Efficient integration schemes for the 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

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 integration schemes

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 $e^{\tau L_H}$, i.e. the solution of Hamilton equations of motion, 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.

As an example, we consider a particular 2nd order symplectic integrator with 5 steps [Laskar & Robutel, Cel. Mech. Dyn. Astr. (2001)]:

$$SABA_2 = e^{\left[\frac{(3-\sqrt{3})}{6}\tau\right] L_A} \, e^{\frac{\tau}{2} L_B} \, e^{\frac{\sqrt{3}\tau}{3} L_A} \, e^{\frac{\tau}{2} L_B} \, e^{\left[\frac{(3-\sqrt{3})}{6}\tau\right] L_A}$$

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 , Eggl, Ch.S., IJBC (2012)].

The Hénon-Heiles system can be split as:

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

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

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

$$e^{\tau L_{AV}}: \begin{cases} x' &= x + p_x \tau \\ y' &= y + p_y \tau \\ px' &= p_x \\ py' &= p_y \\ \delta x' &= \delta x + \delta p_x \tau \\ \delta y' &= \delta y + \delta p_y \tau \\ \delta p_x' &= \delta p_x \\ \delta p_y' &= \delta p_y \end{cases}$$

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

$$e^{\tau L_{BV}}: \begin{cases} x' &= x \\ y' &= y \\ p_x' &= p_x - x(1+2y)\tau \\ p_y' &= p_y + (y^2 - x^2 - y)\tau \\ \delta x' &= \delta x \\ \delta y' &= \delta y \\ \delta p_x' &= \delta p_x - [(1+2y)\delta x + 2x\delta y]\,\tau \\ \delta p_y' &= \delta p_y + [-2x\delta x + (-1+2y)\delta y]\,\tau \end{cases}$$

Disordered lattices

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 H_K**. $\tilde{\varepsilon}_l$ **chosen uniformly from** $\left[\frac{1}{2},\frac{3}{2}\right]$.

The discrete nonlinear Schrödinger (DNLS) equation

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

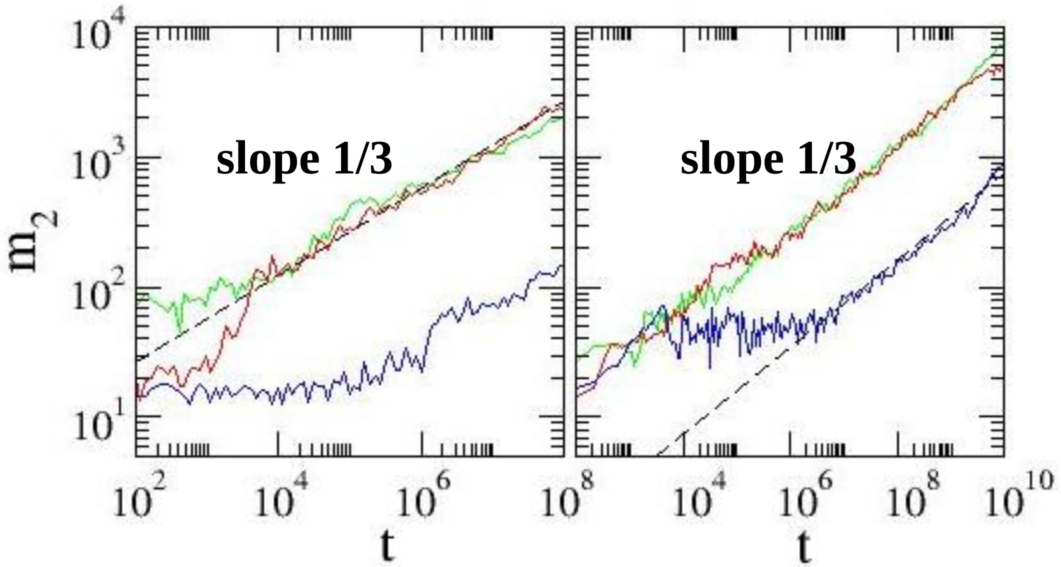
where **ε_l are uniformly chosen from** $\left[-\frac{W}{2},\frac{W}{2}\right]$ and **β is the nonlinear parameter.**

Conserved quantities: The energy H_D and the norm S of the wave packet.

Spreading of wave packets

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)

The KG model

Two part split symplectic integrators

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

A: $\frac{p_l^2}{2}$

B: $\frac{\tilde{\varepsilon}_l}{2} u_l^2 + \frac{1}{4} u_l^4 + \frac{1}{2W} \left(u_{l+1} - u_l \right)^2$

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

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

The DNLS model

A 2nd order SABA Symplectic Integrator with 5 steps, combined with approximate solution for the B part (Fourier Transform): SIFT$_2$

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

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

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

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

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

The DNLS model

Symplectic Integrators produced by Successive Splits (SS)

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

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

B → 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, $SS(SABA_2)_2$:

$$SS(SABA_2)_2 = e^{\left[\frac{(3-\sqrt{3})}{6}\tau\right]L_A} e^{\frac{\tau}{2}L_B} e^{\frac{\sqrt{3}\tau}{3}L_A} e^{\frac{\tau}{2}L_B} e^{\left[\frac{(3-\sqrt{3})}{6}\tau\right]L_A}$$

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

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

The DNLS model

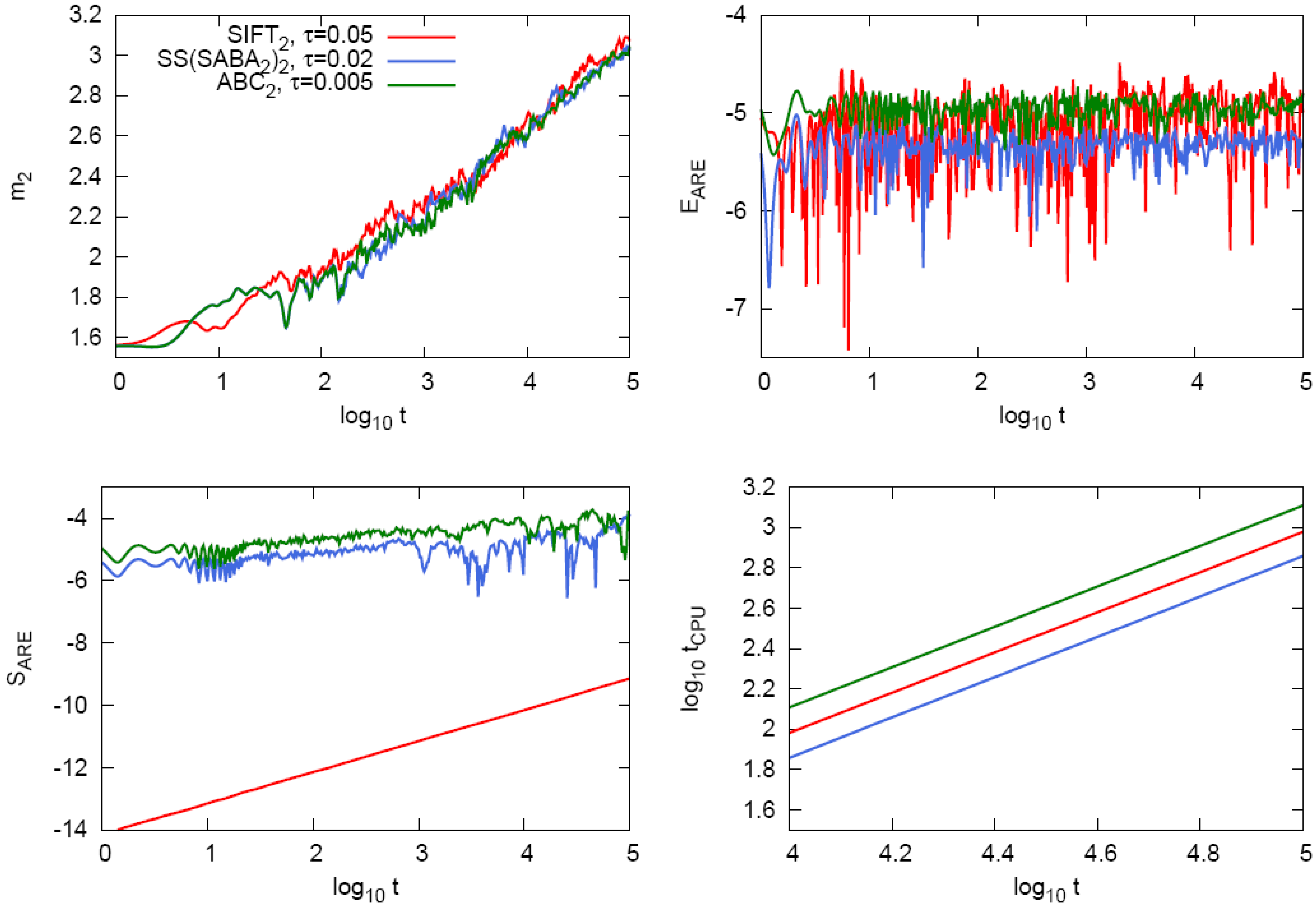
Three part split symplectic integrator of order 2, with 5 steps: ABC_2

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

$$ABC_2 = e^{\frac{\tau}{2}L_A}\, e^{\frac{\tau}{2}L_B}\, e^{\tau L_C}\, e^{\frac{\tau}{2}L_B}\, e^{\frac{\tau}{2}L_A}$$

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

2^{nd} order integrators: Numerical results



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)]:

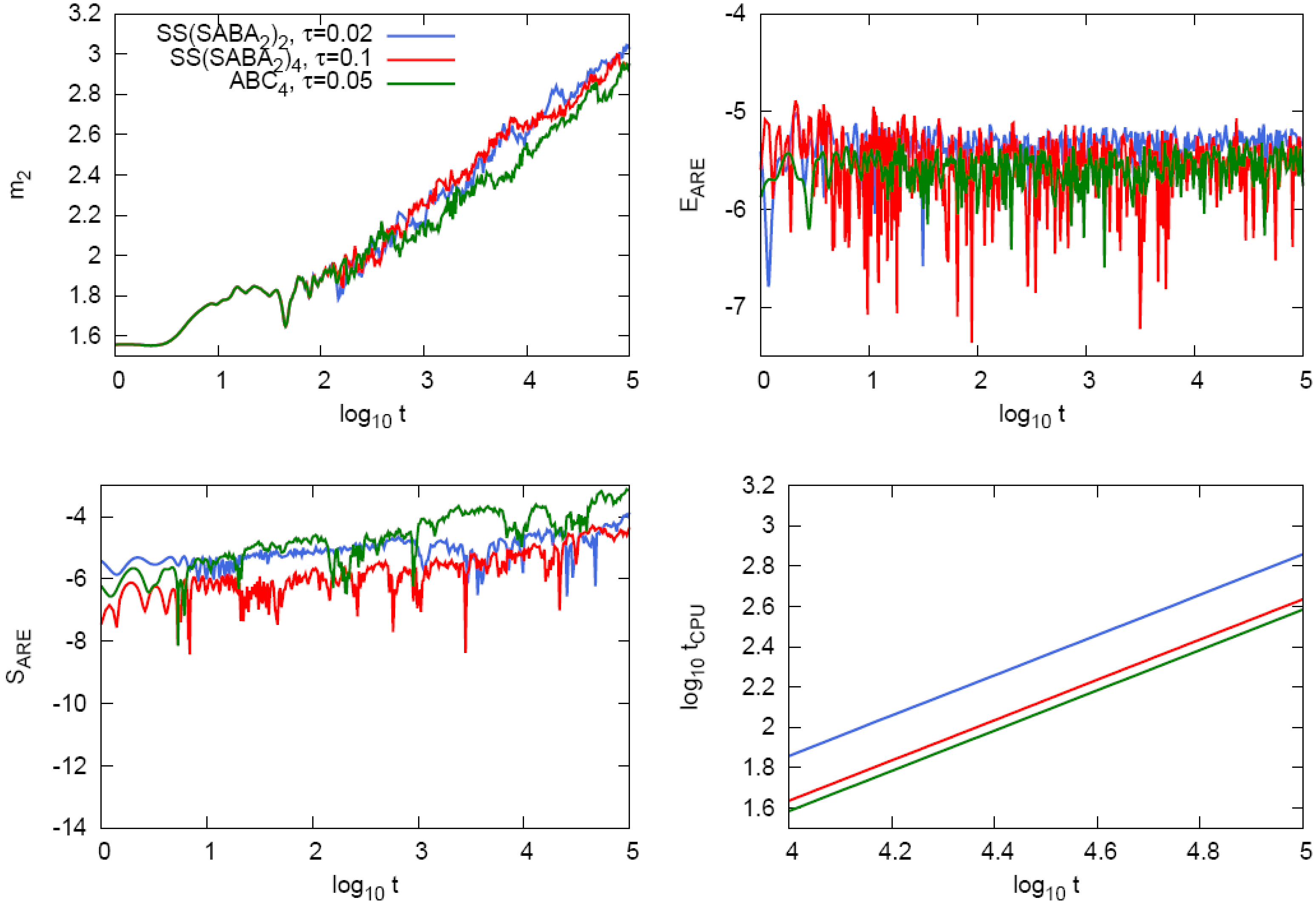
$$S_{4th}(\tau) = S_{2nd}(x_1\tau) \times S_{2nd}(x_0\tau) \times S_{2nd}(x_1\tau)$$

$$x_0 = -\frac{2^{1/3}}{2-2^{1/3}}, \qquad x_1 = \frac{1}{2-2^{1/3}}$$

Starting with the 2^{nd} order integrators $SS(SABA_2)_2$ and ABC_2 we construct the 4^{th} order integrators:

- **$SS(SABA_2)_4$ with 37 steps**
- **ABC_4 with 13 steps**

4th order integrators: Numerical results



Conclusions

- **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} order integrators proved to be quite efficient, allowing integration of the DNLS for very long times.**

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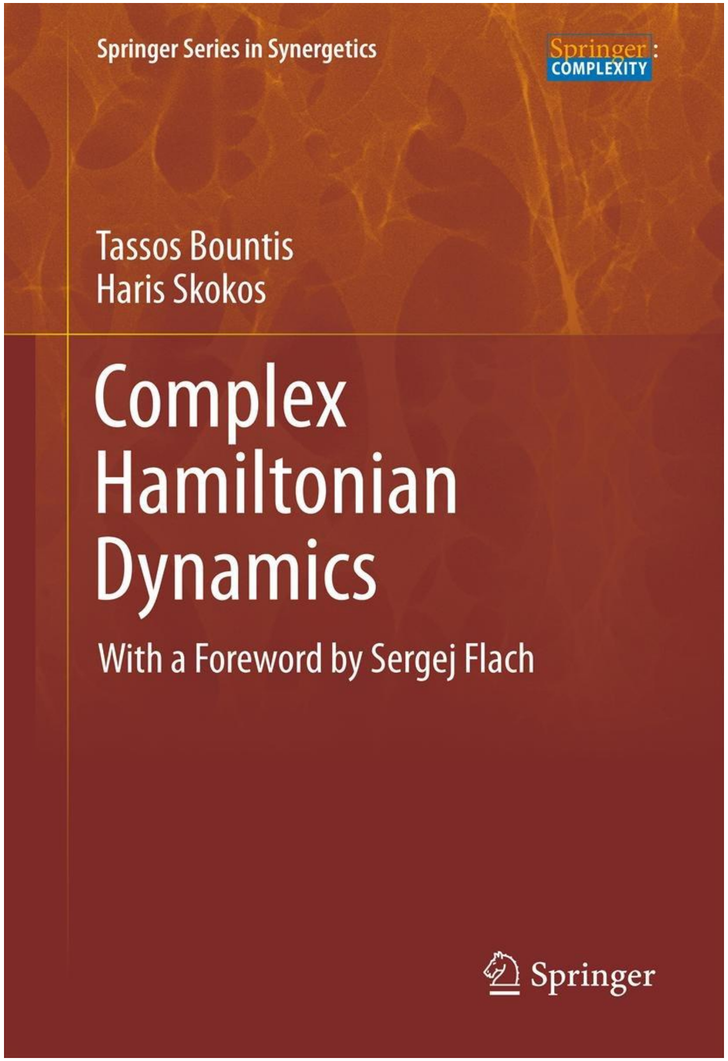

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