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:

$$H(q_1, q_2, \ldots, q_N, p_1, p_2, \ldots, p_N)$$

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:

$$\frac{d\tilde{X}}{dt} = \{H, \tilde{X}\} = L_H \tilde{X} \Rightarrow \tilde{X}(t) = \sum_{n=0}^{t^n} H^n \tilde{X} = e^{tL_H} \tilde{X}$$

where $\tilde{X}$ 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 $t+\tau$ 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 $\tau$ is described by a series of successive acts of Hamiltonians $A$ and $B$.**
Symplectic Integrator SABA\textsubscript{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

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

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:

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

where \( \varepsilon_l \) chosen uniformly from \( \left[ -\frac{W}{2}, \frac{W}{2} \right] \) and \( \beta \) 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

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

where \( A_\nu \) is the amplitude of the \( \nu \)th NM.

Second moment:

\[ m_2 = \sum_{\nu=1}^{N} \left( \nu - \bar{\nu} \right)^2 z_\nu \quad \text{with} \quad \bar{\nu} = \sum_{\nu=1}^{N} \nu z_\nu \]

Different spreading regimes
The KG model

We apply the SABAC\textsubscript{2} integrator scheme to the KG Hamiltonian by using the splitting:

\[
H_{K} = \sum_{l=1}^{N} \left( \frac{p_{l}^{2}}{2} + \frac{\tilde{\varepsilon}_{l}}{2} u_{l}^{2} + \frac{1}{4} u_{l}^{4} + \frac{1}{2W} \left( u_{l+1} - u_{l} \right)^{2} \right)
\]

with a corrector term which corresponds to the Hamiltonian function:

\[
\begin{align*}
\exp^{\tau L_{A}}: & \begin{cases} u_{l}' = p_{l}\tau + u_{l} \\ p_{l}' = p_{l}, \end{cases} \\
\exp^{\tau L_{B}}: & \begin{cases} u_{l}' = u_{l} \\ p_{l}' = \left[ -u_{l}(\tilde{\varepsilon}_{l} + u_{l}^{2}) + \frac{1}{W} (u_{l-1} + u_{l+1} - 2u_{l}) \right] \tau + p_{l}, \end{cases}
\end{align*}
\]

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): SIFT²

\[ H_D = \sum_l \epsilon_l |\psi_l|^2 + \frac{\beta}{2} |\psi_l|^4 - \left( \psi_{l+1} \psi_l^* + \psi_{l+1}^* \psi_l \right), \quad \psi_l = \frac{1}{\sqrt{2}} (q_l + ip_l) \]

\[ H_D = \sum_l \left( \frac{\epsilon_l}{2} (q_l^2 + p_l^2) + \frac{\beta}{8} (q_l^2 + p_l^2)^2 - q_n q_{n+1} - p_n p_{n+1} \right) \]

\[ e^{\tau L_A}: \begin{cases} 
q'_l = q_l \cos(\alpha_l \tau) + p_l \sin(\alpha_l \tau), \\
p'_l = p_l \cos(\alpha_l \tau) - q_l \sin(\alpha_l \tau), \\
\alpha_l = \epsilon_l + \beta(q_l^2 + p_l^2)/2 
\end{cases} \]

\[ e^{\tau L_B}: \begin{cases} 
\varphi_q = \sum_{m=1}^N \psi_m e^{2\pi i q (m-1)/N} \\
\varphi'_q = \varphi_q e^{2i \cos(2\pi (q-1)/N) \tau} \\
\psi'_l = \frac{1}{N} \sum_{q=1}^N \varphi'_q e^{-2\pi il(q-1)/N} 
\end{cases} \]
The DNLS model

Symplectic Integrators produced by Successive Splits (SS)

\[ H_D = \sum_l \left( \frac{\epsilon_l}{2} \left( q_l^2 + p_l^2 \right) + \frac{\beta}{8} \left( q_l^2 + p_l^2 \right)^2 \right) - q_n q_{n+1} - p_n p_{n+1} \]

\[ \begin{align*}
q_l' &= q_l \cos(\alpha_l \tau) + p_l \sin(\alpha_l \tau), \\
p_l' &= p_l \cos(\alpha_l \tau) - q_l \sin(\alpha_l \tau),
\end{align*} \]

Using the SABA₂ integrator we get a 2nd order integrator with 13 steps, SS²:

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

\[ \tau' = \tau / 2 \]
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: ABC²

\[ H_D = \sum_l \left( \frac{\epsilon_l}{2} \left( q_l^2 + p_l^2 \right) + \frac{\beta}{8} \left( q_l^2 + p_l^2 \right)^2 - q_n q_{n+1} - p_n p_{n+1} \right) \]

\[ ABC^2 = e_2^{L_A} e_2^{L_B} e^{\tau L_C} e_2^{L_B} e_2^{L_A} \]

This low order integrator has already been used by e.g. Chambers, MNRAS (1999) – Goździewski et al., MNRAS (2008).
**2nd order integrators: Numerical results**

- **ABC²** $\tau=0.005$
- **SS²** $\tau=0.02$
- **SIFT²** $\tau=0.05$
- **DOP853** $\delta=10^{-16}$

$E_r$: relative energy error
$S_r$: relative norm error
4th order symplectic integrators

Starting from any 2nd order symplectic integrator $S^{2\text{nd}}$, we can construct a 4th order integrator $S^{4\text{th}}$ using a composition method [Yoshida, Phys. Let. A (1990)]:

$$S^{4\text{th}}(\tau) = S^{2\text{nd}}(x_1 \tau) \times S^{2\text{nd}}(x_0 \tau) \times S^{2\text{nd}}(x_1 \tau)$$

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

Starting with the 2nd order integrators $SS^2$ and $ABC^2$ we construct the 4th 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 ABC6 having 29 steps [Yoshida, Phys. Let. A (1990)]:

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

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 integrators: Numerical results

- SIFT\(^2\) \(\tau=0.05\)
- SS\(^4\) \(\tau=0.1\)
- ABC\(^4\) \(\tau=0.05\)
- ABC\(^6\) \(\tau=0.15\)

\(E_r\): 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