High order three part split symplectic integrators. Application to 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://www.mth.uct.ac.za/~hskokos/

This research has been co-financed by the European Union (European Social Fund – ESF) and Greek national funds through the Operational Program "Education and Lifelong Learning" of the National Strategic Reference Framework (NSRF) - Research Funding Program: Thales. Investing in knowledge society through the European Social Fund.

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

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

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

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

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

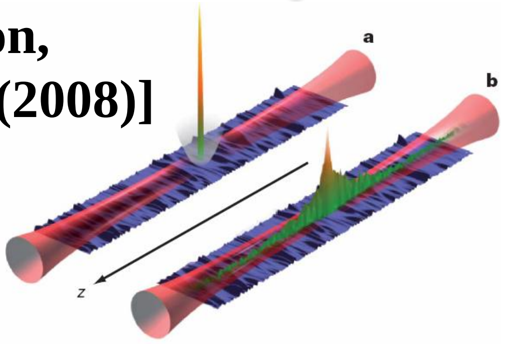
$$\left.\begin{aligned} \dot{x} &= p_x \\ \dot{y} &= p_y \\ \dot{p}_x &= 0 \\ \dot{p}_y &= 0 \\ \dot{\delta x} &= \delta p_x \\ \dot{\delta y} &= \delta p_y \\ \dot{\delta p}_x &= 0 \\ \dot{\delta p}_y &= 0 \end{aligned}\right\} \Rightarrow \frac{d\vec{u}}{dt} = L_{AV}\vec{u} \quad \Rightarrow \quad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

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

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

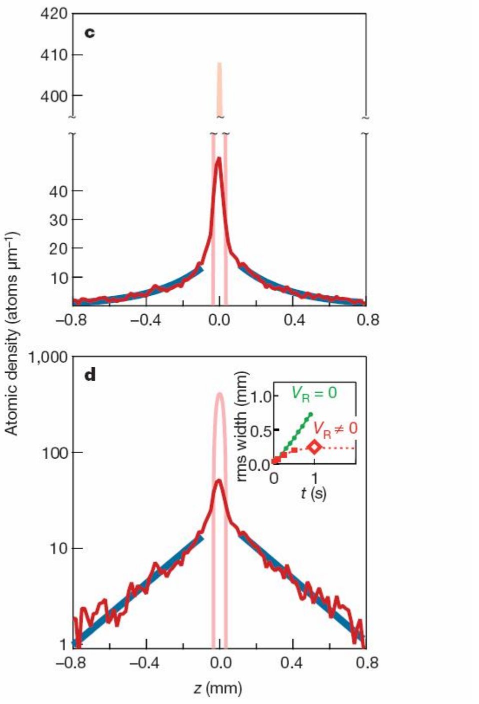
Interplay of disorder and nonlinearity

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

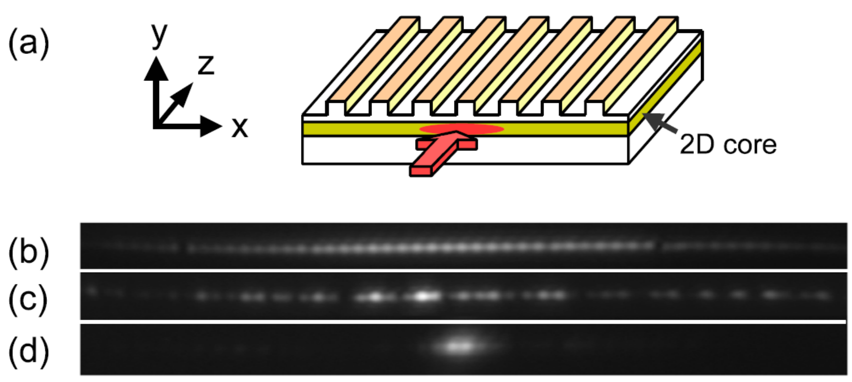


Waves in nonlinear disordered media – localization or delocalization?

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

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

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:

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

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 $S = \sum_l |\psi_l|^2$ of the wave packet.

Distribution characterization

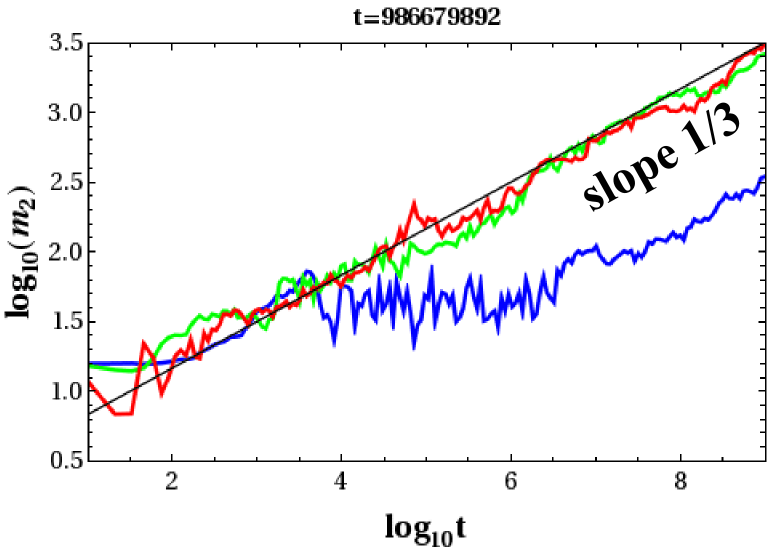
We consider normalized energy distributions in normal mode (NM) space

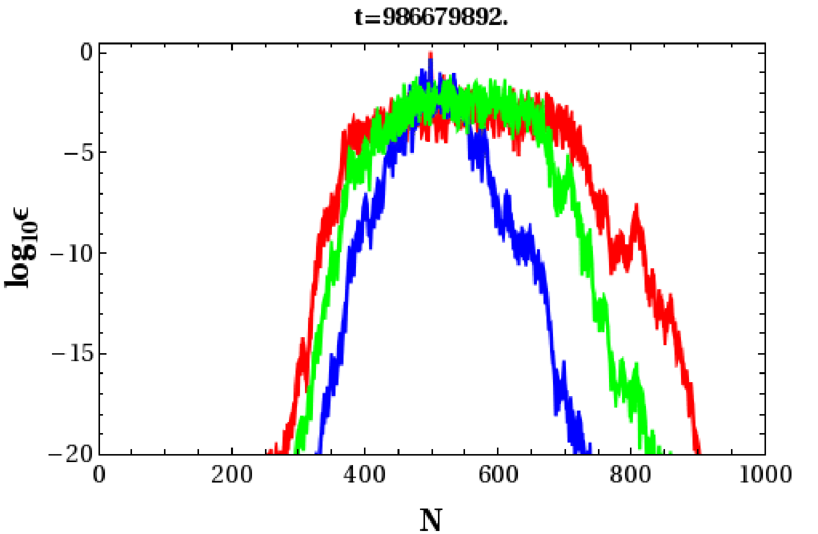
$$z_\nu \equiv \frac{E_\nu}{\sum_m E_m} \quad \text{with} \quad E_\nu = \frac{1}{2}\left(\dot{A}_\nu^2 + \omega_\nu^2 A_\nu^2\right)$$

, where A_ν is the amplitude of the νth NM.

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

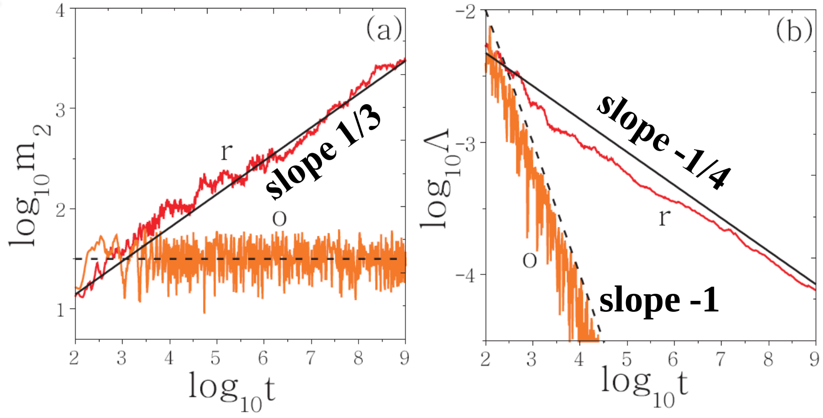
Different spreading regimes

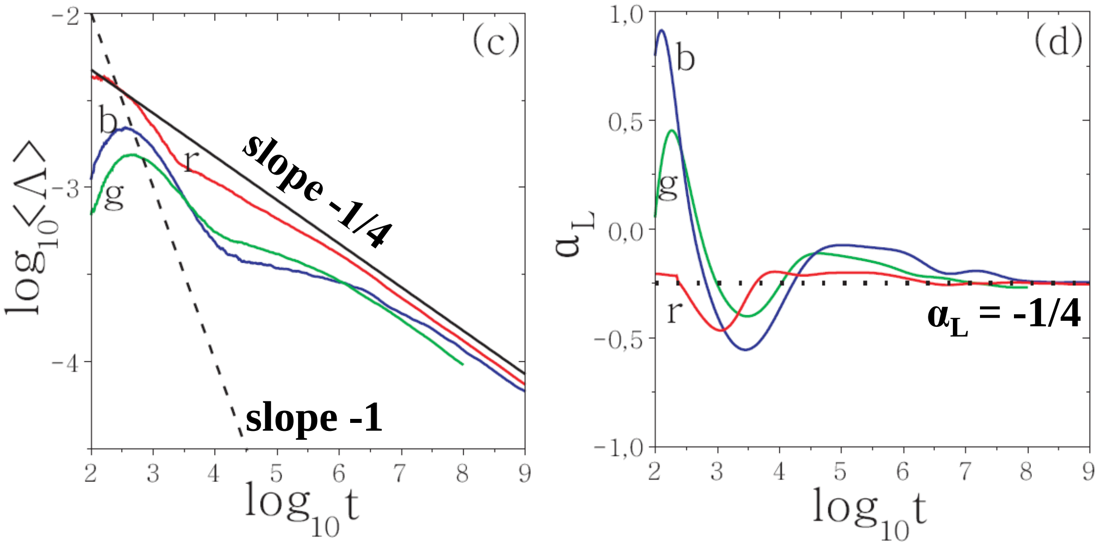




KG: Lyapunov Exponents

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. 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:

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

The DNLS model

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

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

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

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

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

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

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

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

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

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

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

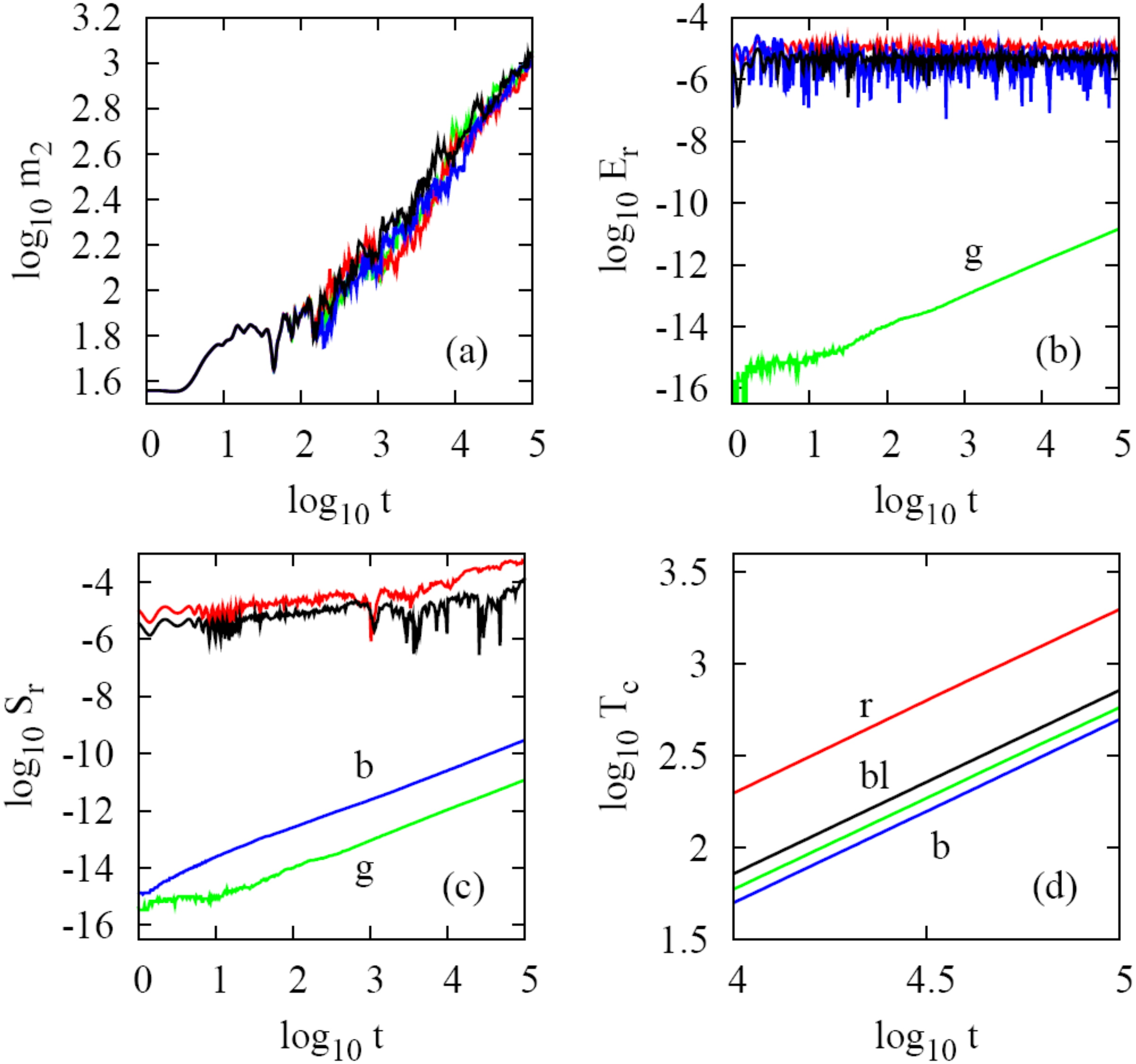
Three part split symplectic integrator of order 2, with 5 steps: ABC^2

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

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

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

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

$SIFT^2$ 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: 4^{th} 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 2^{nd} order integrators SS^2, $SIFT^2$ and ABC^2 we construct the 4^{th} order integrators:

SS^4 with 37 steps **$SIFT^4$ with 13 steps** **$ABC^4_{[Y]}$ with 13 steps**

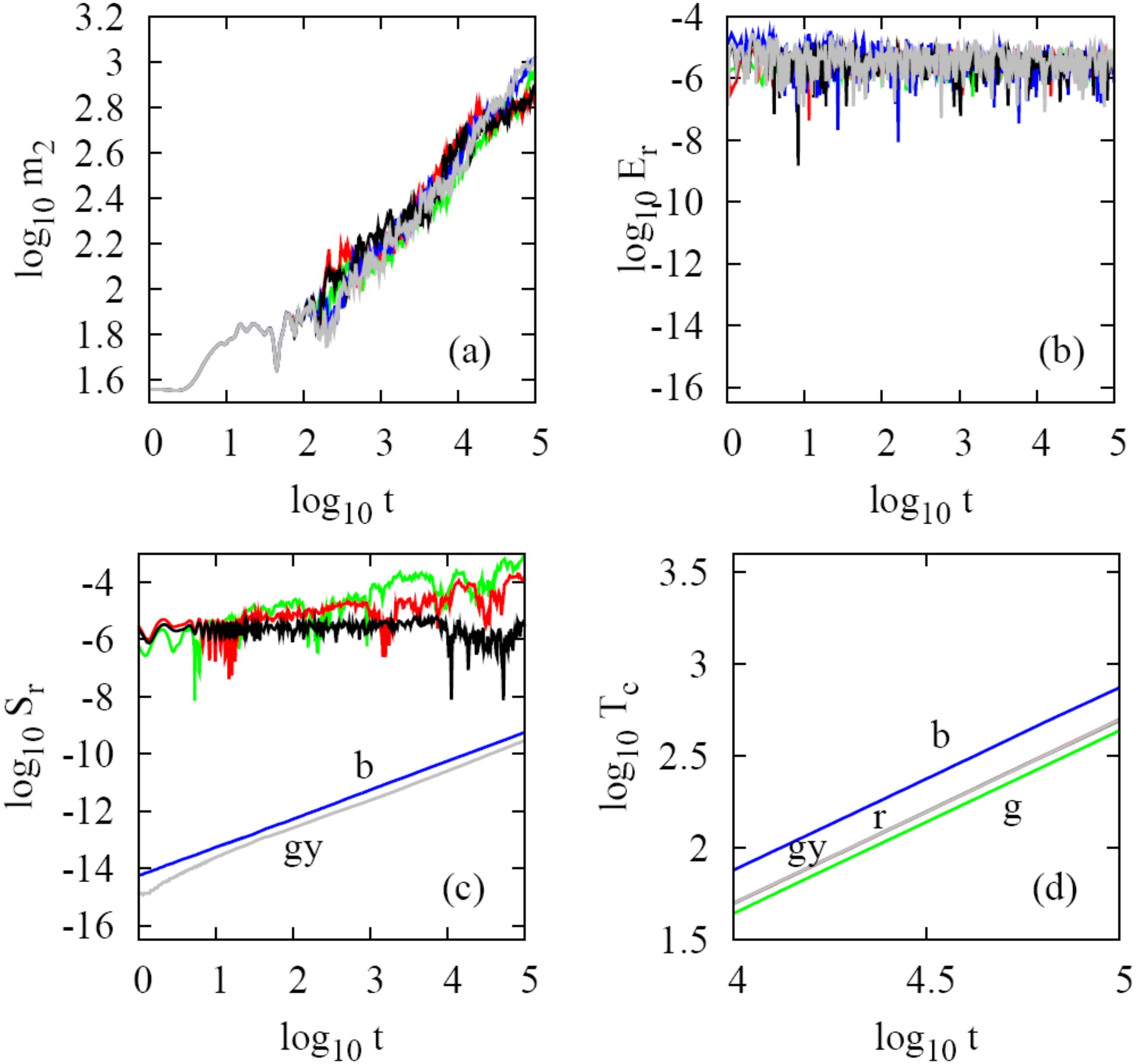
Composition method proposed by Suzuki [Phys. Lett. A (1990)]:

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

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

Starting with the 2^{nd} order integrators ABC^2 we construct the 4^{th} order integrator: $ABC^4_{[S]}$ with 21 steps.

4^{th} order integrators: Numerical results



SIFT^4 τ=0.125

SIFT^2 τ=0.05

ABC$^4_{[S]}$ τ=0.1

SS^4 τ=0.1

ABC$^4_{[Y]}$ 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)

High order composition methods (I)

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

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

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 composition methods (II)

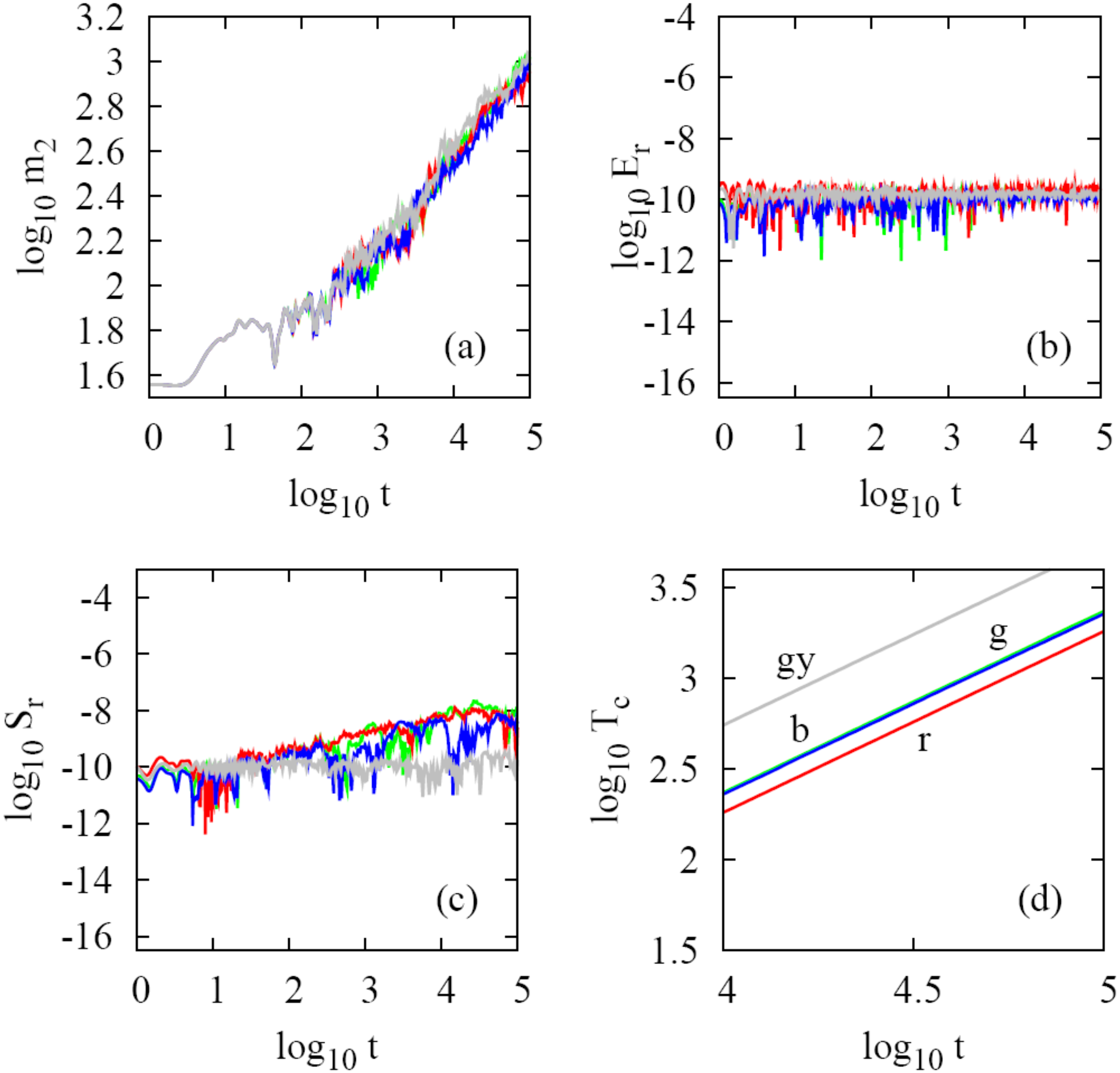
In addition, following the works of
Kahan & Li, Math Comput. (1997), and
Sofroniou & Spaletta, Optim. Methods Softw. (2005)
we implement some efficient high order composition methods,
considering as the basic block the 2nd order ABC^2 integrator.

$ABC^6_{[KL]}$ with 37 steps
$ABC^6_{[SS]}$ with 45 steps

$ABC^8_{[Y]}$ with 61 steps
$ABC^8_{[KL]}$ with 69 steps
$ABC^8_{[SS]}$ with 77 steps

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

High order integrators: Numerical results (I)



SS^4_{864} $\tau=0.015625$

$ABC^6_{[Y]}$ $\tau=0.03$

$ABC^6_{[KL]}$ $\tau=0.04$

$ABC^6_{[SS]}$ $\tau=0.125$

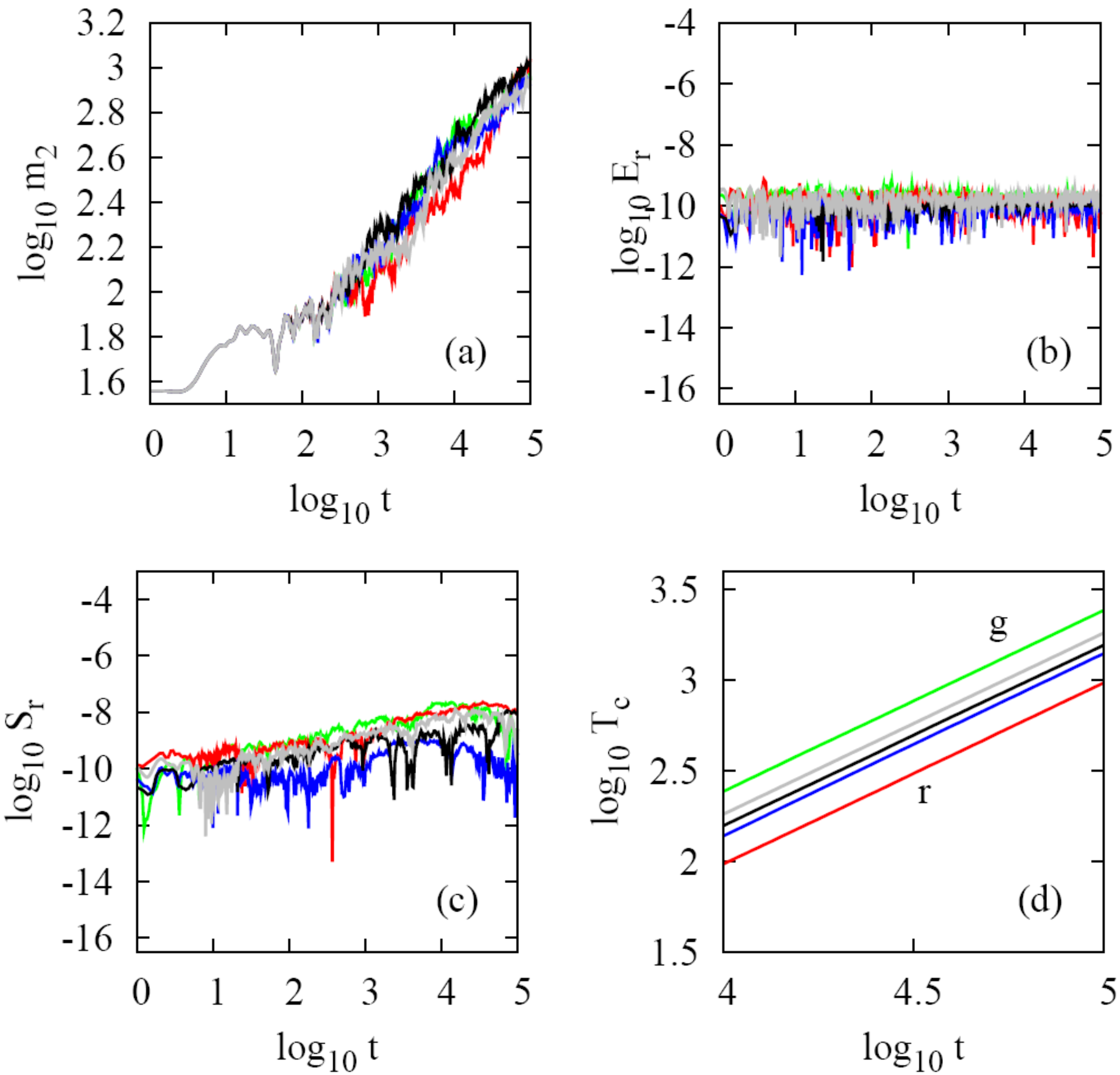
E_r: relative energy error

S_r: relative norm error

T_c: CPU time (sec)

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

High order integrators: Numerical results (II)



$ABC^8_{[Y]}$ $\tau=0.0625$

$ABC^6_{[SS]}$ $\tau=0.125$

$ABC^{10}_{[SS]}$ $\tau=0.2$

$ABC^8_{[KL]}$ $\tau=0.125$

$ABC^8_{[SS]}$ $\tau=0.2$

E_r: relative energy error

S_r: relative norm error

T_c: CPU time (sec)

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

Summary

- **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 $SIFT^2$ and $SIFT^4$ 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.**

References

- **Flach, Krimer, S. (2009) PRL, 102, 024101**
- **S., Krimer, Komineas, Flach (2009) PRE, 79, 056211**
- **S., Flach (2010) PRE, 82, 016208**
- **Laptyeva, Bodyfelt, Krimer, S., Flach (2010) EPL, 91, 30001**
- **Bodyfelt, Laptyeva, S., Krimer, Flach (2011) PRE, 84, 016205**
- **Bodyfelt, Laptyeva, Gligoric, S., Krimer, Flach (2011) Int. J. Bifurc. Chaos, 21, 2107**
- **S., Gkolias, Flach (2013) PRL, 111, 064101**
- **Tieleman, S., Lazarides (2014) EPL, 105, 20001**

- **S., Gerlach (2010) PRE, 82, 036704**
- **Gerlach, S. (2011) Discr.Cont. Dyn. Sys.-Supp. 2011, 475**
- **Gerlach, Eggl, S. (2012) Int. J. Bifurc. Chaos, 22, 1250216**
- **Gerlach, Eggl, S., Bodyfelt, Papamikos (2013) nlin.CD/1306.0627**
- **S., Gerlach, Bodyfelt, Papamikos, Eggl (2014) Phys. Lett. A, 378, 1809**

Thank you for your attention