High order three part split symplectic integrators. Application to the disordered discrete nonlinear Schrödinger 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:

$$\begin{align*}
\dot{x} &= p_x \\
\dot{y} &= p_y \\
\dot{p}_x &= -x - 2xy \\
\dot{p}_y &= y^2 - x^2 - y
\end{align*}$$

Variational equations:

$$\begin{align*}
\dot{\delta x} &= \delta p_x \\
\dot{\delta y} &= \delta p_y \\
\dot{\delta p}_x &= -(1 + 2y) \delta x - 2x \delta y \\
\dot{\delta p}_y &= -2x \delta x + (-1 + 2y) \delta y
\end{align*}$$
Symplectic Integrators (SIs)

Formally the solution of the Hamilton equations of motion can be written as:

\[
\frac{d\vec{X}}{dt} = \{H, \vec{X}\} = L_H \dot{X} \Rightarrow \dot{X}(t) = \sum_{n \geq 0} \frac{t^n}{n!} L^n_H \ddot{X} = e^{tL_H} \ddot{X}
\]

where $\dot{X}$ 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

\[
e^{\tau L_H} = e^{\tau(L_A + L_B)} = \prod_j e^{c_j \tau L_A} e^{d_j \tau L_B} + O(\tau^{n+1})
\]

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\(_2\)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.
Tangent Map (TM) Method


The Hénon-Heiles system can be split as:

\[
\begin{align*}
\dot{x} &= p_x \\
\dot{y} &= p_y \\
\dot{p}_x &= -x - 2xy \\
\dot{p}_y &= y^2 - x^2 - y
\end{align*}
\]

\[
\begin{align*}
A(\vec{p}) &\rightarrow \dot{\vec{u}} = \frac{1}{2}(p_x^2 + p_y^2) \\
B(\vec{q}) &\rightarrow \dot{\vec{u}} = L_{AV} \vec{u} \Rightarrow e^{\tau L_{AV}} \\
\Rightarrow \frac{d\vec{u}}{dt} = L_{BV} \vec{u} \Rightarrow e^{\tau L_{BV}} : \\
\begin{align*}
x' &= x + p_x \tau \\
y' &= y + p_y \tau \\
p_x' &= p_x \\
p_y' &= p_y \\
\delta x' &= \delta x + \delta p_x \tau \\
\delta y' &= \delta y + \delta p_y \tau \\
\delta p_x' &= \delta p_x \\
\delta p_y' &= \delta p_y
\end{align*}
\]
Interplay of disorder and nonlinearity


Waves in nonlinear disordered media – localization or delocalization?


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

**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 \( \varepsilon_l \) 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

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

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

Second moment:

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

Different spreading regimes
KG: Lyapunov Exponents

Individual runs
Linear case
E=0.4, W=4

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

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

with a corrector term which corresponds to the Hamiltonian function:

\[ C = \sum_{l=1}^{N} \left[ u_l (\tilde{\epsilon}_l + u_l^2) - \frac{1}{W} (u_{l-1} + u_{l+1} - 2u_l) \right]^2. \]
The DNLS model

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

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

\[ H_D = \sum_{l} \left( \frac{\varepsilon_l}{2} (q_l^2 + p_l^2) + \frac{\beta}{8} (q_l^2 + p_l^2)^2 \right) - q_{n}q_{n+1} - p_{n}p_{n+1} \]

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

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

Symplectic Integrators produced by Successive Splits (SS)

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

Using the SABA_2 integrator we get a 2^{nd} order integrator with 13 steps, SS^2:

\[ \tau' = \tau / 2 \]

\[ \tau = \frac{(3-\sqrt{3})}{6} \]

\[ \tau' = \frac{\sqrt{3}\tau}{6} \]

\[ \tau' = \frac{(3-\sqrt{3})}{6} \]

\[ \tau' = \frac{\sqrt{3}\tau'}{6} \]
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.

Three part split symplectic integrators for the DNLS model

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

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

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

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

\[ \text{ABC}^2 \quad \tau = 0.005 \]
\[ \text{SS}^2 \quad \tau = 0.02 \]
\[ \text{DOP853} \quad \delta = 10^{-16} \]
\[ \text{SIFT}^2 \quad \tau = 0.05 \]

- \( E_r \): relative energy error
- \( S_r \): relative norm error
- \( T_c \): CPU time (sec)

Composition Methods: 4\textsuperscript{th} order SIs

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

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

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

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


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

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

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

SIFT\textsuperscript{4} \(\tau=0.125\)
SIFT\textsuperscript{2} \(\tau=0.05\)
ABC\textsuperscript{4}[S] \(\tau=0.1\)
SS\textsuperscript{4} \(\tau=0.1\)
ABC\textsuperscript{4}[Y] \(\tau=0.05\)

\(E_r\): relative energy error
\(S_r\): relative norm error
\(T_c\): CPU time (sec)

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 2\textsuperscript{nd} order ABC\textsuperscript{2} integrator.

\[
\begin{align*}
\text{ABC}_6^{[\text{KL}]} & \quad \text{with 37 steps} \\
\text{ABC}_6^{[\text{SS}]} & \quad \text{with 45 steps} \\
\text{ABC}_8^{[\text{Y}]} & \quad \text{with 61 steps} \\
\text{ABC}_8^{[\text{KL}]} & \quad \text{with 69 steps} \\
\text{ABC}_8^{[\text{SS}]} & \quad \text{with 77 steps} \\
\text{ABC}_{10}^{[\text{SS}]} & \quad \text{with 125 steps}
\end{align*}
\]
High order integrators: Numerical results (I)

\[ SS^4_{864} \tau = 0.015625 \]

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

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

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

\[ E_r: \text{relative energy error} \]

\[ S_r: \text{relative norm error} \]

\[ T_c: \text{CPU time (sec)} \]

High order integrators: Numerical results (II)

\[ \text{ABC}^8_{[Y]} \quad \tau=0.0625 \]
\[ \text{ABC}^6_{[SS]} \quad \tau=0.125 \]
\[ \text{ABC}^{10}_{[SS]} \quad \tau=0.2 \]
\[ \text{ABC}^8_{[KL]} \quad \tau=0.125 \]
\[ \text{ABC}^8_{[SS]} \quad \tau=0.2 \]

\( E_r: \) relative energy error
\( S_r: \) relative norm error
\( T_c: \) CPU time (sec)

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.
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Thank you for your attention