Efficient integration techniques for the long time simulation of the disordered discrete nonlinear Schrödinger equation

Haris Skokos

Department of Mathematics and Applied Mathematics, University of Cape Town, Cape Town, South Africa

E-mail: haris.skokos@uct.ac.za
URL: http://math_research.uct.ac.za/~hskokos/

Work in collaboration with Enrico Gerlach

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**

Autonomous Hamiltonian systems

Let us consider an N degree of freedom autonomous Hamiltonian systems of the 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:

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

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:

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

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 $SABA_2C$

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

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

$A(\vec{p})$ →

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

$B(\vec{q})$ →

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

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

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:

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

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

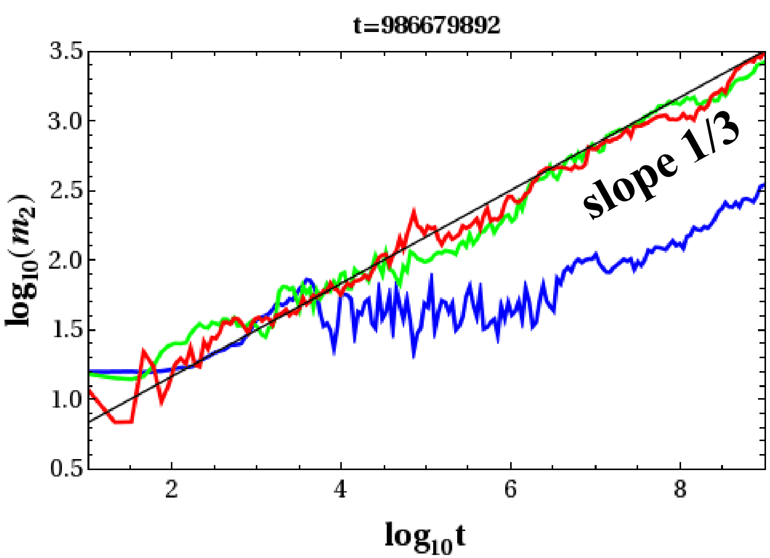
We consider normalized energy distributions in normal mode (NM) space

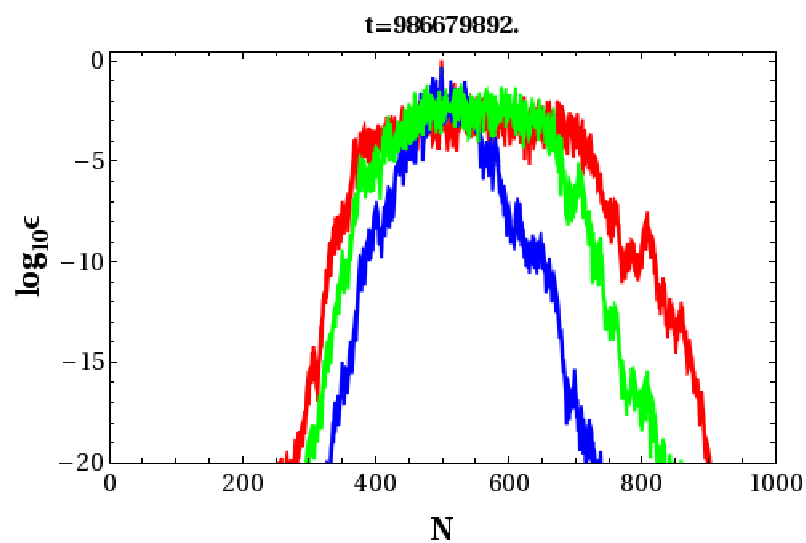
$$z_\nu \equiv \frac{E_\nu}{\sum_m E_m} \quad \text{with} \quad E_\nu = \frac{1}{2}\left(\dot{A}_\nu^2 + \omega_\nu^2 A_\nu^2\right)$$

, 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



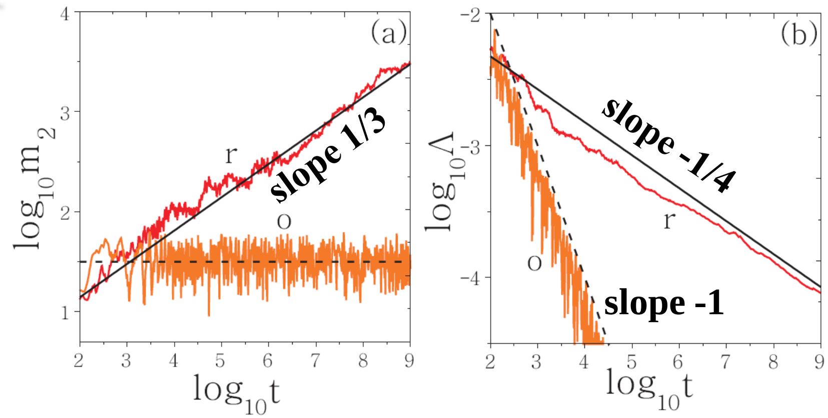


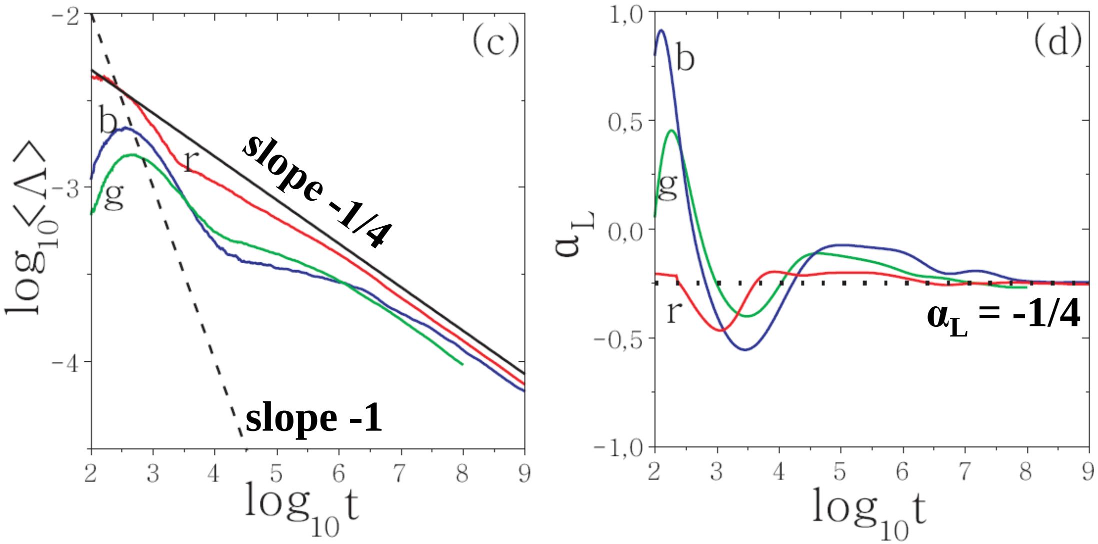
KG: Lyapunov Exponents

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:

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

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

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

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

How can we use Symplectic Integrators for the DNLS model?

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

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

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

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

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

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)**

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

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

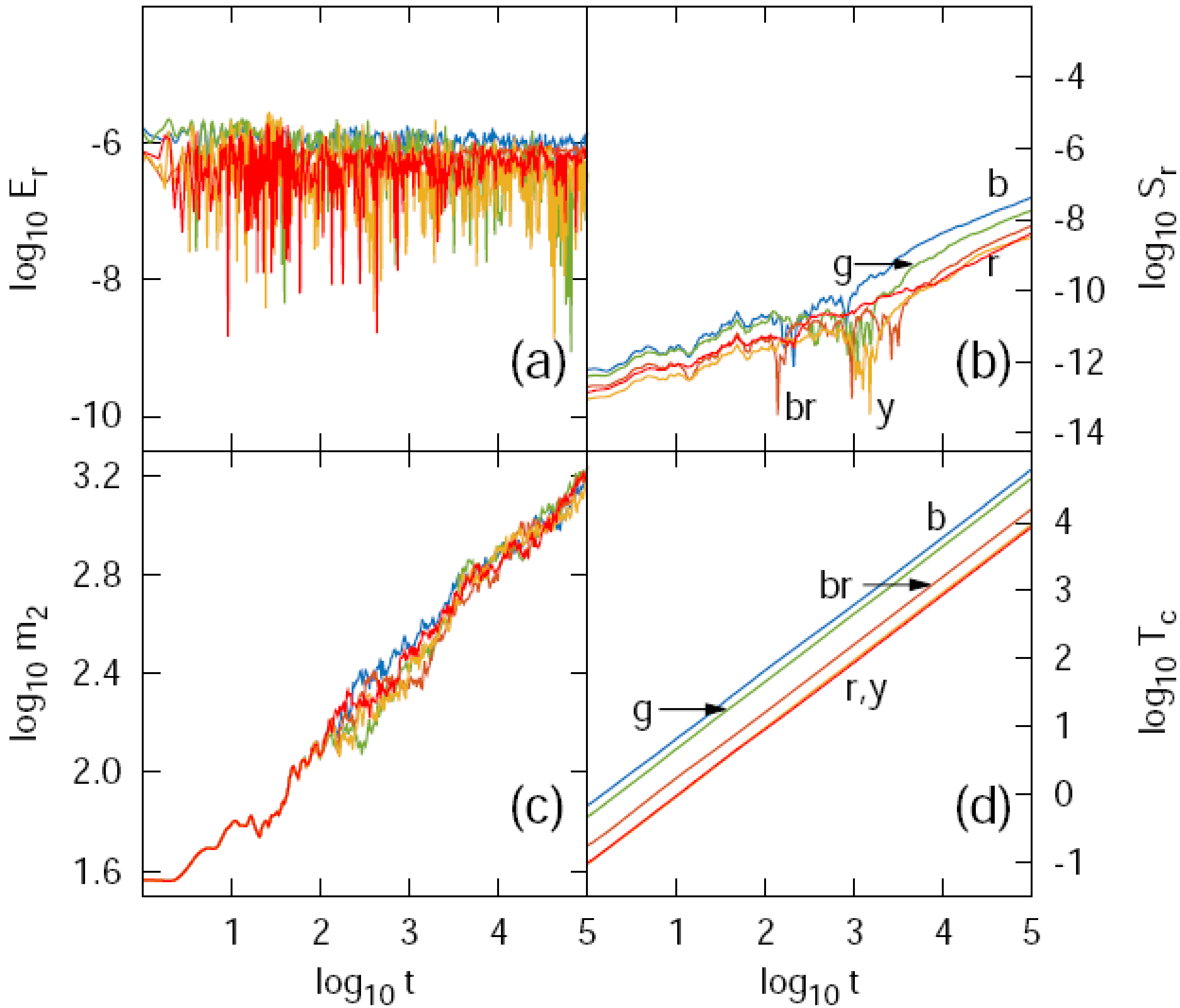
ABA864 [Blanes et al., 2013, App. Num. Math.] (15 steps)

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)

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

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 2nd order integrator with 13 steps, SS^2:

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

$\tau' = \tau / 2$

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

DNLS model: 3 part split SIs

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).

DNLS model: 3 part split SIs

Order 4: 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)]:

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

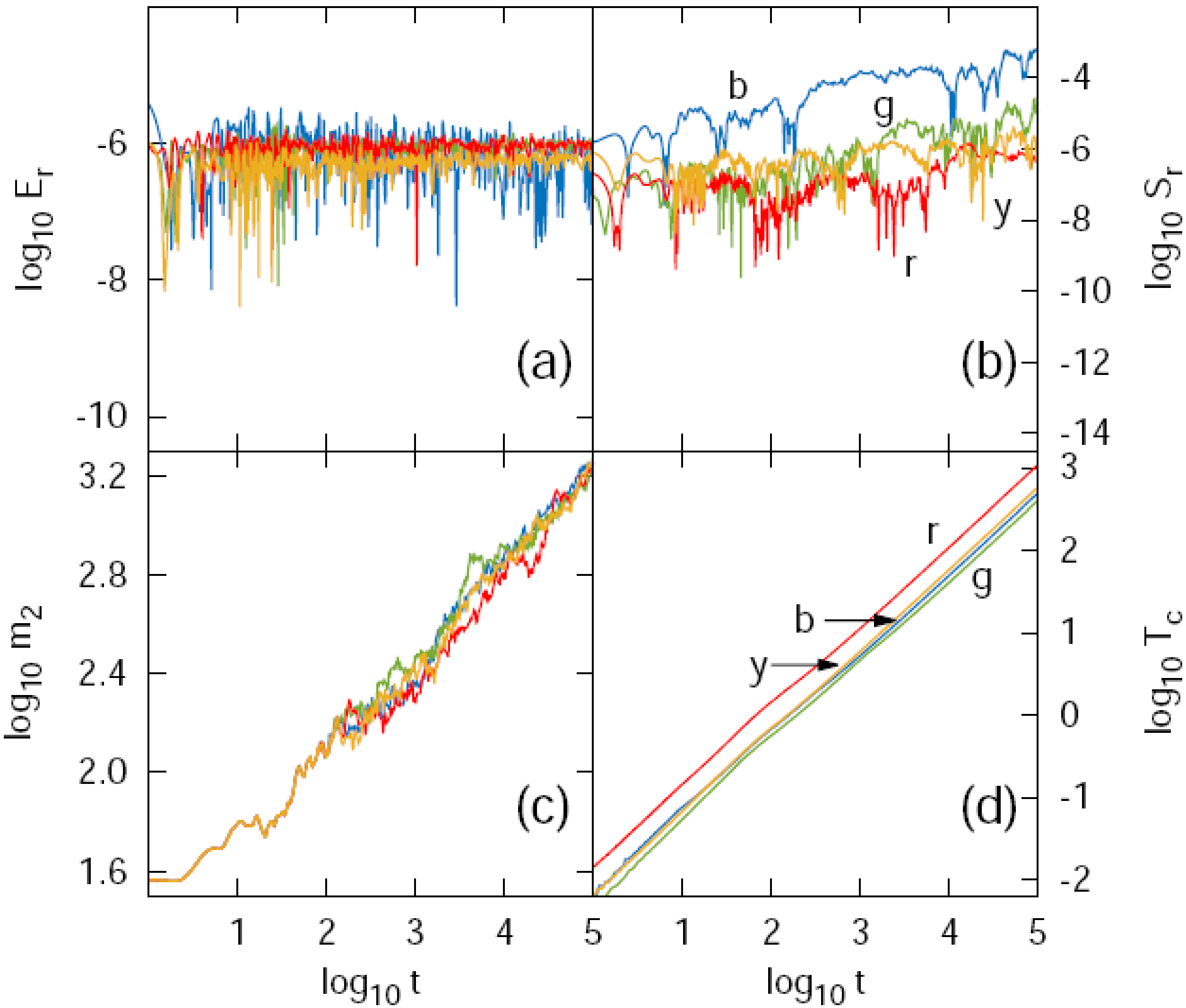
In this way, starting with the 2^{nd} order integrators SS^2 and ABC^2 we construct the 4^{th} order integrators:

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

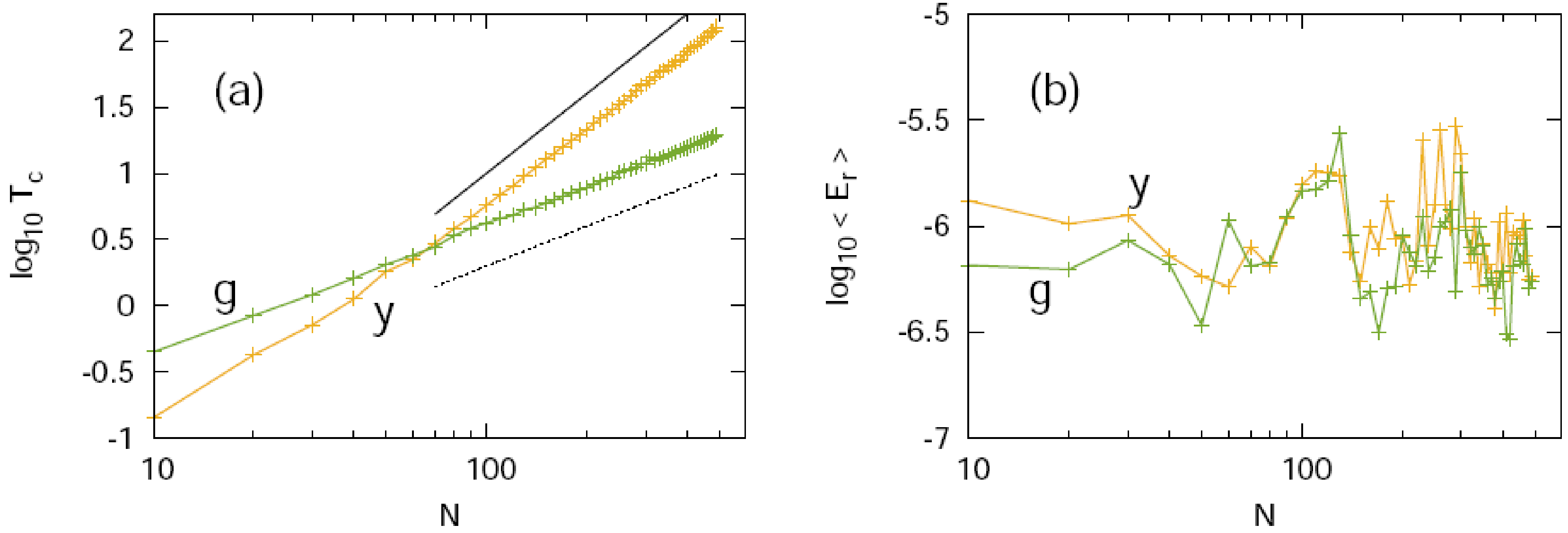
E_r: relative energy error

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 2 and 3 part split 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

•Ch.S., Gerlach (2010) PRE, 82, 036704

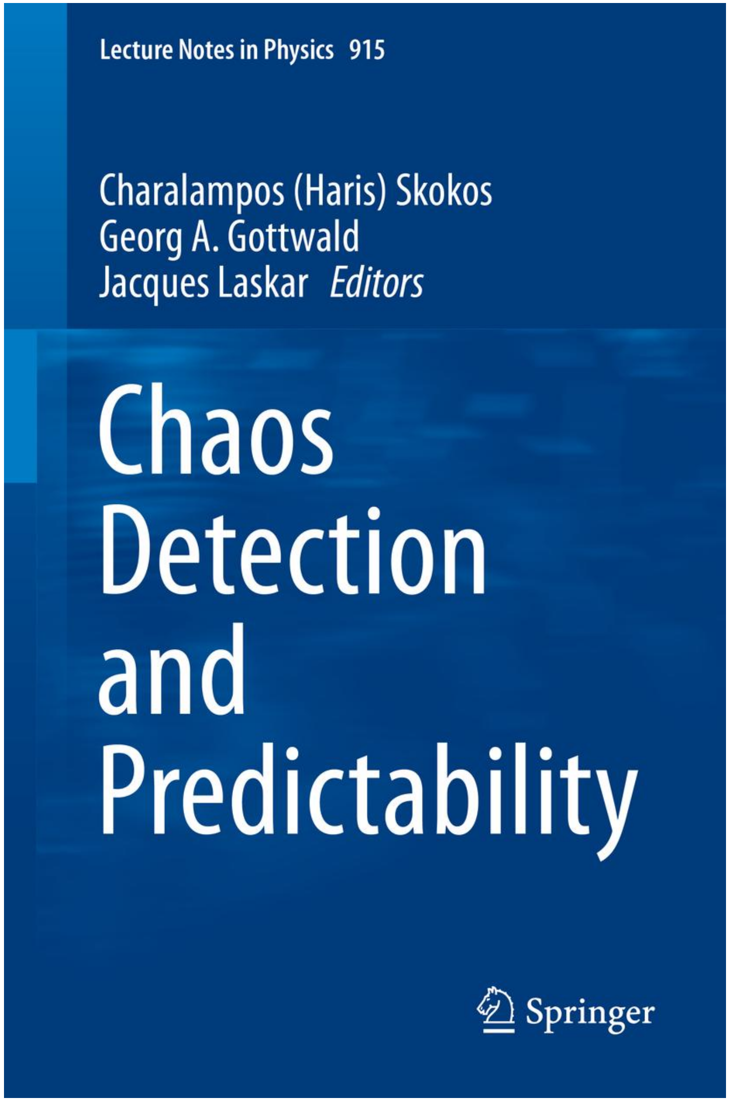
•Gerlach, Ch.S. (2011) Discr.Cont. Dyn. Sys.-Supp. 2011, 475

•Gerlach, Eggl, Ch.S. (2012) Int. J. Bifurc. Chaos, 22, 1250216

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

•Gerlach, Meichsner, Ch.S. (2016) Eur. Phys. J. Sp. Top., 225, 1103

A …shameless promotion



2016, Lect. Notes Phys., 915, Springer

Contents