

# **Efficient integration techniques for the long time simulation of the disordered discrete nonlinear Schrödinger equation**

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# Outline

- **Symplectic Integrators – Tangent Map Method**
- **Disordered lattices and their dynamical behavior**
- **Different 2-part and 3-part split symplectic integrators for the disordered discrete nonlinear Schrödinger equation (DNLS)**
- **Summary**

# 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:

$$H_2 = \frac{1}{2}(p_x^2 + p_y^2) + \frac{1}{2}(x^2 + y^2) + x^2y - \frac{1}{3}y^3$$

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:

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

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  $t+\tau$**  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<sub>2</sub>C

The operator  $e^{\tau L_H}$  can be approximated by the symplectic integrator [Laskar & Robutel, Cel. Mech. Dyn. Astr. (2001)]:

$$S A B A_2 = e^{c_1 \tau L_A} e^{d_1 \tau L_B} e^{c_2 \tau L_A} e^{d_1 \tau L_B} e^{c_1 \tau L_A}$$

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<sub>2</sub> = C (SABA<sub>2</sub>) 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 [Ch.S. & Gerlach, PRE (2010) – Gerlach & Ch.S., Discr. Cont. Dyn. Sys. (2011) – Gerlach et al., IJBC (2012)].

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

$$\begin{array}{l}
 \dot{x} = p_x \\
 \dot{y} = p_y \\
 \dot{p}_x = -x - 2xy \\
 \dot{p}_y = y^2 - x^2 - y \\
 \dot{\delta x} = \delta p_x \\
 \dot{\delta y} = \delta p_y \\
 \dot{\delta p}_x = -(1 + 2y)\delta x - 2x\delta y \\
 \dot{\delta p}_y = -2x\delta x + (-1 + 2y)\delta y
 \end{array}
 \xrightarrow{A(\vec{p})}
 \left. \begin{array}{l}
 \dot{x} = p_x \\
 \dot{y} = p_y \\
 \dot{p}_x = 0 \\
 \dot{p}_y = 0 \\
 \dot{\delta x} = \delta p_x \\
 \dot{\delta y} = \delta p_y \\
 \dot{\delta p}_x = 0 \\
 \dot{\delta p}_y = 0
 \end{array} \right\} \Rightarrow \frac{d\vec{u}}{dt} = L_{AV}\vec{u} \Rightarrow e^{\tau L_{AV}} : \left\{ \begin{array}{l}
 x' = x + p_x\tau \\
 y' = y + p_y\tau \\
 px' = p_x \\
 py' = p_y \\
 \delta x' = \delta x + \delta p_x\tau \\
 \delta y' = \delta y + \delta p_y\tau \\
 \delta p'_x = \delta p_x \\
 \delta p'_y = \delta p_y
 \end{array} \right.$$
  

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

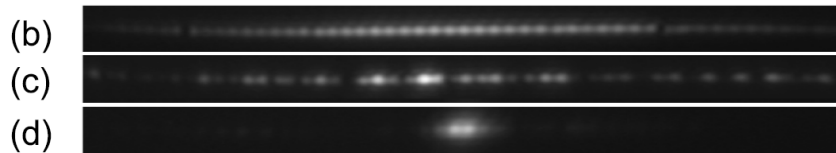
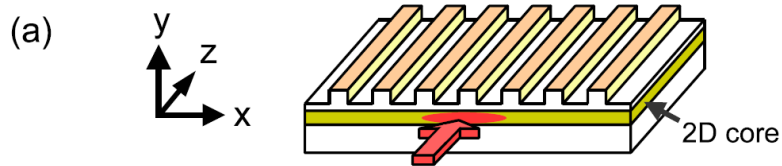
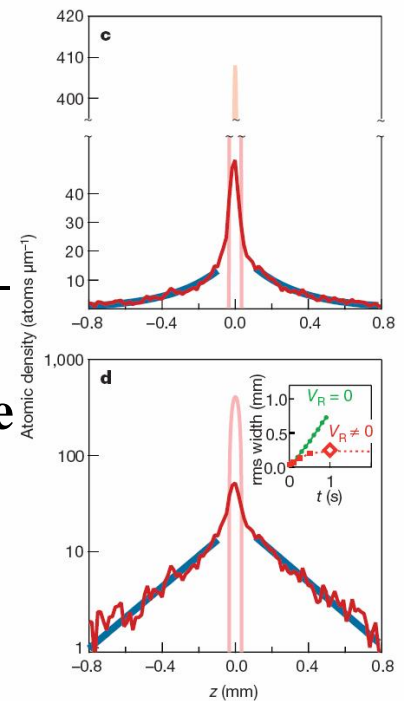
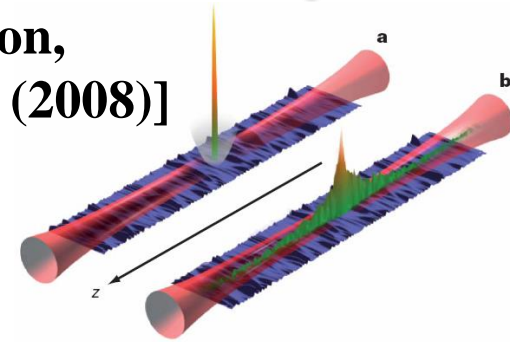
# Interplay of disorder and nonlinearity

**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) – Lapytyeva 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

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

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)  $A_{v,l}$  - 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:

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

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

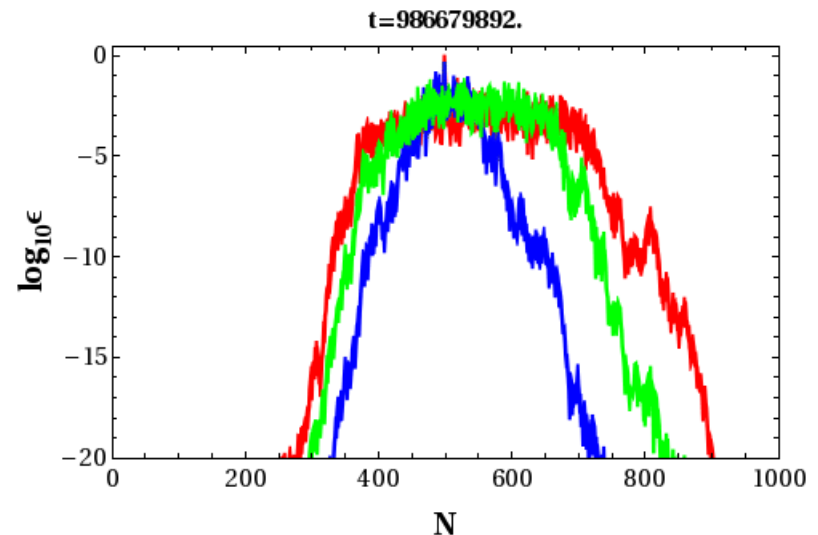
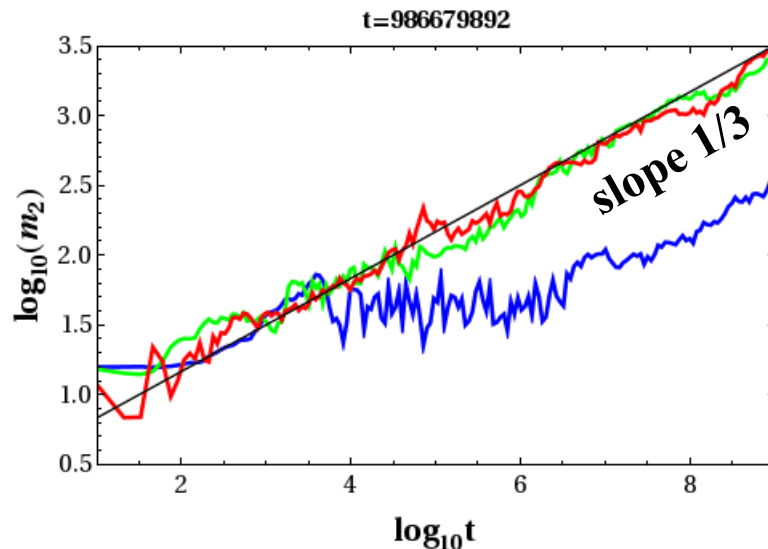
We consider normalized **energy distributions** in normal mode (NM) space

$$z_v \equiv \frac{E_v}{\sum_m E_m} \quad \text{with} \quad E_v = \frac{1}{2} \left( \dot{A}_v^2 + \omega_v^2 A_v^2 \right) , \quad \text{where } A_v \text{ is the amplitude}$$

of the  $v$ th NM.

**Second moment:** 
$$m_2 = \sum_{v=1}^N (v - \bar{v})^2 z_v \quad \text{with} \quad \bar{v} = \sum_{v=1}^N v z_v$$

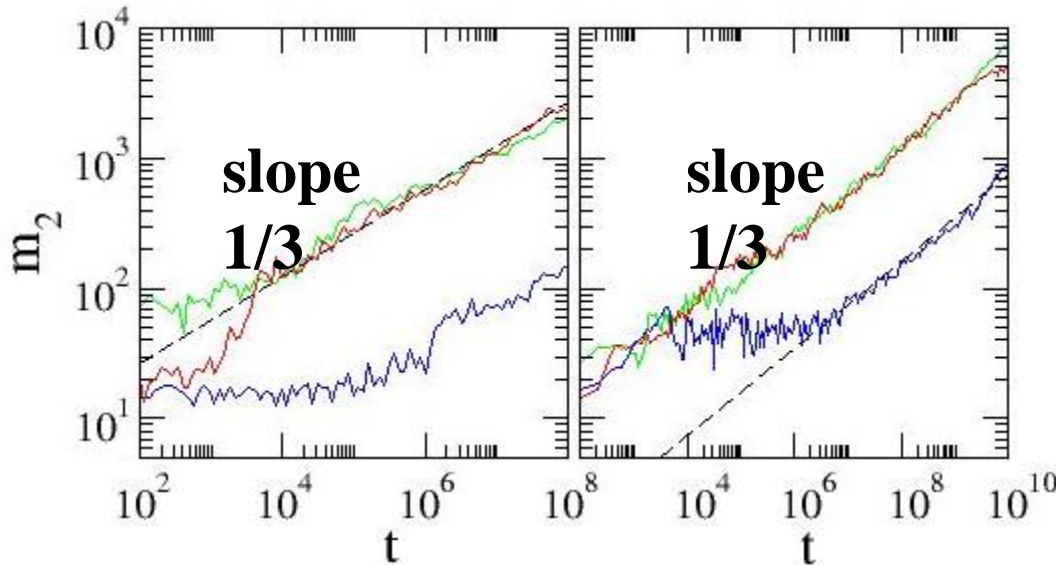
## Different spreading regimes



# Different spreading regimes

Single site excitations  $\alpha=1/3$

**DNLS**  $W=4$ ,  $\beta=$  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  $\alpha=1/3$  or  $\alpha=1/2$ , 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)**

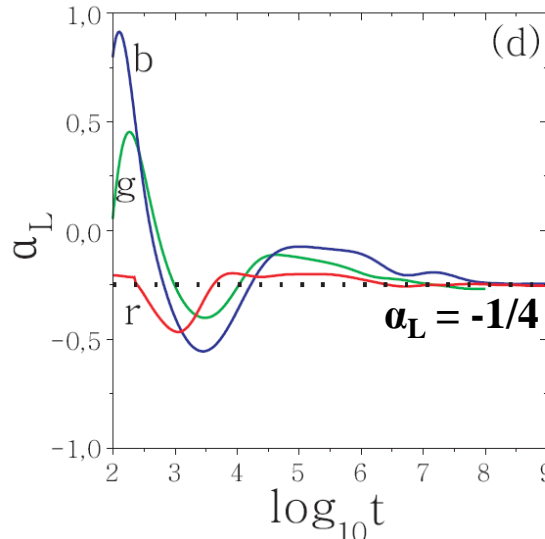
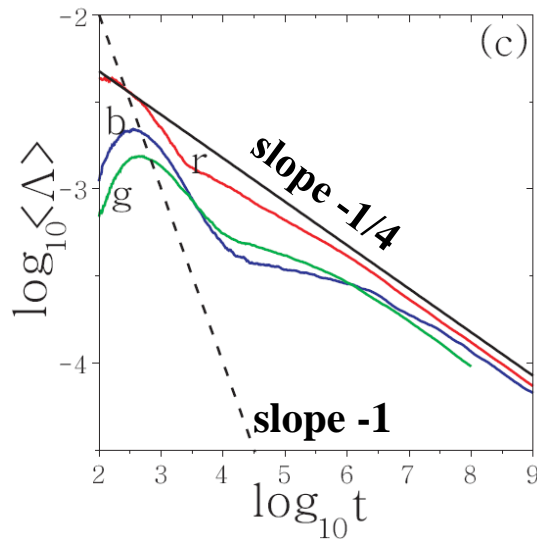
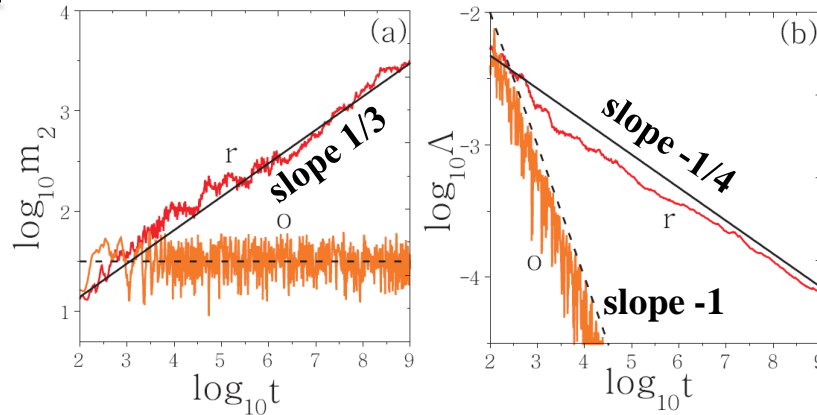
**Bodyfelt, Laptyeva, Ch.S., Krimer, Flach S., PRE (2011)**

# KG: Lyapunov Exponents

**Individual runs**

**Linear case**

**E=0.4, W=4**



$$\alpha_L = \frac{d(\log \langle \Lambda \rangle)}{d \log t}$$

**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.Ch. et al. PRL (2013)**


# The KG model

We apply the **SABAC<sub>2</sub>** integrator scheme to the KG Hamiltonian by using the **splitting**:

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



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



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

with a **corrector term** which corresponds to the Hamiltonian function:

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

# The DNLS model

How can we use Symplectic Integrators for the DNLS model?

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

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

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

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

$$e^{\tau L_B} : (\mathbf{q}', \mathbf{p}')^T = \mathbf{C}(\tau) \cdot (\mathbf{q}, \mathbf{p})^T$$

# Evaluation of the $\mathbf{C}(\tau)$ matrix

The equations of motion for the Hamiltonian B can be written as:

$$\dot{\mathbf{x}}^T = \begin{pmatrix} \mathbf{0} & \mathbf{A} \\ -\mathbf{A} & \mathbf{0} \end{pmatrix} \mathbf{x}^T \quad \text{with} \quad \mathbf{A} = \begin{pmatrix} 0 & -1 & 0 & \dots & 0 & 0 \\ -1 & 0 & -1 & \dots & 0 & 0 \\ 0 & -1 & 0 & \dots & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & \dots & 0 & -1 \\ 0 & 0 & 0 & \dots & -1 & 0 \end{pmatrix}$$

Then the matrix  $\mathbf{C}(\tau)$  is given by

$$\mathbf{C}(\tau) = \begin{pmatrix} \cos(\mathbf{A}\tau) & \sin(\mathbf{A}\tau) \\ -\sin(\mathbf{A}\tau) & \cos(\mathbf{A}\tau) \end{pmatrix}$$

$$\cos(\mathbf{A}\tau) = \sum_{k=0}^{\infty} \frac{(-1)^k}{(2k)!} \mathbf{A}^{2k} \tau^{2k}, \quad \sin(\mathbf{A}\tau) = \sum_{k=0}^{\infty} \frac{(-1)^k}{(2k+1)!} \mathbf{A}^{2k+1} \tau^{2k+1}.$$

The evaluation of the elements of matrices  $\cos(\mathbf{A}\tau)$  and  $\sin(\mathbf{A}\tau)$  can be obtained through the determination of the eigenvalues and eigenvectors of matrix A itself **(Gerlach, Meichsner, Ch.S., 2016, Eur. Phys. J. Sp. Top).**

# DNLS model: 2 part split SIs

Order 2: **Leap-frog** (3 steps)  $LF(\tau) = e^{\frac{\tau}{2}L_A} e^{\tau L_B} e^{\frac{\tau}{2}L_A}$   
**SABA<sub>2</sub>** (5 steps)

Order 4: **Yoshida**, 1990, Phys. Lett. A (7 steps)

$$S^4(\tau) = e^{c_1 \tau L_A} e^{d_1 \tau L_B} e^{c_2 \tau L_A} e^{d_2 \tau L_B} e^{c_2 \tau L_A} e^{d_1 \tau L_B} e^{c_1 \tau L_A},$$

with  $c_1 = \frac{1}{2(2-2^{1/3})}$ ,  $c_2 = \frac{1-2^{1/3}}{2(2-2^{1/3})}$ ,  $d_1 = \frac{1}{2-2^{1/3}}$ ,  $d_2 = -\frac{2^{1/3}}{2-2^{1/3}}$ .

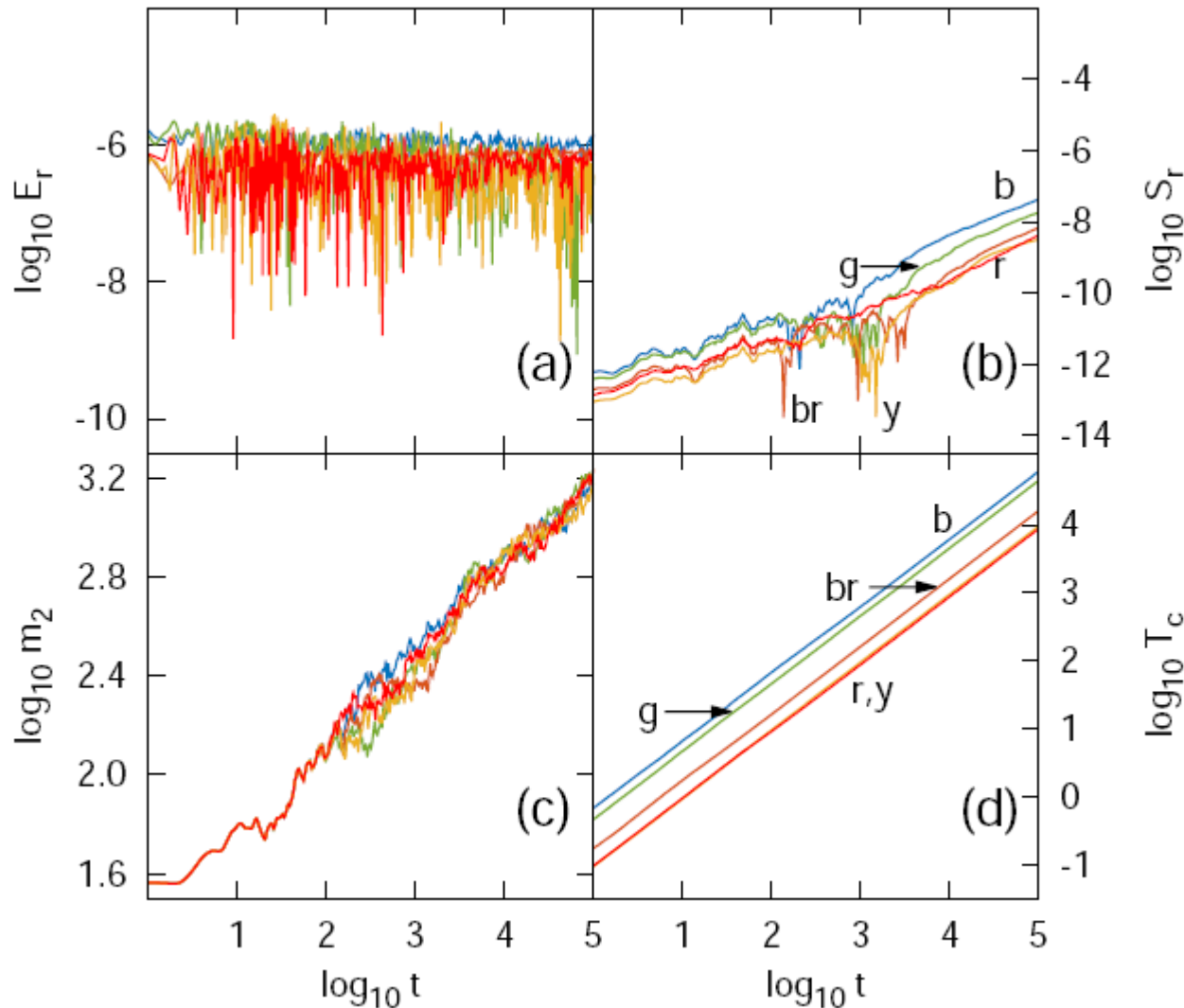
**ABA864** [Blanes et al., 2013, App. Num. Math.] (15 steps)

Order 6: Using the composition method refereed as ‘solution A’ in [Yoshida, 1990, Phys. Lett. A] we construct the 6th order symplectic integrator **S<sup>6</sup>** having 29 steps

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

where  $S^2$  is the SABA<sub>2</sub> integrator, while the values of  $w_0, w_1, w_2, w_3$  can be found in [Yoshida, 1990, Phys. Lett. A]

# 2 part split SIs: Numerical results



$N=1000, W=4, \beta=0.72, H_D=-28.5$

LF  $\tau=0.0025$

SABA<sub>2</sub>  $\tau=0.01$

S<sup>4</sup>  $\tau=0.05$

ABA864  $\tau=0.175$

S<sup>6</sup>  $\tau=0.25$

$E_r$ : relative energy error

$S_r$ : relative norm error

$T_c$ : CPU time (sec)

Gerlach, Meichsner,  
Ch.S., 2016, Eur. Phys.  
J. Sp. Top.



# DNLS model: 3 part split SIs

Symplectic Integrators produced by **Successive Splits (SS)**

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

$$\left\{ \begin{array}{l} q'_l = q_l \cos(\alpha_l \tau) + p_l \sin(\alpha_l \tau), \\ p'_l = p_l \cos(\alpha_l \tau) - q_l \sin(\alpha_l \tau), \end{array} \right\} \begin{array}{l} \left\{ \begin{array}{l} q'_l = q_l, \\ p'_l = p_l + (q_{l-1} + q_{l+1})\tau \end{array} \right\} \left\{ \begin{array}{l} p'_l = p_l, \\ q'_l = q_l - (p_{l-1} + p_{l+1})\tau \end{array} \right\} \end{array}$$

Using the **SABA<sub>2</sub>** integrator we get a **2<sup>nd</sup> order integrator with 13 steps, SS<sup>2</sup>:**

$$SS^2 = e^{\left[ \frac{(3-\sqrt{3})}{6} \tau \right] L_A} \underbrace{e^{\frac{\tau}{2} L_B}}_{\mathbf{B}_1} e^{\frac{\sqrt{3}\tau}{3} L_A} \underbrace{e^{\frac{\tau}{2} L_B}}_{\mathbf{B}_2} e^{\left[ \frac{(3-\sqrt{3})}{6} \tau \right] L_A}$$

$$\tau' = \tau / 2 \quad \underbrace{e^{\left[ \frac{(3-\sqrt{3})}{6} \tau' \right] L_{B_1}} e^{\frac{\tau'}{2} L_{B_2}} e^{\frac{\sqrt{3}\tau'}{3} L_{B_1}} e^{\frac{\tau'}{2} L_{B_2}}}_{\mathbf{B}_1} e^{\left[ \frac{(3-\sqrt{3})}{6} \tau' \right] L_{B_1}}}_{\mathbf{B}_1} \underbrace{e^{\left[ \frac{(3-\sqrt{3})}{6} \tau' \right] L_{B_1}} e^{\frac{\tau'}{2} L_{B_2}} e^{\frac{\sqrt{3}\tau'}{3} L_{B_1}} e^{\frac{\tau'}{2} L_{B_2}}}_{\mathbf{B}_2} e^{\left[ \frac{(3-\sqrt{3})}{6} \tau' \right] L_{B_1}}}_{\mathbf{B}_2}$$

# DNLS model: 3 part split SIs

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

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

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

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

# DNLS model: 3 part split SIs

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

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

In this way, starting with the 2<sup>nd</sup> order integrators  $SS^2$  and  $ABC^2$  we construct the 4<sup>th</sup> order integrators:

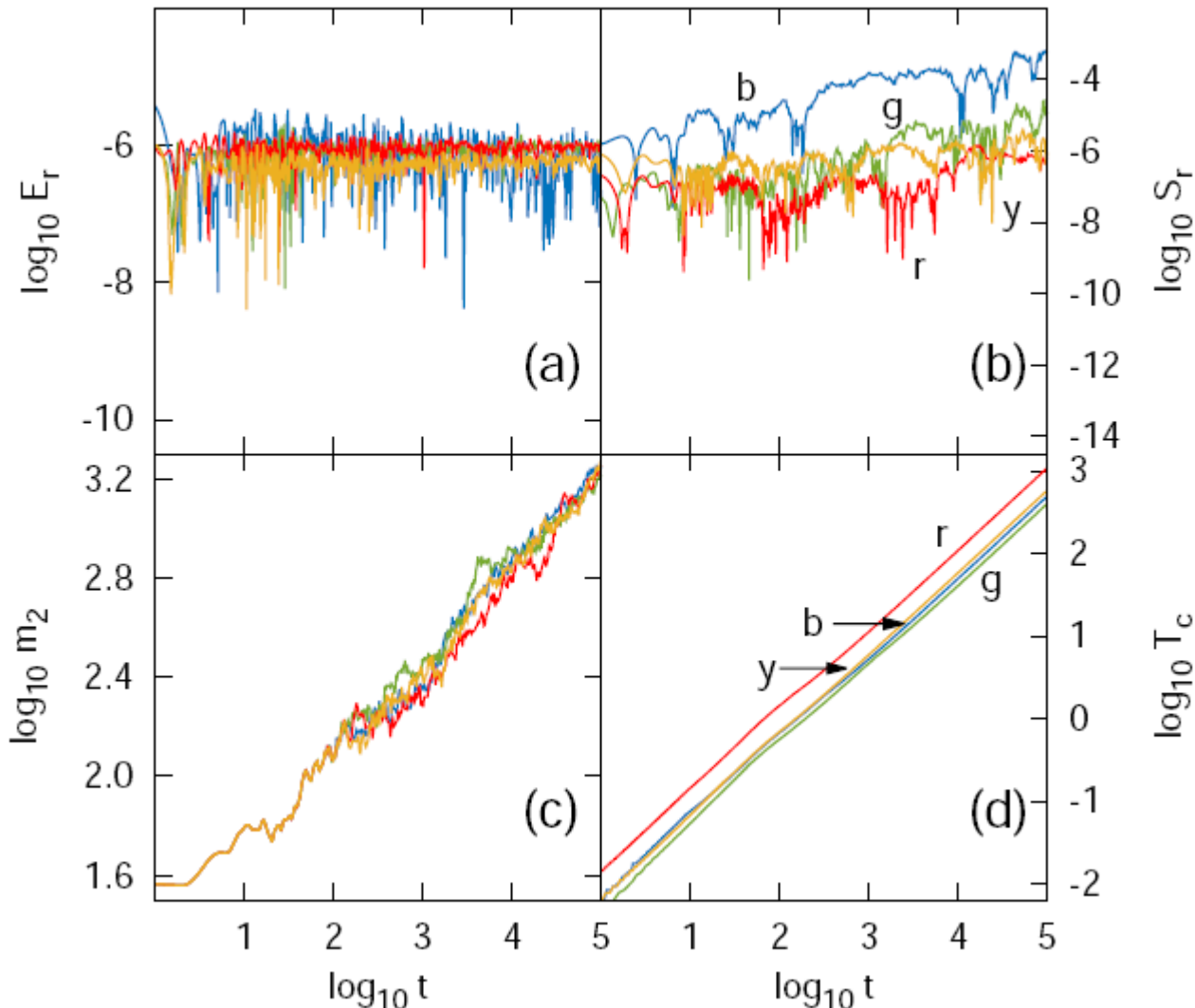
**$SS^4$**  with 37 steps

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

Using the ABAH864 integrator [Blanes et al., 2013, App. Num. Math.], where the B part is integrated by the  $SABA_2$  scheme, we construct the 4th order integrator:  **$SS^4_{864}$**  integrator with 49 steps.

**Order 6:** Using the composition method proposed in [Sofroniou & Spaletta, 2005, Optim. Methods Softw.] we construct the 6th order symplectic integrator  **$ABC^6_{[SS]}$**  with 45 steps.

# 3 part split SIs: Numerical results



$N=1000, W=4, \beta=0.72, H_D=-28.5$

$ABC^4_{[Y]} \tau=0.05$

$SS^4 \tau=0.05$

$SS^4_{864} \tau=0.125$

$ABC^6_{[SS]} \tau=0.225$

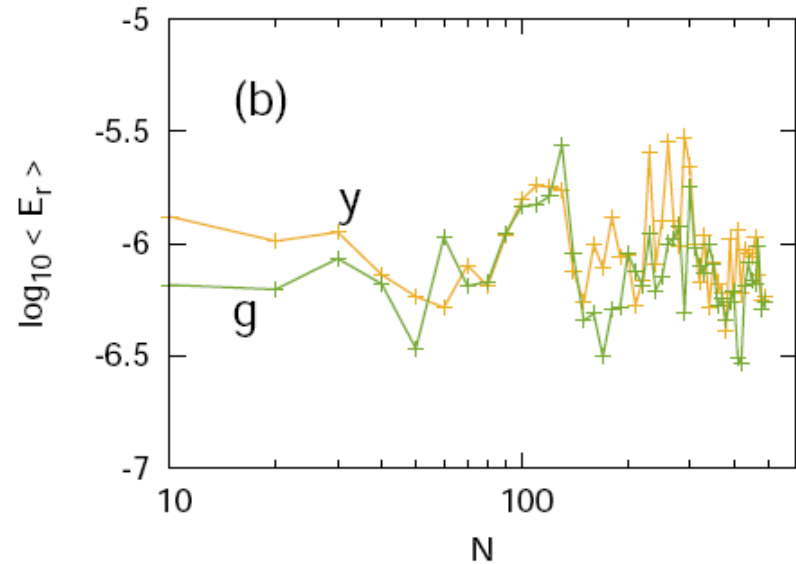
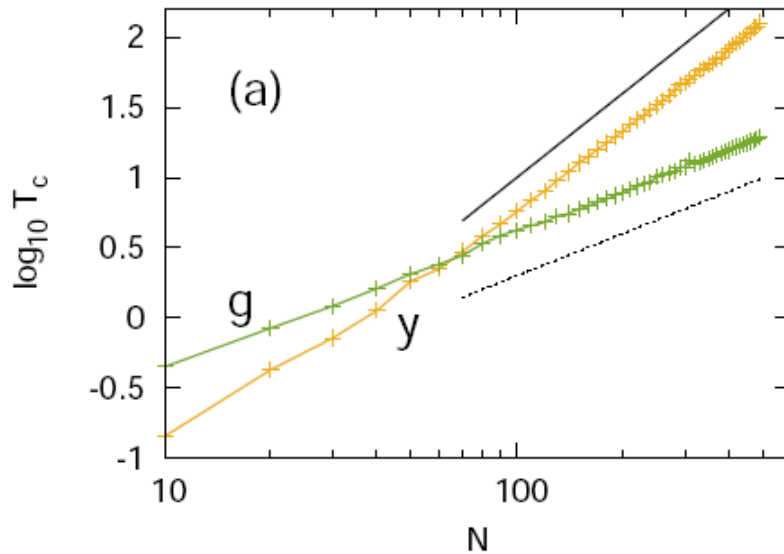
$E_r$ : relative energy error

$S_r$ : relative norm error

$T_c$ : CPU time (sec)

Gerlach, Meichsner,  
Ch.S., 2016, Eur. Phys.  
J. Sp. Top.

# 2 and 3 part split SIs: Comparing their efficiency



Best 2 part split: **ABA864**  $\tau=0.125$

Best 3 part split: **ABC<sup>6</sup><sub>[SS]</sub>**  $\tau=0.225$

$N$  = number of sites,  $t = 10^4$

$E_r$ : relative energy error,  $T_c$ : CPU time (sec)

# Summary

- We presented several efficient symplectic integration methods suitable for the integration of the DNLS model, which are based on 2 and 3 part split of the Hamiltonian.
  - ✓ 2 part split methods preserve better the second integral of the system (i.e. the norm)
  - ✓ For small lattices ( $N \lesssim 70$ ) 2 part split methods are computationally more efficient, while for larger lattice 3 part split method should be used.

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# Chaos Detection and Predictability

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