High order three part split symplectic integration schemes

Haris Skokos

Physics Department, Aristotle University of Thessaloniki
Thessaloniki, Greece

E-mail: hskokos@auth.gr
URL: http://users.auth.gr/hskokos/

Work in collaboration with
Joshua Bodyfelt, Siegfried Eggl, Enrico Gerlach, Georgios Papamikos

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

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

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

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.

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$_2$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 $c_1 = \frac{1}{2} - \frac{\sqrt{3}}{6},\ c_2 = \frac{\sqrt{3}}{3},\ d_1 = \frac{1}{2}.$

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

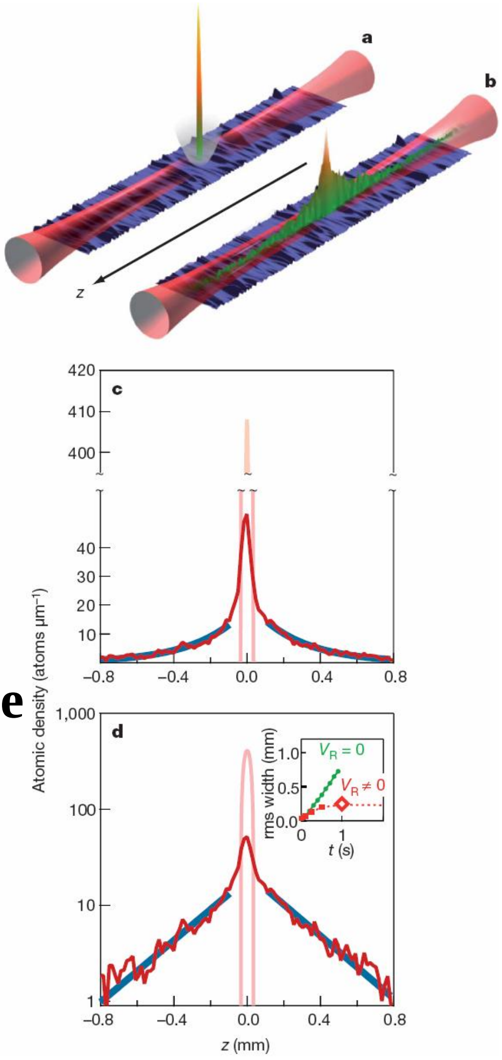
Waves in disordered media – Anderson localization

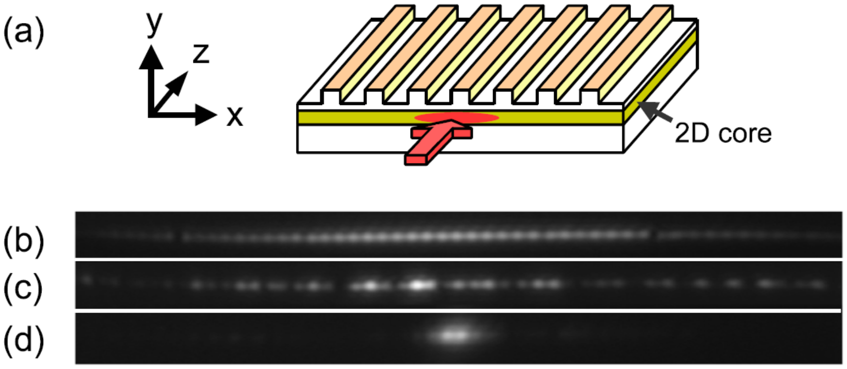
[Anderson, Phys. Rev. (1958)]. Experiments on BEC [Billy et al., Nature (2008)]

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) - Flach et al., PRL (2009) - Ch.S. et al., PRE (2009) - Ch.S. & Flach, PRE (2010) – Laptyeva et al., EPL (2010) - 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** $\left[\frac{1}{2},\frac{3}{2}\right]$.

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.

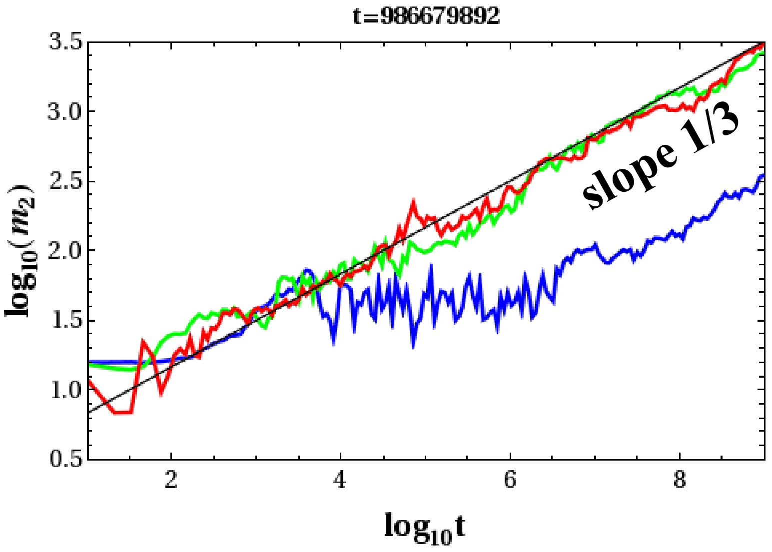
Distribution characterization

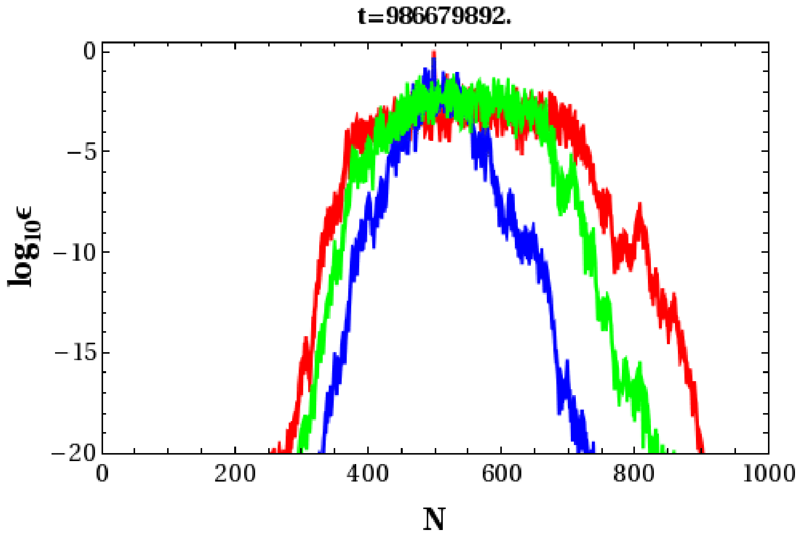
We consider normalized energy distributions in normal mode (NM) space

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





The KG model

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

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

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

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

with a corrector term which corresponds to the Hamiltonian function:

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

The DNLS model

A 2nd order SABA Symplectic Integrator with 5 steps, combined with approximate solution for the B part (Fourier Transform): SIFT²

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

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

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

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

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

The DNLS model

Symplectic Integrators produced by Successive Splits (SS)

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

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

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:

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

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

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

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

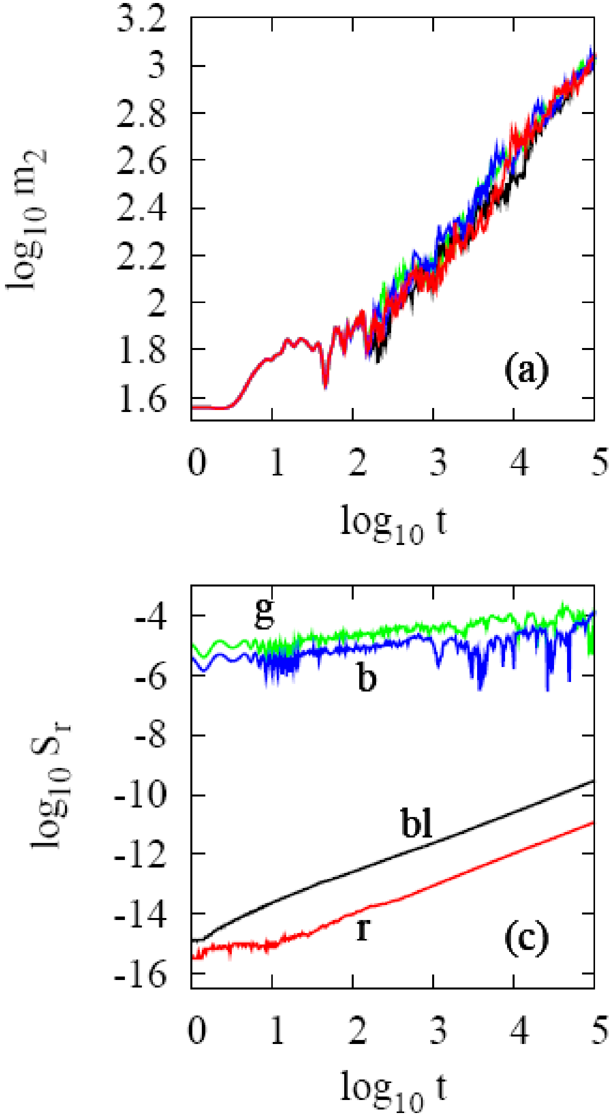
Three part split symplectic integrator of order 2, with 5 steps: ABC^2

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

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

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

2nd order integrators: Numerical results



ABC^2 $\tau=0.005$

SS^2 $\tau=0.02$

SIFT^2 $\tau=0.05$

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**

6th order symplectic integrators

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

$$\mathbf{ABC^6(\tau) = ABC^2(w_3\tau)\times ABC^2(w_2\tau)\times ABC^2(w_1\tau)\times}$$

$$\mathbf{\times ABC^2(w_0\tau)\times ABC^2(w_1\tau)\times ABC^2(w_2\tau)\times ABC^2(w_3\tau)}$$

whose coefficients $\mathbf{w_1 = -1.17767998417887}$

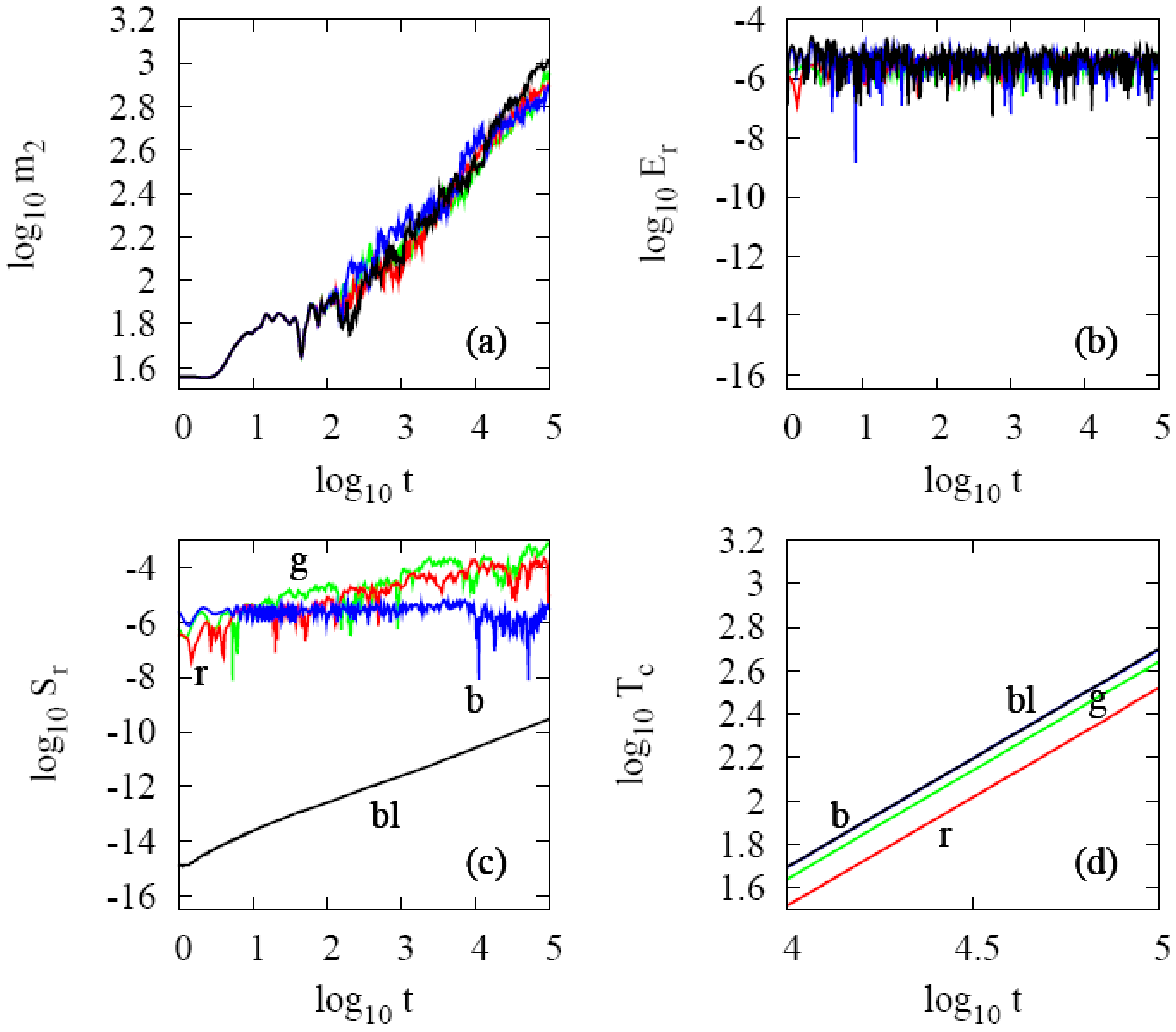
$$\mathbf{w_2 = 0.235573213359357}$$

$$\mathbf{w_3 = 0.784513610477560}$$

$$\mathbf{w_0 = 1 - 2(w_1 + w_2 + w_3)}$$

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 4th and 6th 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.

Ch.S., Gerlach, Bodyfelt, Papamikos, Eggl (2013)
arXiv:1302.1788