Numerical tools for investigating the dynamics of Hamiltonian systems

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Outline

- **Application of the Generalized ALignment Index (GALI) method of chaos detection to time dependent Hamiltonians**
  - ✓ **Definition of the GALI**
  - ✓ **Behavior of the GALI for chaotic and regular motion**
  - ✓ **Application to a time dependent galactic potential**

- **Symplectic integration schemes for the disordered discrete nonlinear Schrödinger equation (DNLS)**
  - ✓ **Disordered lattices and their dynamical behavior**
  - ✓ **Different 2-part and 3-part spilt symplectic integrators**

- **Summary**

Autonomous Hamiltonian systems

Consider an **N degree of freedom** autonomous Hamiltonian system having a Hamiltonian function of the form:

$$\underbrace{H(q_1, q_2, \ldots, q_N}_{\text{positions}}, \underbrace{p_1, p_2, \ldots, p_N)}_{\text{momenta}}$$

The time evolution of an orbit (trajectory) with initial condition

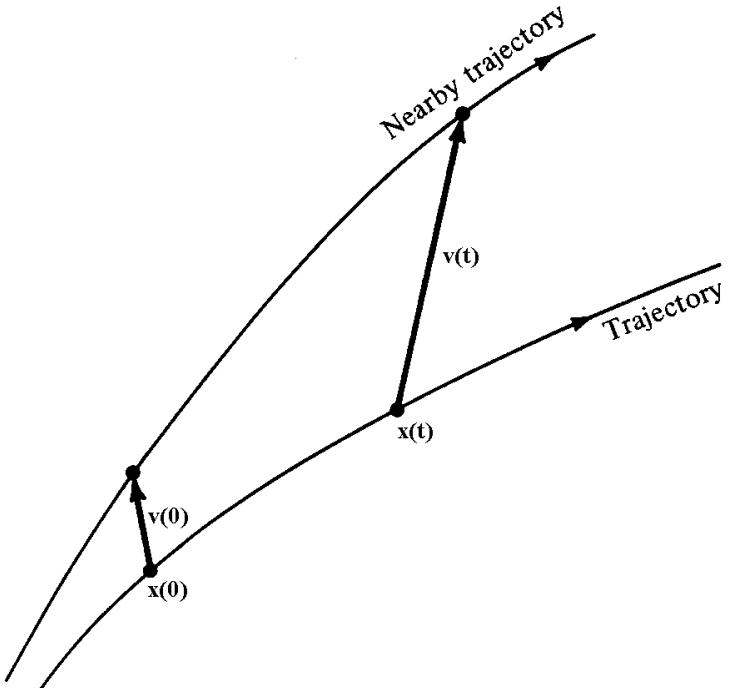$$P(0) = (q_1(0), q_2(0), \ldots, q_N(0), p_1(0), p_2(0), \ldots, p_N(0))$$

is governed by the **Hamilton's equations of motion**

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

Variational Equations

We use the notation $\mathbf{x} = (q_1, q_2, \ldots, q_N, p_1, p_2, \ldots, p_N)^T$. The **deviation vector** from a given orbit is denoted by

$$\mathbf{v} = (\delta x_1, \delta x_2, \ldots, \delta x_n)^T \text{, with } n = 2N$$

The time evolution of **v** is given by the so-called **variational equations:**

$$\frac{d\mathbf{v}}{dt} = -\mathbf{J} \cdot \mathbf{P} \cdot \mathbf{v}$$

where

$$\mathbf{J} = \begin{pmatrix} \mathbf{0}_N & -\mathbf{I}_N \\ \mathbf{I}_N & \mathbf{0}_N \end{pmatrix} , \quad \mathbf{P}_{ij} = \frac{\partial^2 \mathbf{H}}{\partial \mathbf{x}_i \partial \mathbf{x}_j} \quad i, j = 1, 2, \ldots, n$$

Benettin & Galgani, 1979, in Laval and Gressillon (eds.), op cit, 93

Definition of GALI

In the case of an N degree of freedom Hamiltonian system or a 2N symplectic map we follow the evolution of

k deviation vectors with 2≤k≤2N,

and define (Ch.S., Bountis, Antonopoulos, 2007, Physica D) the Generalized Alignment Index (GALI) of order k :

$$GALI_k(t) = \left\| \hat{v}_1(t) \wedge \hat{v}_2(t) \wedge \ldots \wedge \hat{v}_k(t) \right\|$$

where

$$\hat{v}_1(t) = \frac{v_1(t)}{\left\| v_1(t) \right\|}$$

Behavior of GALI$_k$ for chaotic motion

GALI$_k$ ($2 \leq k \leq 2N$) tends exponentially to zero with exponents that involve the values of the first k largest Lyapunov exponents $\sigma_1, \sigma_2, \ldots, \sigma_k$:

$$GALI_k(t) \propto e^{-\left[(\sigma_1 - \sigma_2) + (\sigma_1 - \sigma_3) + \ldots + (\sigma_1 - \sigma_k)\right]t}$$
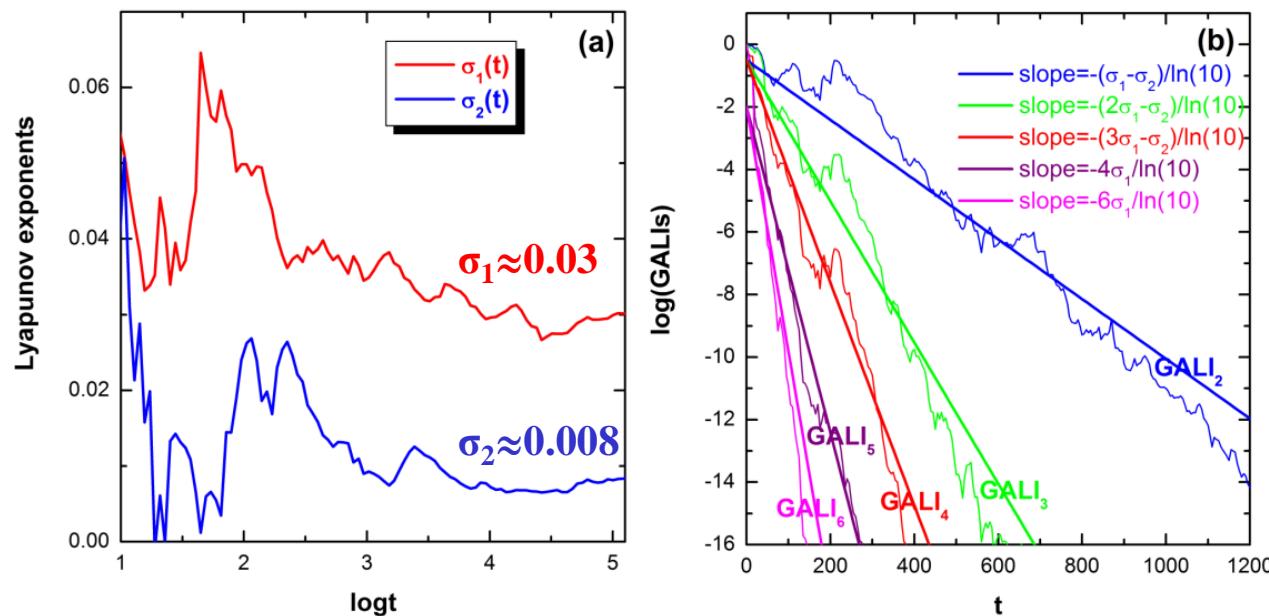
The above relation is valid even if some Lyapunov exponents are equal, or very close to each other.

Behavior of GALI$_k$ for chaotic motion

3D system:

$$H_3 = \sum_{i=1}^{3} \frac{\omega_i}{2}(q_i^2 + p_i^2) + q_1^2 q_2 + q_1^2 q_3$$

with $\omega_1 = 1$, $\omega_2 = \sqrt{2}$, $\omega_3 = \sqrt{3}$, $H_3 = 0.09$.

Behavior of GALI$_k$ for regular motion

If the motion occurs on an **s-dimensional torus with s≤N** then the behavior of GALI$_k$ is given by **(Ch.S., Bountis, Antonopoulos, 2008, Eur. Phys. J. Sp. Top.):**
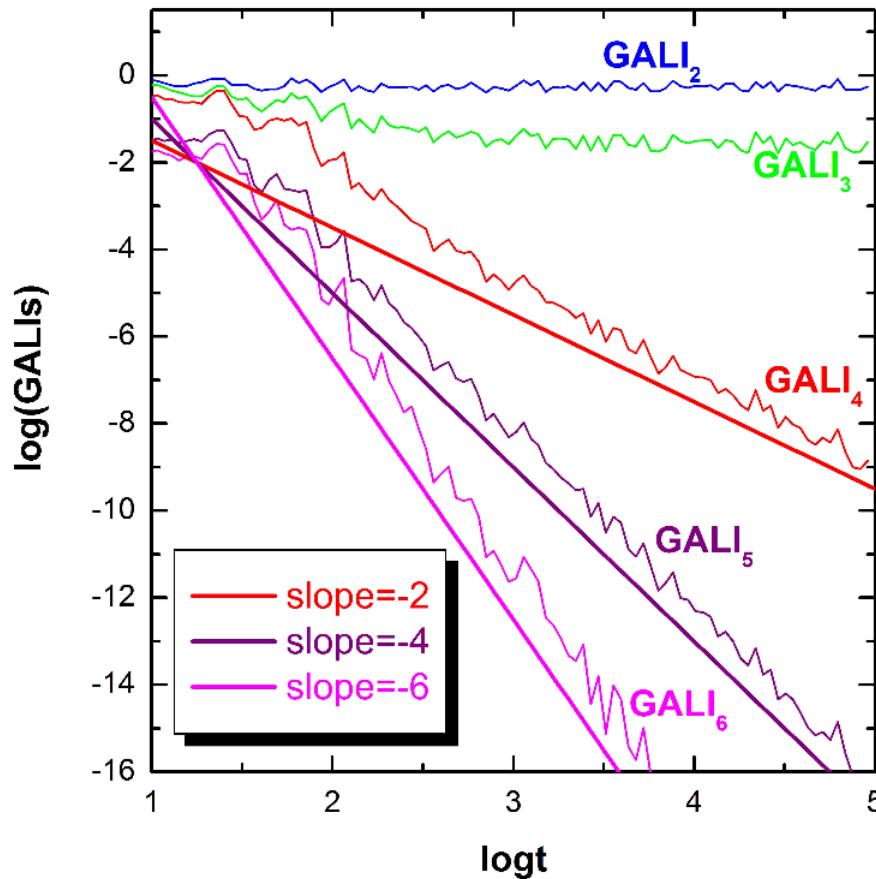
$$GALI_k(t) \propto \begin{cases} \text{constant} & \text{if} \quad 2 \leq k \leq s \\ \dfrac{1}{t^{k-s}} & \text{if} \quad s < k \leq 2N - s \\ \dfrac{1}{t^{2(k-N)}} & \text{if} \quad 2N - s < k \leq 2N \end{cases}$$

while in the **common case with s=N** we have :

$$GALI_k(t) \propto \begin{cases} \text{constant} & \text{if} \quad 2 \leq k \leq N \\ \dfrac{1}{t^{2(k-N)}} & \text{if} \quad N < k \leq 2N \end{cases}$$

Behavior of GALI_k for regular motion

3D Hamiltonian

Behavior of GALI$_k$

Chaotic motion:

GALI$_k \rightarrow 0$ exponential decay

$$GALI_k(t) \propto e^{-\left[(\sigma_1 - \sigma_2) + (\sigma_1 - \sigma_3) + ... + (\sigma_1 - \sigma_k)\right]t}$$

Regular motion:

GALI$_k \rightarrow$ constant $\neq 0$ or GALI$_k \rightarrow 0$ power law decay

$$GALI_k(t) \propto \begin{cases} \text{constant} & \text{if} \quad 2 \leq k \leq s \\[2mm] \dfrac{1}{t^{k-s}} & \text{if} \quad s < k \leq 2N - s \\[2mm] \dfrac{1}{t^{2(k-N)}} & \text{if} \quad 2N - s < k \leq 2N \end{cases}$$
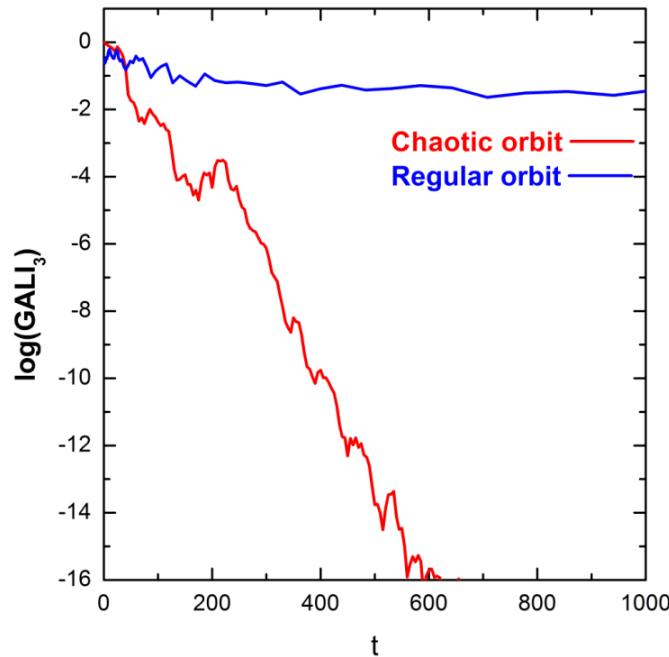
Global dynamics

- **GALI$_2$ (practically equivalent to the use of SALI)**
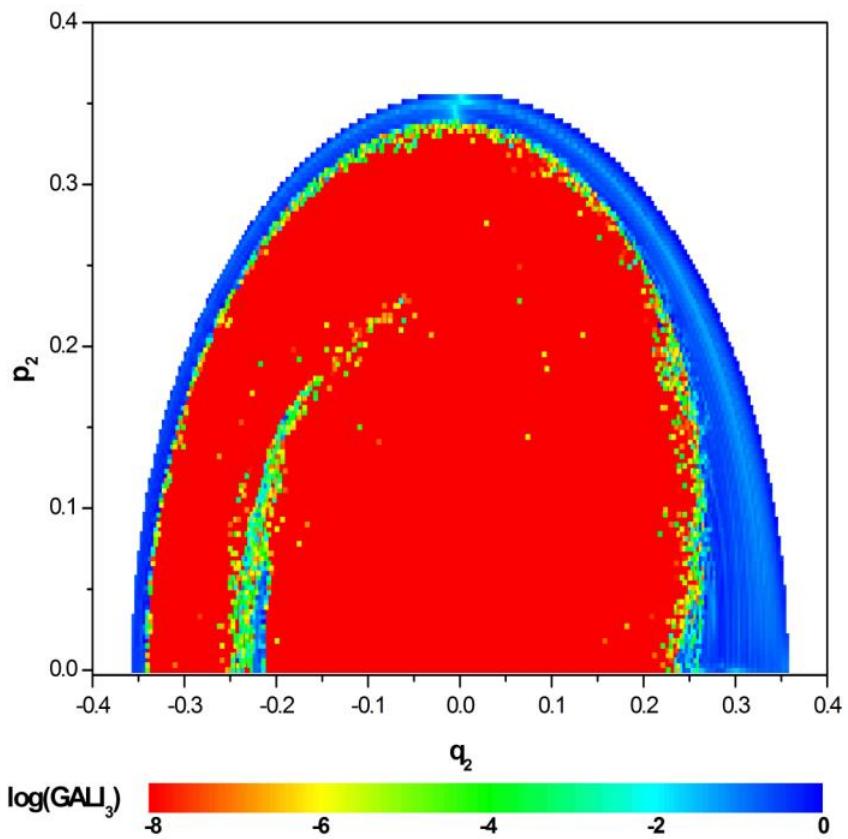
- **GALI$_N$**

Chaotic motion: GALI$_N$→0 (exponential decay)

Regular motion: GALI$_N$→constant≠0

3D Hamiltonian

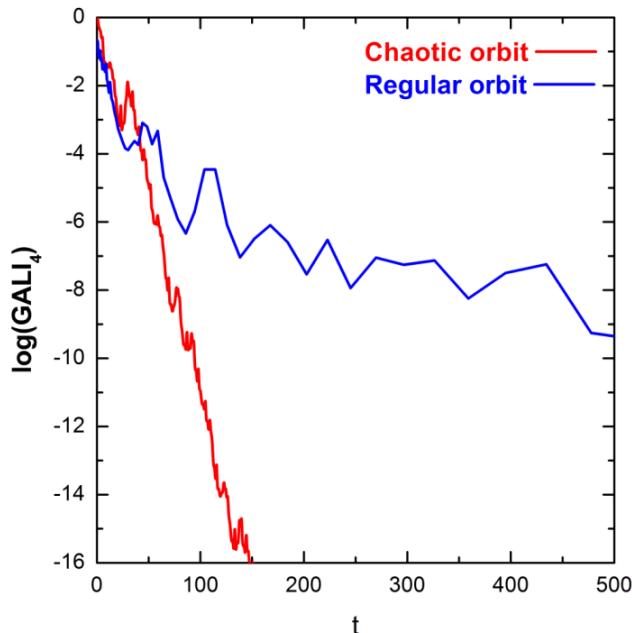**Subspace $q_3=p_3=0$, $p_2 \geq 0$ for t=1000.**
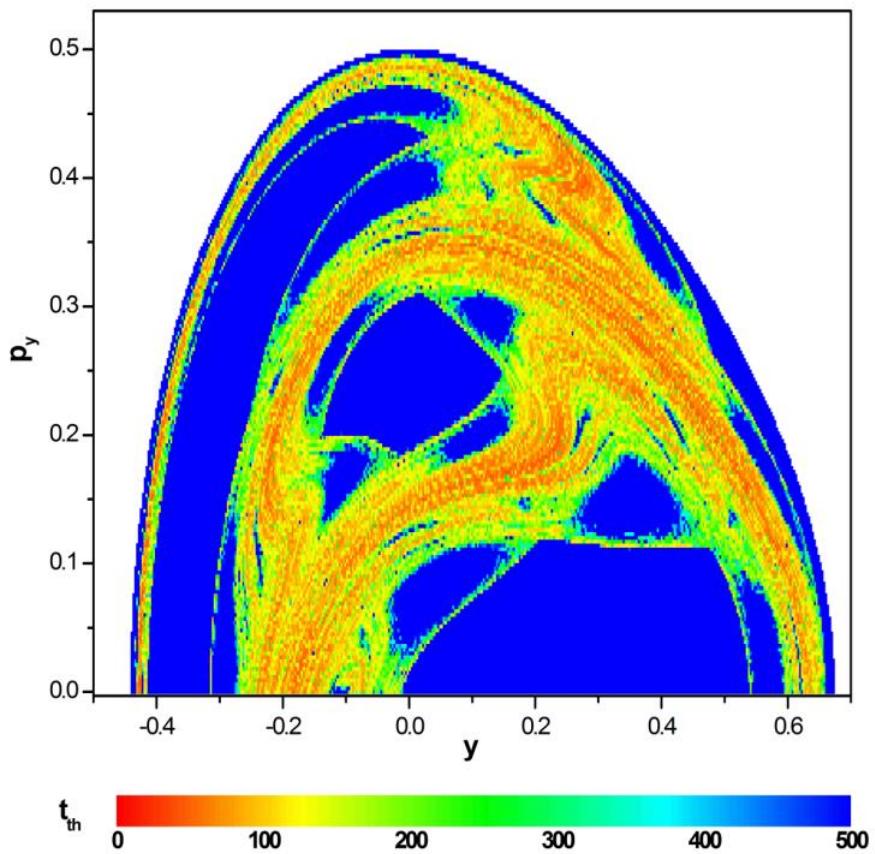
Global dynamics

GALI$_k$ with k>N

The index tends to zero both for regular and chaotic orbits but with completely different time rates:

Chaotic motion: exponential decay
Regular motion: power law

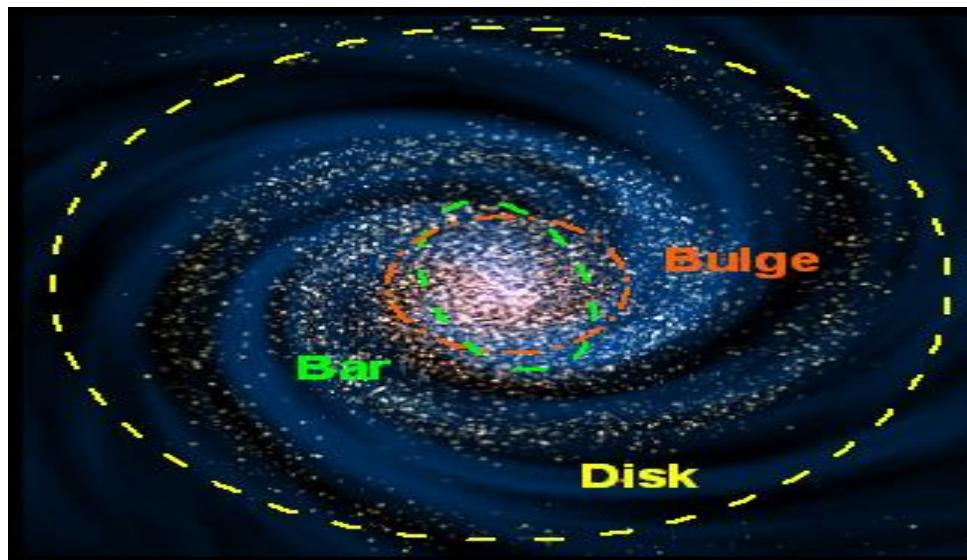**2D Hamiltonian (Hénon-Heiles)**
Time needed for GALI$_4$<10^{-12}

Barred galaxies

NGC 1433

NGC 2217

Bar

Bulge

Disk

Barred galaxy model

The 3D bar rotates around its short z-axis (x: long axis and y: intermediate). The Hamiltonian that describes the motion for this model is:

$$H = \frac{1}{2}(p_x^2 + p_y^2 + p_z^2) + V(x, y, z) - \Omega_b (x p_y - y p_x) \equiv Energy$$

This model consists of the superposition of potentials describing an **axisymmetric** part and a **bar** component of the galaxy **(Manos, Bountis, Ch.S., 2013, J. Phys. A).**

a) Axisymmetric component:

i) Plummer sphere:

$$V_{sphere}(x, y, z) = -\frac{GM_S}{\sqrt{x^2 + y^2 + z^2 + \varepsilon_s^2}}$$

ii) Miyamoto–Nagai disc:

$$V_{disc}(x, y, z) = -\frac{GM_D}{\sqrt{x^2 + y^2 + (A + \sqrt{B^2 + z^2})^2}}$$

b) Bar component: $V_{bar}(x, y, z) = -\pi G a b c \frac{\rho_c}{n+1} \int_\lambda^\infty \frac{du}{\Delta(u)} (1 - m^2(u))^{n+1},$

(Ferrers bar)

$where \; m^2(u) = \frac{x^2}{a^2 + u} + \frac{y^2}{b^2 + u} + \frac{z^2}{c^2 + u}, \; \Delta^2(u) = (a^2 + u)(b^2 + u)(c^2 + u),$

$$\boxed{\rho_c = \frac{105}{32\pi} \frac{GM_B}{abc}}$$

n: positive integer ($n = 2$ for our model) , λ: the unique positive solution of $m^2(\lambda) = 1$

Its density is: $\rho = \begin{cases} \rho_c (1 - m^2)^n, & \text{for } m \leq 1 \\ 0, & \text{for } m > 1 \end{cases}$, where $m^2 = \frac{x^2}{a^2} + \frac{y^2}{b^2} + \frac{z^2}{c^2}$, $a > b > c$ and $n = 2$.

Time-dependent barred galaxy model

The 3D bar rotates around its short *z*-axis (*x*: long axis and *y*: intermediate). The Hamiltonian that describes the motion for this model is:

$$H = \frac{1}{2}(p_x^2 + p_y^2 + p_z^2) + V(x, y, z, t) - \Omega_b(xp_y - yp_x) \equiv Energy$$

This model consists of the superposition of potentials describing an **axisymmetric** part and a **bar** component of the galaxy **(Manos, Bountis, Ch.S., 2013, J. Phys. A).**

a) Axisymmetric component:

$$M_S + M_B(t) + M_D(t) = 1, \quad \text{with} \quad M_B(t) = M_B(0) + \alpha t$$

i) Plummer sphere:

$$V_{sphere}(x, y, z) = -\frac{GM_S}{\sqrt{x^2 + y^2 + z^2 + \varepsilon_s^2}}$$

ii) Miyamoto–Nagai disc:

$$V_{disc}(x, y, z) = -\frac{GM_D(t)}{\sqrt{x^2 + y^2 + (A + \sqrt{B^2 + z^2})^2}}$$

b) Bar component:
$$V_{bar}(x, y, z) = -\pi Gabc\frac{\rho_c}{n+1}\int_\lambda^\infty \frac{du}{\Delta(u)}(1 - m^2(u))^{n+1},$$

(Ferrers bar)
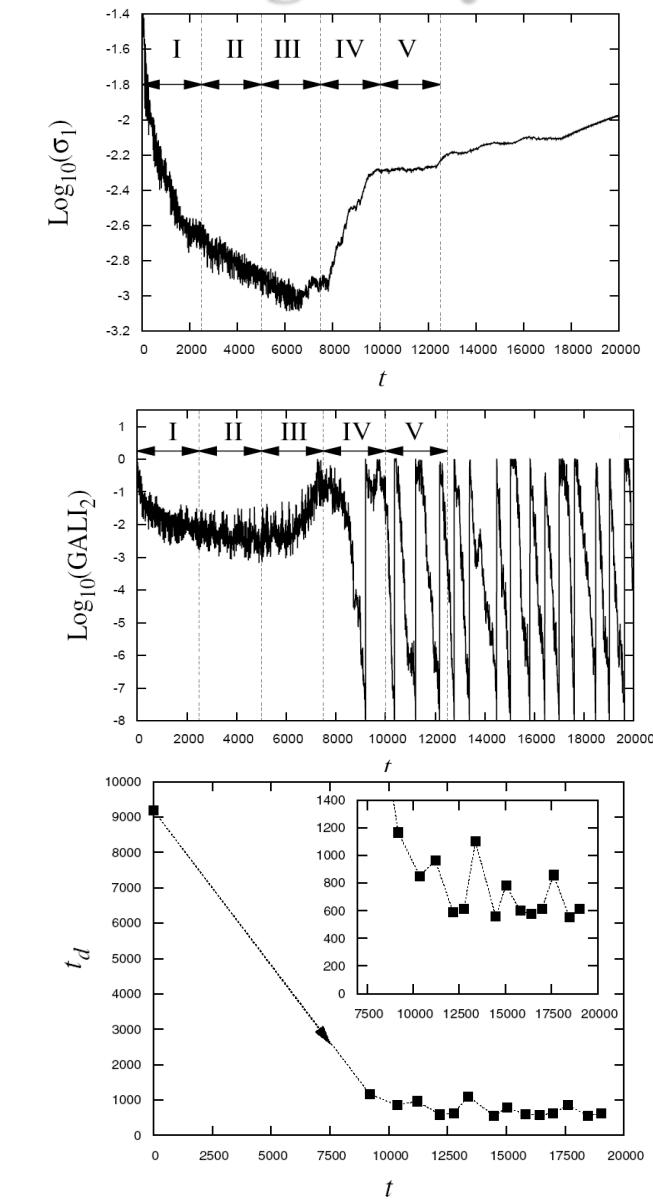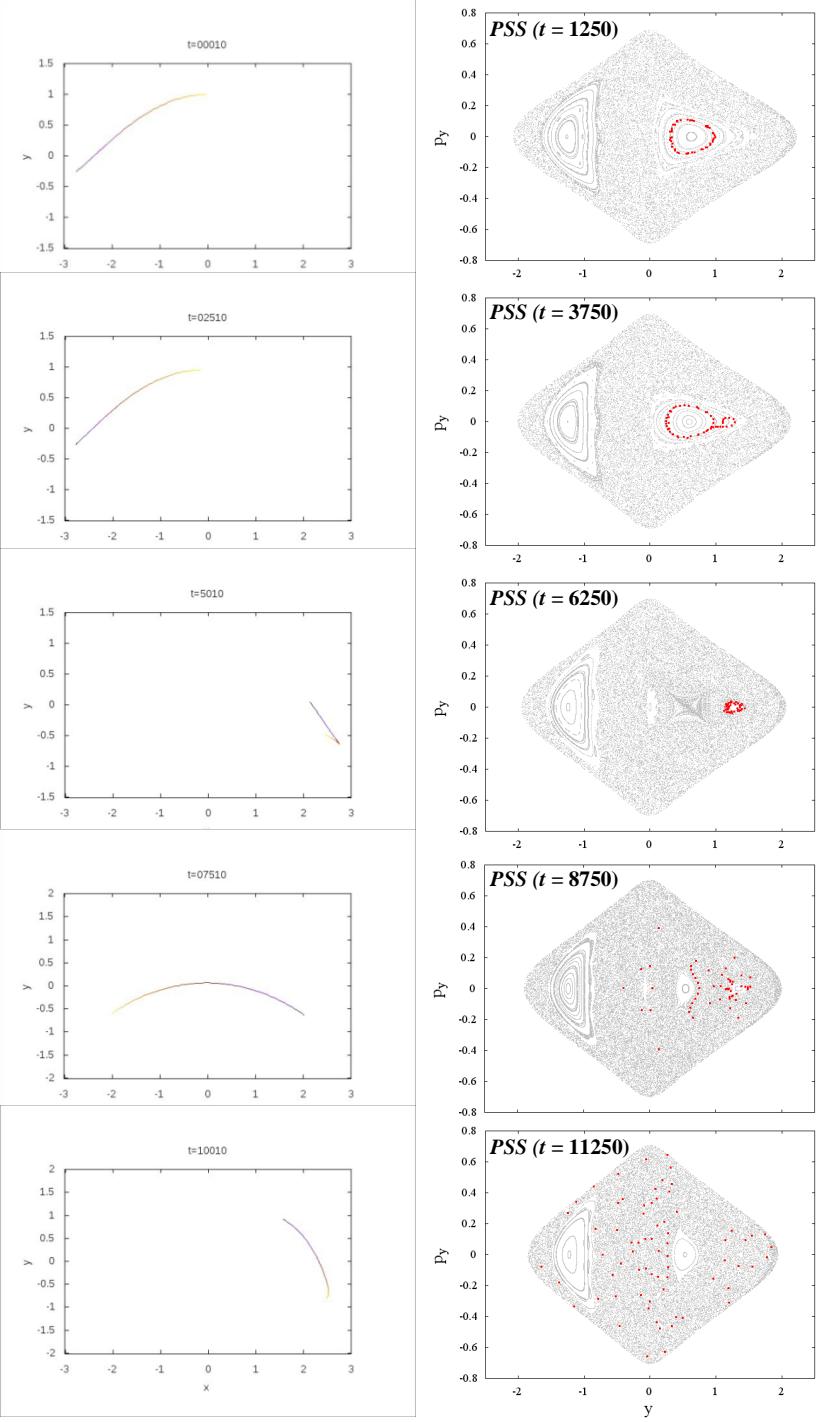
$$\rho_c = \frac{105}{32\pi}\frac{GM_B(t)}{abc}$$

where $m^2(u) = \frac{x^2}{a^2+u} + \frac{y^2}{b^2+u} + \frac{z^2}{c^2+u}$, $\Delta^2(u) = (a^2+u)(b^2+u)(c^2+u)$,

n: positive integer ($n = 2$ for our model), λ: the unique positive solution of $m^2(\lambda) = 1$

Its density is:
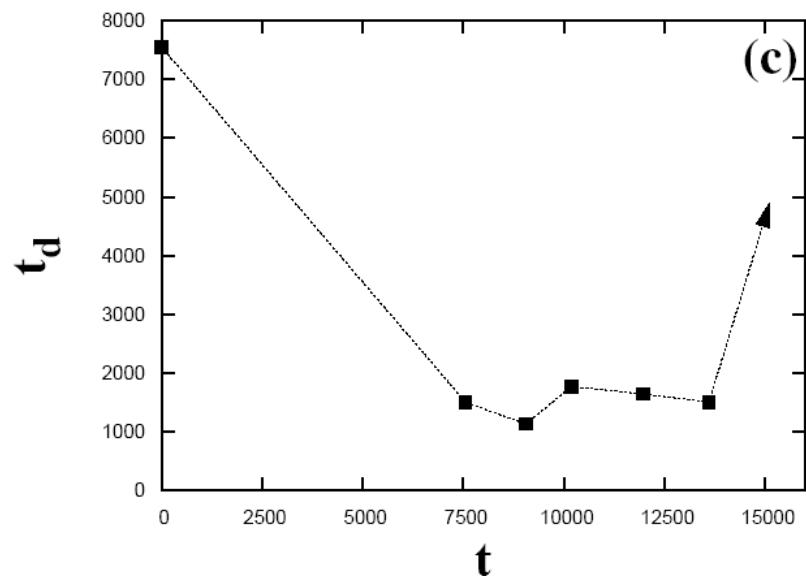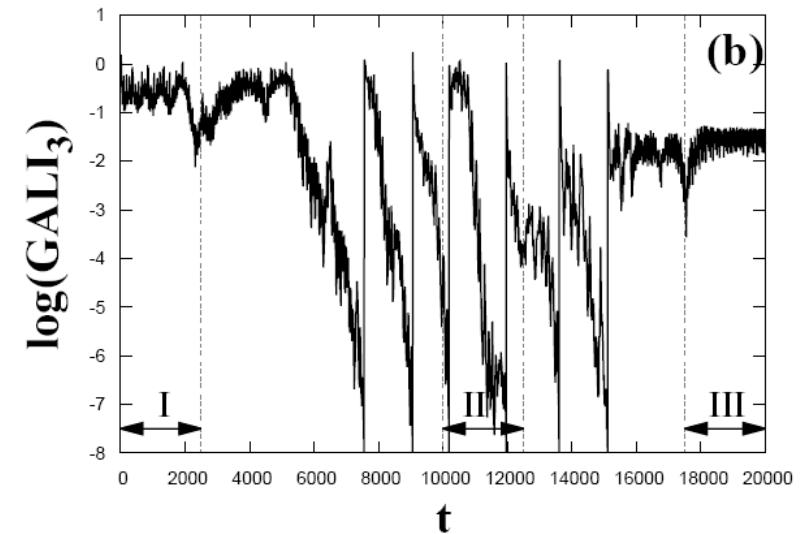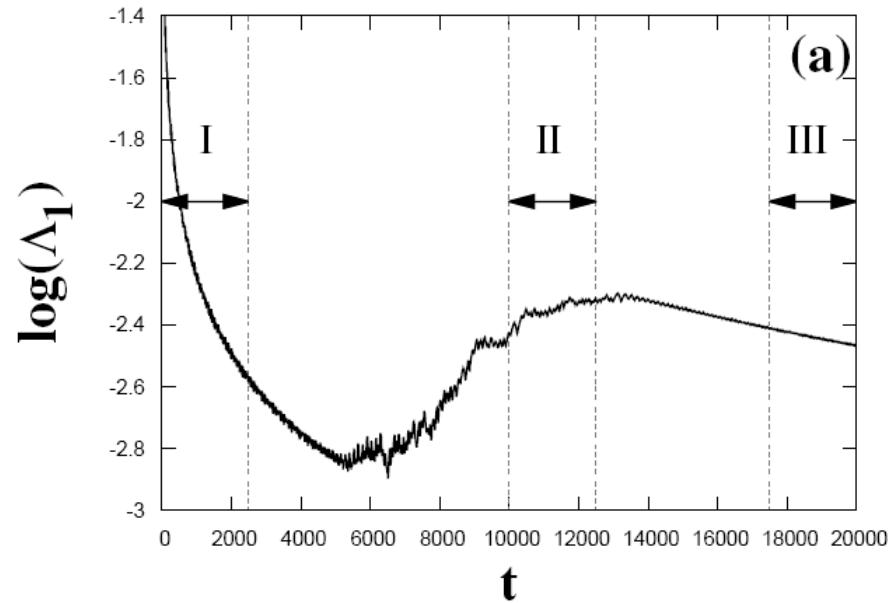$$\rho = \begin{cases} \rho_c(1-m^2)^n, & \text{for } m \le 1 \\ 0, & \text{for } m > 1 \end{cases}, \text{ where } m^2 = \frac{x^2}{a^2} + \frac{y^2}{b^2} + \frac{z^2}{c^2}, \ a > b > c \text{ and } n = 2.$$

Time-dependent 2D barred galaxy model

Time-dependent 3D barred galaxy model

Interplay between chaotic and regular motion

Symplectic Integrators (SIs)

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

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

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

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 $c = \dfrac{2-\sqrt{3}}{24}$.

Thus the full integrator scheme becomes: *SABAC$_2$ = C (SABA$_2$) C* and its error is of order 4.

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** $\left[\frac{1}{2}, \frac{3}{2} \right]$.

<u>Linear case</u> (neglecting the term $u_l^4/4$)

Ansatz: $u_l = A_l \exp(i\omega t)$. **Normal modes (NMs)** $A_{v,l}$ **- Eigenvalue problem:**

$\lambda A_l = \varepsilon_l A_l - (A_{l+1} + A_{l-1})$ with $\lambda = W\omega^2 - W - 2$, $\varepsilon_l = W(\tilde{\varepsilon}_l - 1)$

The discrete nonlinear Schrödinger (DNLS) equation

We also consider the system:

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

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.
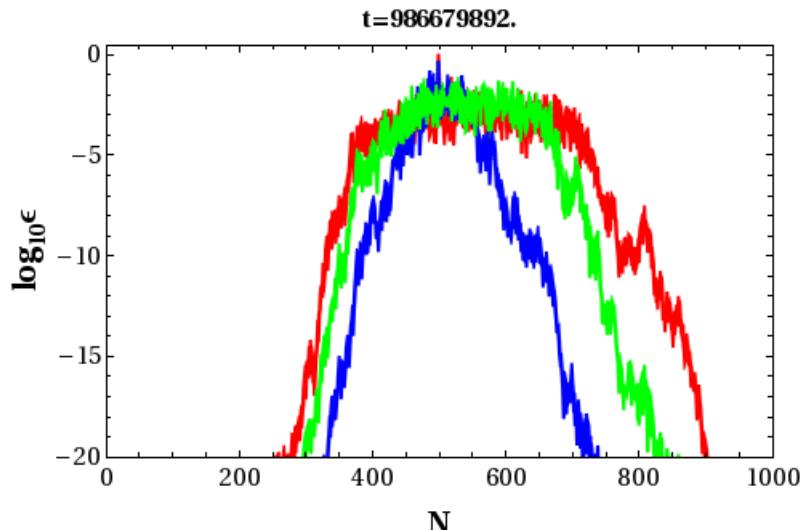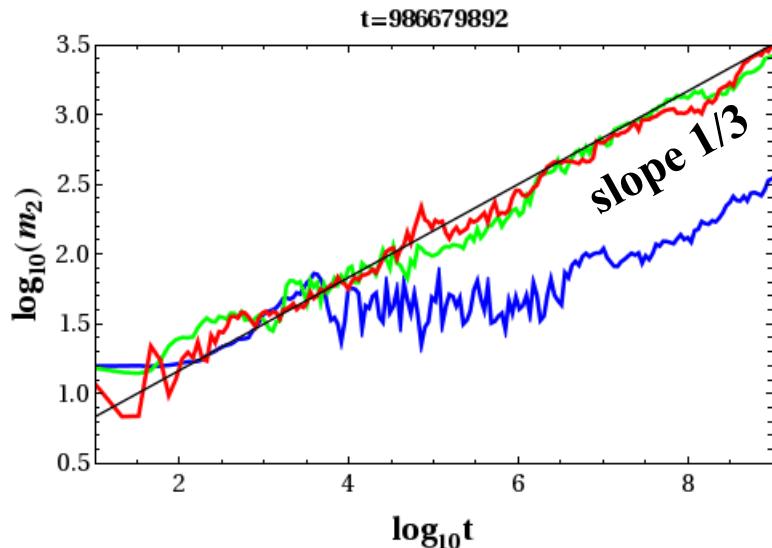
Distribution characterization

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

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

of the vth NM.

Second moment: $\qquad m_2 = \sum_{v=1}^{N}\left(v - \bar{v}\right)^2 z_v \qquad$ with $\ \bar{v} = \sum_{v=1}^{N} v z_v$

Different spreading regimes

The KG model

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

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

A   **B**

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

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

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

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

The DNLS model

How can we use Symplectic Integrators for the DNLS model?

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

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

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

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

$$e^{\tau L_{\mathcal{B}}} : (\mathbf{q}', \mathbf{p}')^{\mathrm{T}} = \mathbf{C}(\tau) \cdot (\mathbf{q}, \mathbf{p})^{\mathrm{T}}$$

Evaluation of the C(τ) matrix

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

$$\dot{\mathbf{x}}^{\mathrm{T}} = \begin{pmatrix} \mathbf{0} & \mathbf{A} \\ -\mathbf{A} & \mathbf{0} \end{pmatrix} \mathbf{x}^{\mathrm{T}} \qquad \textbf{with} \qquad \mathbf{A} = \begin{pmatrix} 0 & -1 & 0 & \cdots & 0 & 0 \\ -1 & 0 & -1 & \cdots & 0 & 0 \\ 0 & -1 & 0 & \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & 0 & -1 \\ 0 & 0 & 0 & \cdots & -1 & 0 \end{pmatrix}$$

Then the matrix C(τ) 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(Aτ) and sin(Aτ) 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)** $\quad LF(\tau) = e^{\frac{\tau}{2}L_{\mathcal{A}}} e^{\tau L_{\mathcal{B}}} e^{\frac{\tau}{2}L_{\mathcal{A}}}$

SABA$_2$ **(5 steps)**

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

$$S^4(\tau) = e^{c_1 \tau L_{\mathcal{A}}} e^{d_1 \tau L_{\mathcal{B}}} e^{c_2 \tau L_{\mathcal{A}}} e^{d_2 \tau L_{\mathcal{B}}} e^{c_2 \tau L_{\mathcal{A}}} e^{d_1 \tau L_{\mathcal{B}}} e^{c_1 \tau L_{\mathcal{A}}},$$

with $c_1 = \frac{1}{2(2-2^{1/3})}$, $c_2 = \frac{1-2^{1/3}}{2(2-2^{1/3})}$, $d_1 = \frac{1}{2-2^{1/3}}$, $d_2 = -\frac{2^{1/3}}{2-2^{1/3}}$
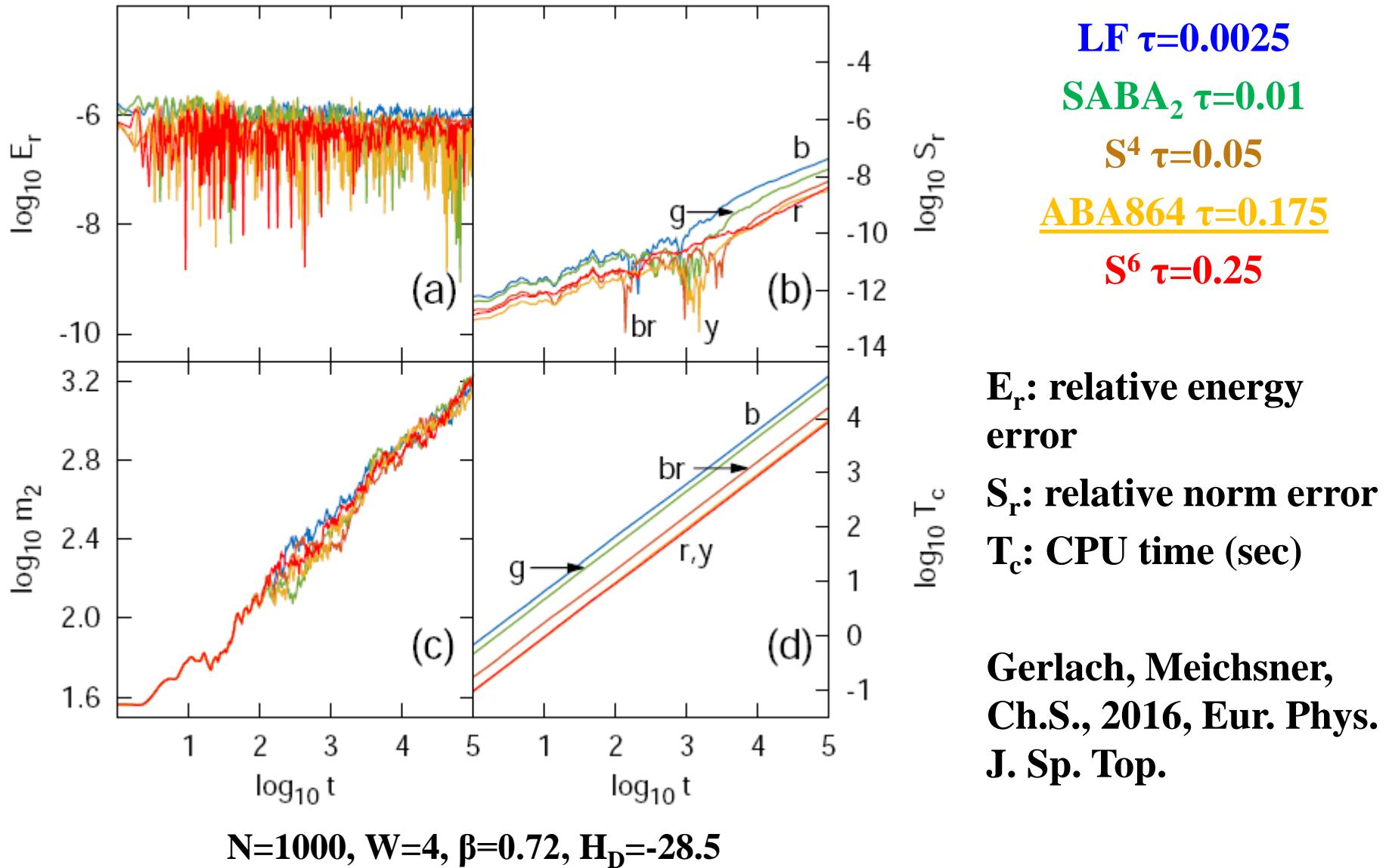
ABA864 **[Blanes et al., 2013, App. Num. Math.] (15 steps)**

Order 6: **Using the composition method refereed as 'solution A' in [Yoshida, 1990, Phys. Lett. A] we construct the 6th order symplectic integrator S^6 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$_2$ 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

LF τ=0.0025

SABA$_2$ τ=0.01

S^4 τ=0.05

ABA864 τ=0.175

S^6 τ=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.

N=1000, W=4, β=0.72, H$_D$=-28.5

DNLS model: 3 part split SIs

Symplectic Integrators produced by Successive Splits (SS)

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

$$\begin{cases} q_l' = q_l \cos(\alpha_l \tau) + p_l \sin(\alpha_l \tau), \\ p_l' = p_l \cos(\alpha_l \tau) - q_l \sin(\alpha_l \tau), \end{cases} \begin{cases} q_l' = q_l, \\ p_l' = p_l + (q_{l-1} + q_{l+1})\tau \end{cases} \begin{cases} p_l' = p_l, \\ q_l' = q_l - (p_{l-1} + p_{l+1})\tau \end{cases}$$

Using the SABA$_2$ integrator we get a 2nd order integrator with 13 steps, SS^2:

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

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

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

DNLS model: 3 part split SIs

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

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

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

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

DNLS model: 3 part split SIs

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

$$S^{4th}(\tau) = S^{2nd}(x_1\tau) \times S^{2nd}(x_0\tau) \times S^{2nd}(x_1\tau), \qquad x_0 = -\frac{2^{1/3}}{2 - 2^{1/3}}, \qquad x_1 = \frac{1}{2 - 2^{1/3}}$$
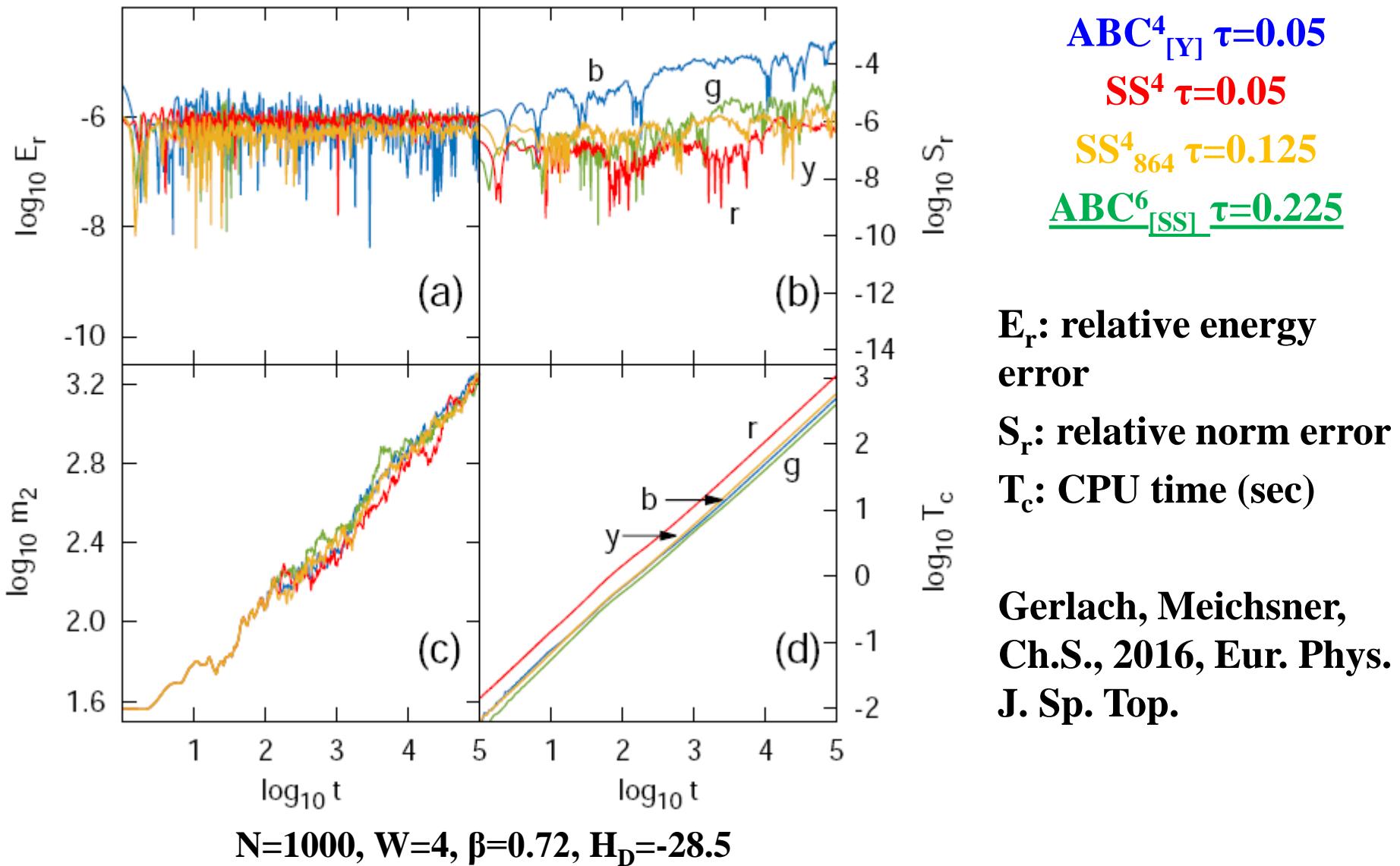
In this way, starting with the 2nd order integrators SS^2 and ABC^2 we construct the 4th order integrators:

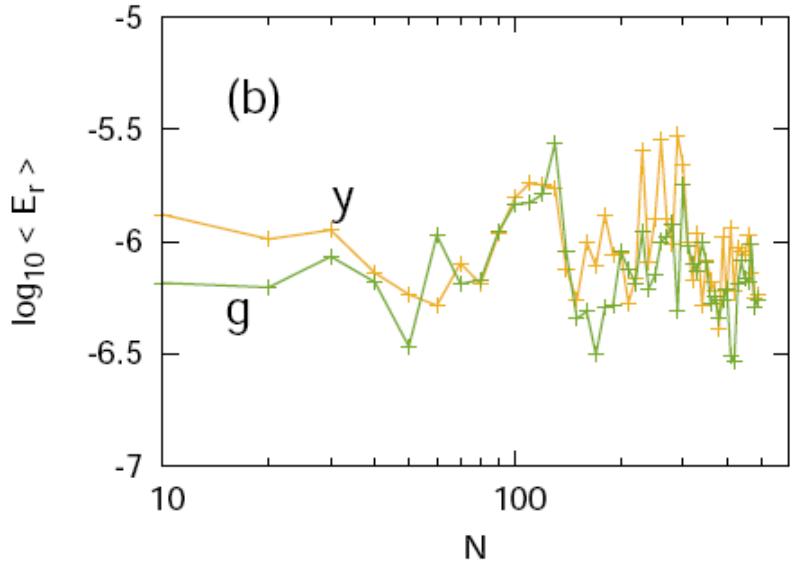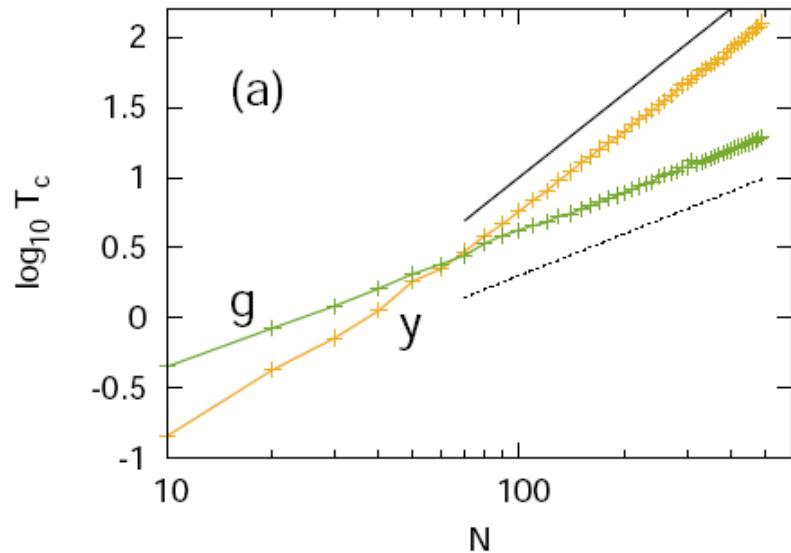$$SS^4 \text{ with 37 steps} \qquad ABC^4_{[Y]} \text{ with 13 steps}$$

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

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

SS^4 $\tau=0.05$

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

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

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.

N=1000, W=4, β=0.72, H_D=-28.5

2 and 3 part split SIs: Comparing their efficiency

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

Best 3 part split: $ABC^6_{[SS]}$ $\tau=0.225$

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

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

Summary

- **GALI$_k$ indices are perfectly suited for studying the dynamics of time-dependent models as they able to <u>capture subtle changes in the nature of an orbit even for relatively small time intervals.</u>**

- **We presented several efficient symplectic integration methods suitable for the integration of the DNLS model, which are based on <u>2 and 3 part split</u> of the Hamiltonian.**

  - ✓ **2 part split methods preserve better the second integral of the system (i.e. the norm)**

  - ✓ **For small lattices (N ≲ 70) 2 part split methods are computationally more efficient, while for larger lattice 3 part split method should be used.**

References
- **Manos T., Bountis T. & Ch.S. (2013) J. Phys. A, 46, 254017**
- **Gerlach, Meichsner, Ch.S. (2016) Eur. Phys. J. Sp. Top., 225, 1103**

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