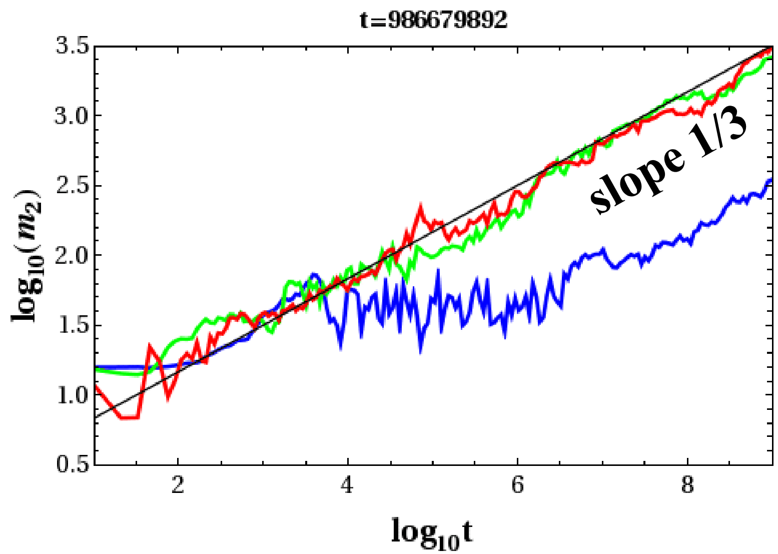
We consider normalized energy distributions in normal mode (NM) space

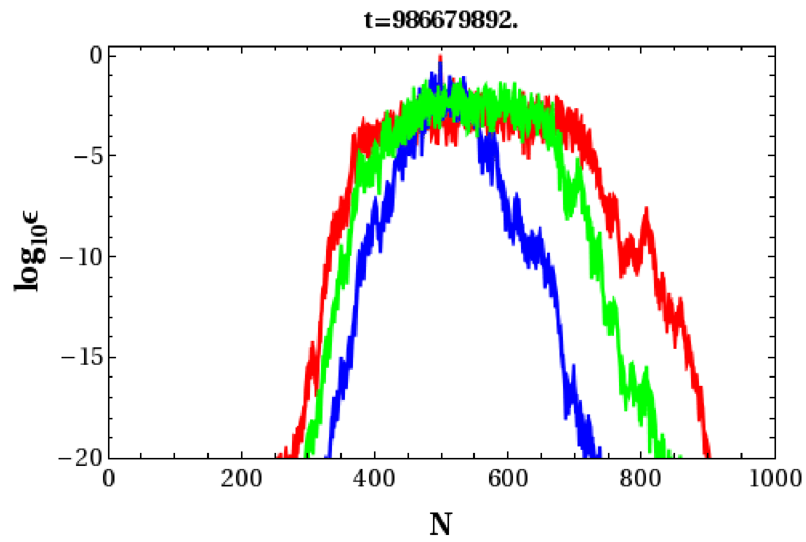
$$z_\nu \equiv \frac{E_\nu}{\sum_m E_m} \quad \text{with} \quad E_\nu = \frac{1}{2}\left(\dot{A}_\nu^2 + \omega_\nu^2 A_\nu^2\right)$$

, where A_ν is the amplitude of the νth NM.

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

Different spreading regimes

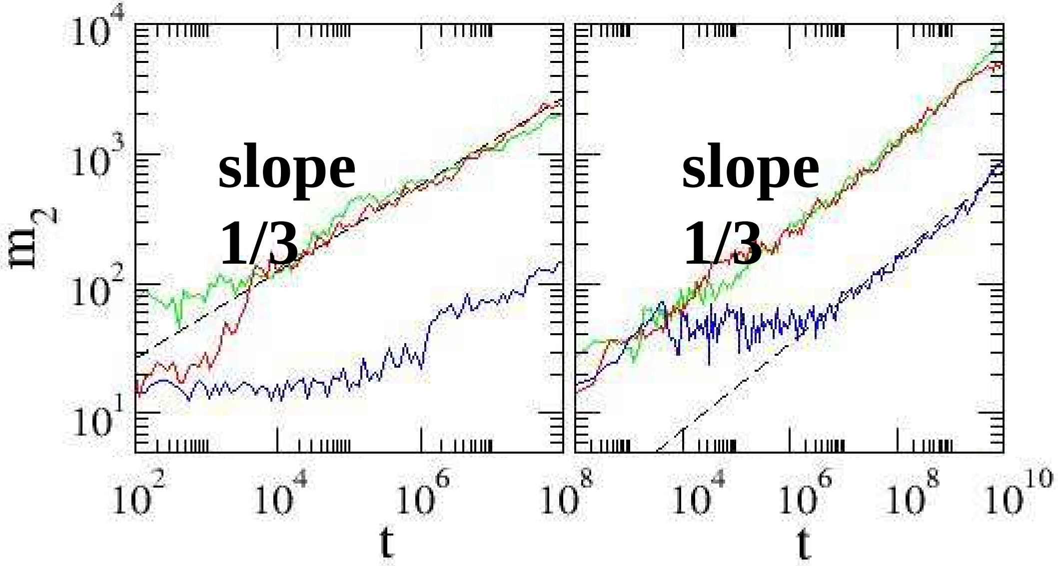




Different spreading regimes

Single site excitations α=1/3

DNLS W=4, β= 0.1, 1, 4.5 KG W = 4, E = 0.05, 0.4, 1.5



Characteristics of wave packet spreading:

$$m_2 \sim t^{\alpha}$$

with α=1/3 or α=1/2, for particular chaotic regimes.

Flach, Krimer, Ch.S., PRL (2009)

Ch.S., Krimer, Komineas, Flach, PRE (2009)

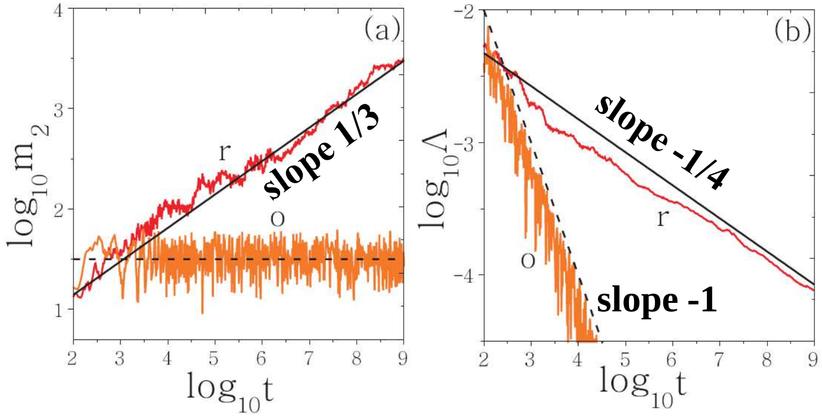
Ch.S., Flach, PRE (2010)

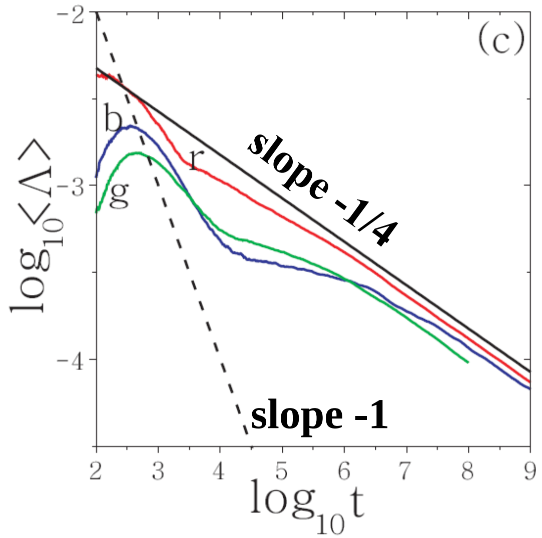
Laptyeva, Bodyfelt, Krimer, Ch.S., Flach , EPL (2010)

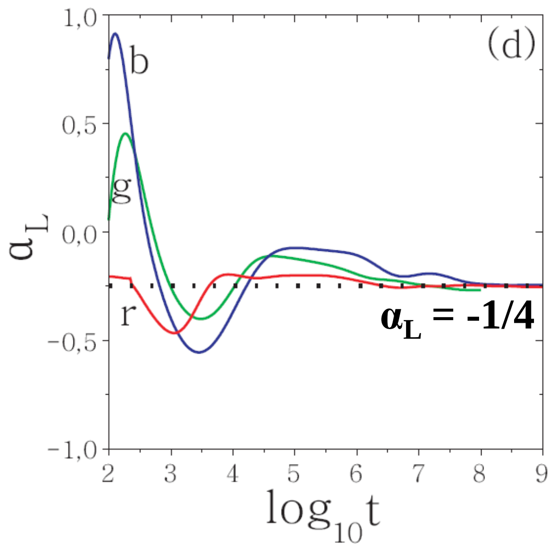
Bodyfelt, Laptyeva, Ch.S., Krimer, Flach S., PRE (2011)

KG: Lyapunov Exponents

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.Ch. et al. PRL (2013)

The KG model

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

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

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

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

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

How can we use Symplectic Integrators for the DNLS model?

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

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

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

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

$$e^{\tau L_B} : (\mathbf{q}', \mathbf{p}')^{\mathrm{T}} = \mathbf{C}(\tau) \cdot (\mathbf{q}, \mathbf{p})^{\mathrm{T}}$$

Evaluation of the C(τ) matrix

The equations of motion for the Hamiltonian B can be written as:

$$\dot{\mathbf{x}}^{\mathrm{T}} = \begin{pmatrix} \mathbf{0} & \mathbf{A} \\ -\mathbf{A} & \mathbf{0} \end{pmatrix} \mathbf{x}^{\mathrm{T}}$$

with

$$\mathbf{A} = \begin{pmatrix} 0 & -1 & 0 & \cdots & 0 & 0 \\ -1 & 0 & -1 & \cdots & 0 & 0 \\ 0 & -1 & 0 & \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & 0 & -1 \\ 0 & 0 & 0 & \cdots & -1 & 0 \end{pmatrix}$$

Then the matrix C(τ) is given by

$$\mathbf{C}(\tau) = \begin{pmatrix} \cos(\mathbf{A}\tau) & \sin(\mathbf{A}\tau) \\ -\sin(\mathbf{A}\tau) & \cos(\mathbf{A}\tau) \end{pmatrix}$$

$$\cos(\mathbf{A}\tau) = \sum_{k=0}^{\infty} \frac{(-1)^k}{(2k)!} \mathbf{A}^{2k} \tau^{2k}, \quad \sin(\mathbf{A}\tau) = \sum_{k=0}^{\infty} \frac{(-1)^k}{(2k+1)!} \mathbf{A}^{2k+1} \tau^{2k+1}.$$

The evaluation of the elements of matrices cos(Aτ) and sin(Aτ) can be obtained through the determination of the eigenvalues and eigenvectors of matrix A itself **(Gerlach, Meichsner, Ch.S., 2016, Eur. Phys. J. Sp. Top).**

DNLS model: 2 part split SIs

Order 2: **Leap-frog (3 steps)** $LF(\tau) = e^{\frac{\tau}{2}L_{\mathcal{A}}} e^{\tau L_{\mathcal{B}}} e^{\frac{\tau}{2}L_{\mathcal{A}}}$

SABA_2 (5 steps)

Order 4: **Yoshida, 1990, Phys. Lett. A (7 steps)**

$$S^4(\tau) = e^{c_1\tau L_{\mathcal{A}}} e^{d_1\tau L_{\mathcal{B}}} e^{c_2\tau L_{\mathcal{A}}} e^{d_2\tau L_{\mathcal{B}}} e^{c_2\tau L_{\mathcal{A}}} e^{d_1\tau L_{\mathcal{B}}} e^{c_1\tau L_{\mathcal{A}}},$$

$$\text{with } c_1 = \frac{1}{2(2-2^{1/3})},\ c_2 = \frac{1-2^{1/3}}{2(2-2^{1/3})},\ d_1 = \frac{1}{2-2^{1/3}},\ d_2 = -\frac{2^{1/3}}{2-2^{1/3}}.$$

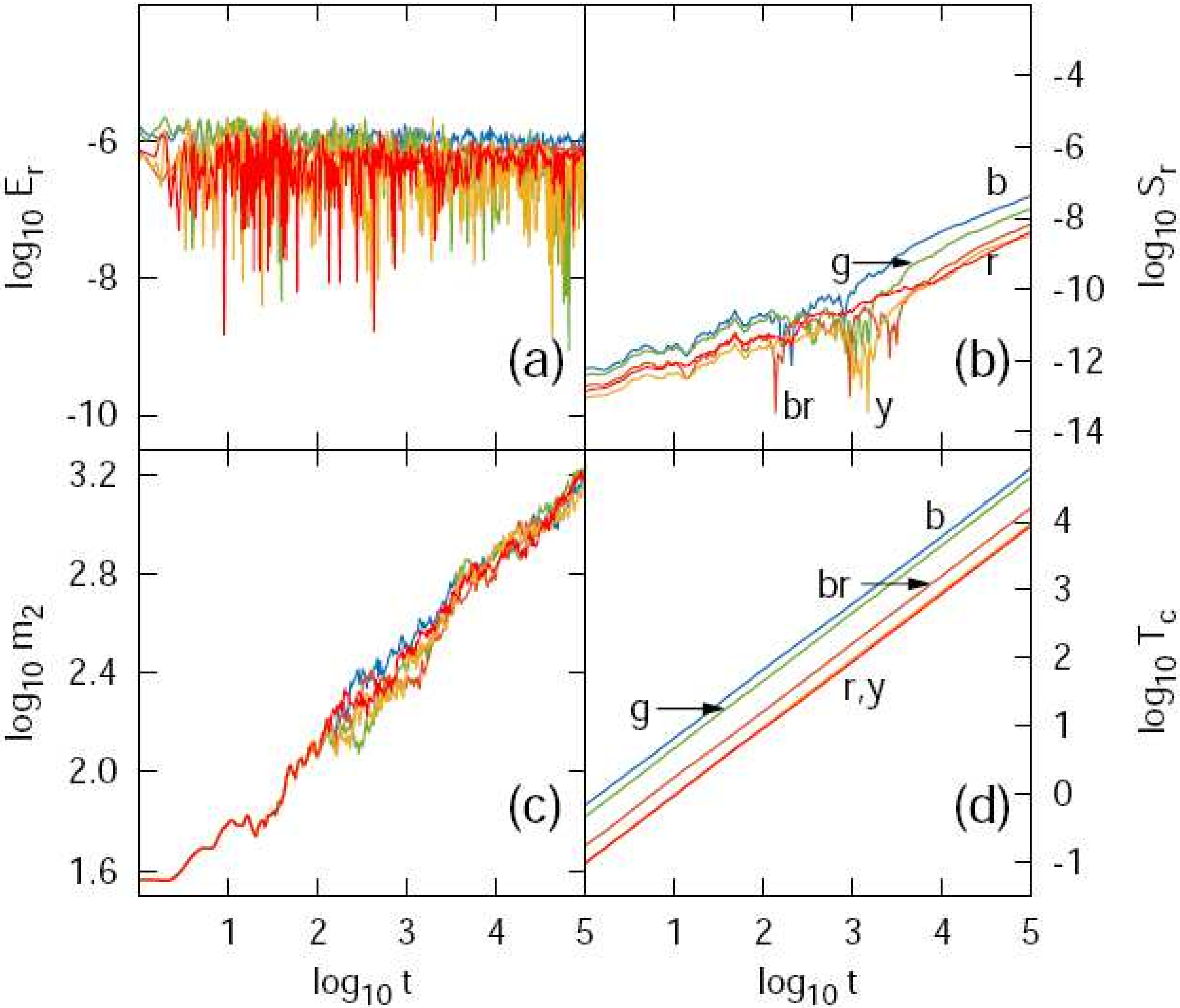
ABA864 [Blanes et al., 2013, App. Num. Math.] (15 steps)

Order 6: **Using the composition method refereed as 'solution A' in [Yoshida, 1990, Phys. Lett. A] we construct the 6th order symplectic integrator S^6 having 29 steps**

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

where S^2 is the SABA_2 integrator, while the values of w_0, w_1, w_2, w_3 can be found in [Yoshida, 1990, Phys. Lett. A]

2 part split SIs: Numerical results



N=1000, W=4, β=0.72, H_D=-28.5

LF τ=0.0025

$SABA_2$ τ=0.01

S^4 τ=0.05

ABA864 τ=0.175

S^6 τ=0.25

E_r: relative energy error

S_r: relative norm error

T_c: CPU time (sec)

Gerlach, Meichsner, Ch.S., 2016, Eur. Phys. J. Sp. Top.

DNLS model: 3 part split SIs

Symplectic Integrators produced by Successive Splits (SS)

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

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

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

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

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

DNLS model: 3 part split SIs

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

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

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

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

DNLS model: 3 part split SIs

Order 4: 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)]:

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

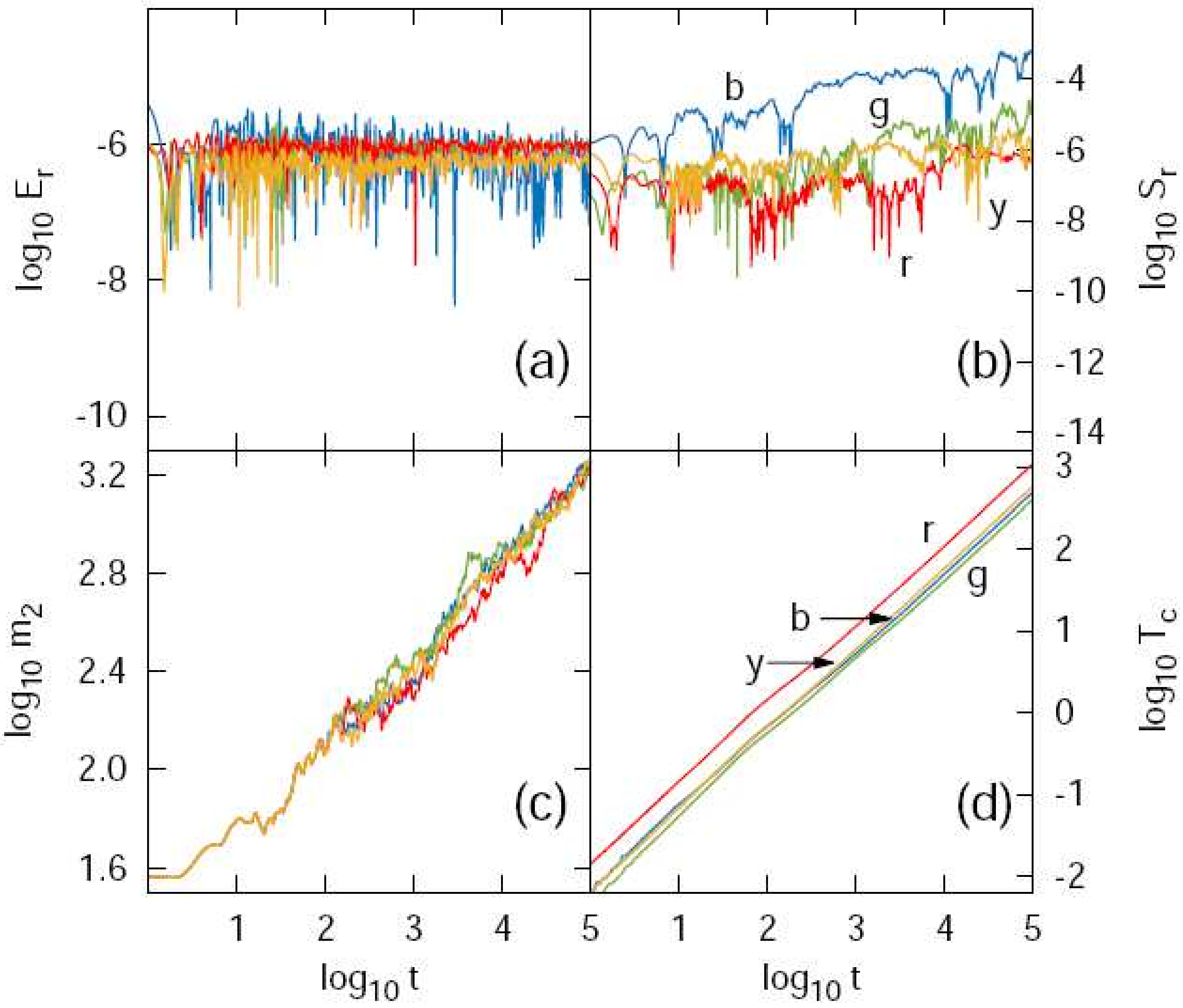
In this way, starting with the 2nd order integrators SS^2 and ABC^2 we construct the 4th order integrators:

SS^4 with 37 steps $\qquad$ $ABC^4_{[Y]}$ with 13 steps

Using the ABAH864 integrator [Blanes et al., 2013, App. Num. Math.], where the B part is integrated by the $SABA_2$ scheme, we construct the 4th order integrator: SS^4_{864} integrator with 49 steps.

Order 6: Using the composition method proposed in [Sofroniou & Spaletta, 2005, Optim. Methods Softw.] we construct the 6th order symplectic integrator $ABC^6_{[SS]}$ with 45 steps.

3 part split SIs: Numerical results



N=1000, W=4, β=0.72, H_D=-28.5

$ABC^4_{[Y]}$ τ=0.05

SS^4 τ=0.05

SS^4_{864} τ=0.125

$ABC^6_{[SS]}$ τ=0.225

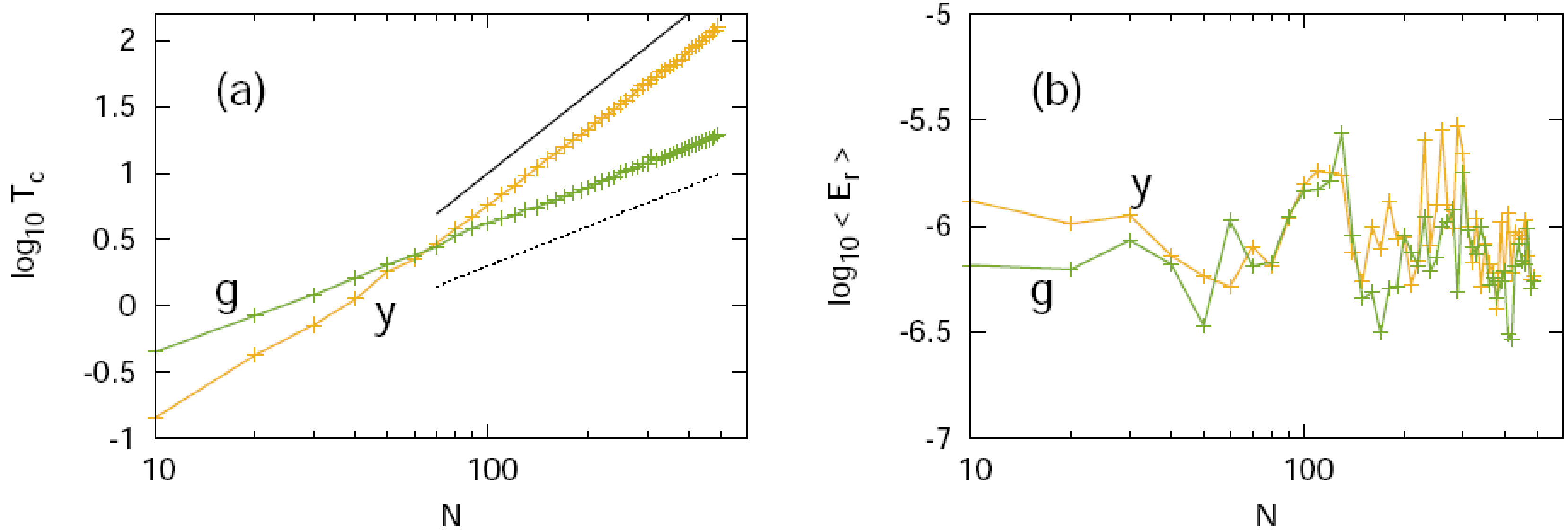
E_r: relative energy error

S_r: relative norm error

T_c: CPU time (sec)

Gerlach, Meichsner, Ch.S., 2016, Eur. Phys. J. Sp. Top.

2 and 3 part split SIs: Comparing their efficiency



Best 2 part split: ABA864 τ=0.125

Best 3 part split: $ABC^6_{[SS]}$ τ=0.225

N = number of sites, t = 10^4

E_r: relative energy error, T_c: CPU time (sec)

Summary

- **We presented several efficient symplectic integration methods suitable for the integration of the DNLS model, which are based on <u>2 and 3 part split</u> of the Hamiltonian.**
  - ✓ **2 part split methods preserve better the second integral of the system (i.e. the norm)**
  - ✓ **For small lattices (N $\lesssim$ 70) 2 part split methods are computationally more efficient, while for larger lattice 3 part split method should be used.**

References

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•**Ch.S., Gerlach, Bodyfelt, Papamikos, Eggl (2014) Phys. Lett. A, 378, 1809**

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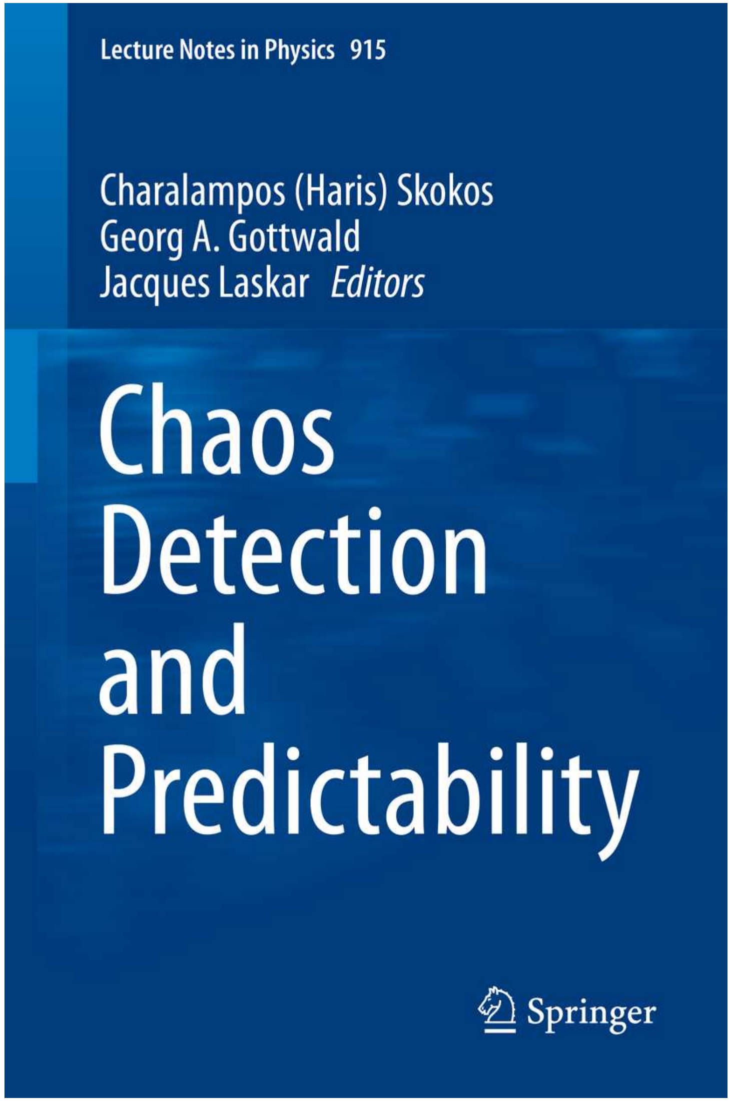
A …shameless promotion



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Contents