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:

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

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

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

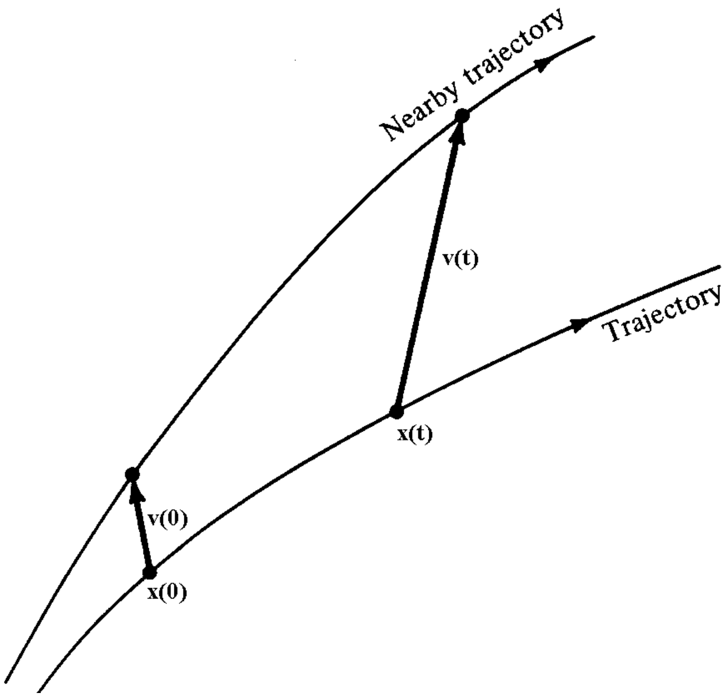
is governed by the Hamilton's equations of motion

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

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

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



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

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

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

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 $2 \leq k \leq 2N$,

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 $\sigma_1, \sigma_2, \ldots, \sigma_k$:

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

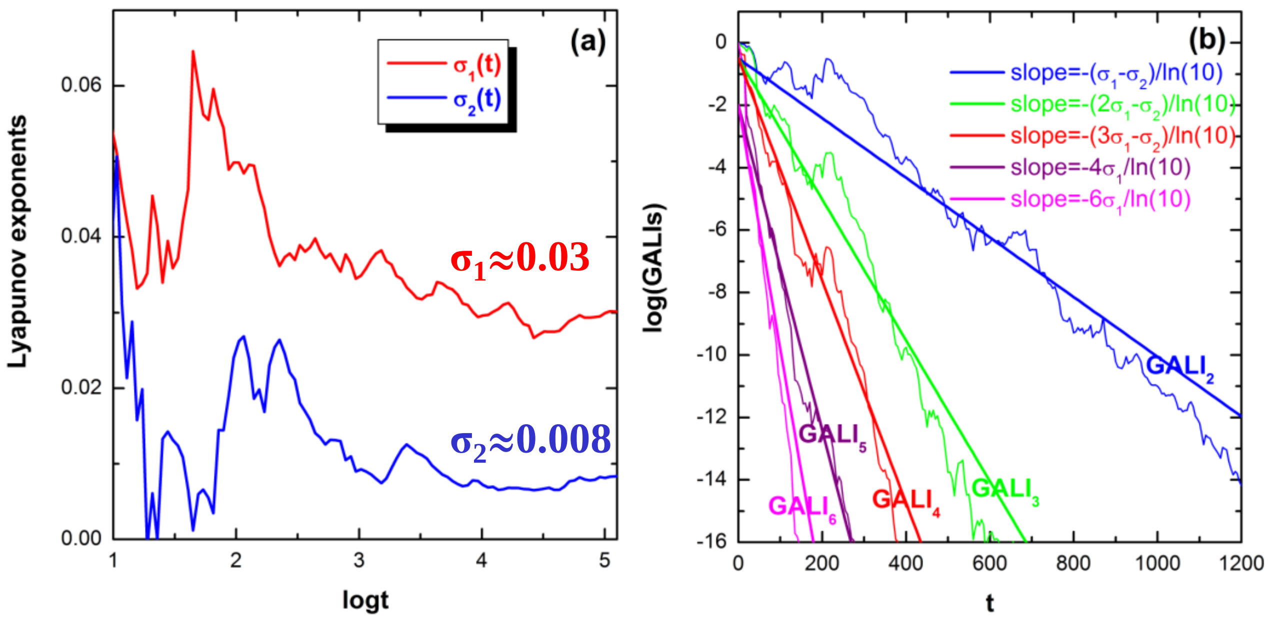
The above relation is valid even if some Lyapunov exponents are equal, or very close to each other.

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 ω_1=1, ω_2=$\sqrt{2}$, ω_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.):

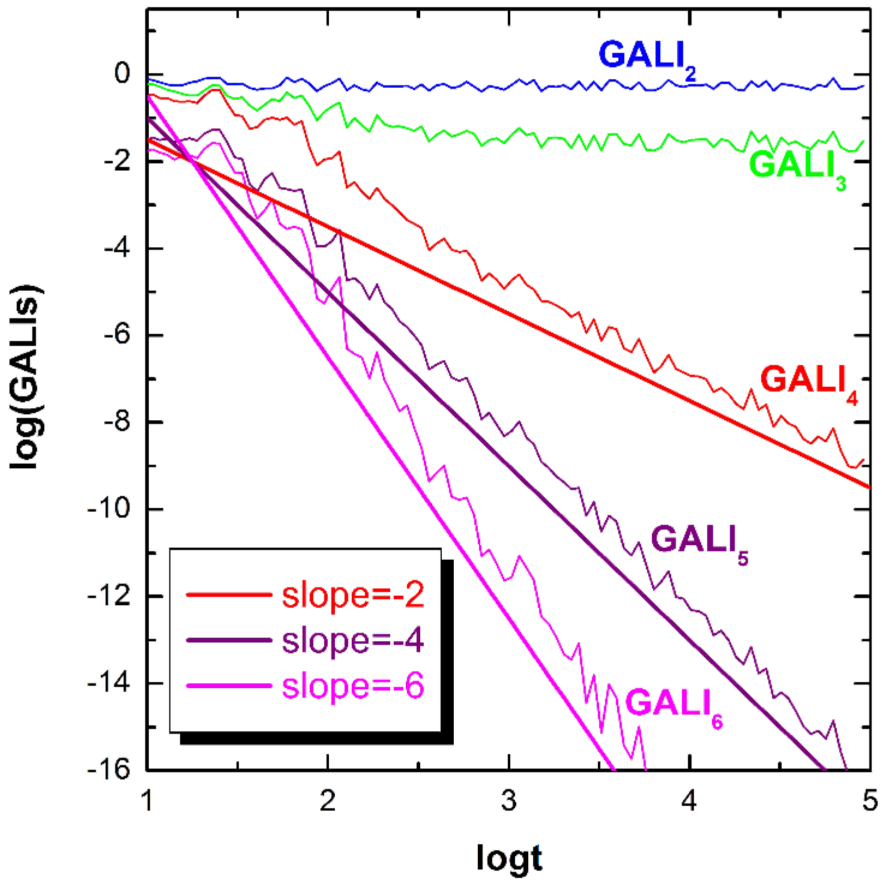
$$GALI_k(t) \propto \begin{cases} \text{constant} & \text{if} \quad 2 \leq k \leq s \\ \dfrac{1}{t^{k-s}} & \text{if} \quad s < k \leq 2N-s \\ \dfrac{1}{t^{2(k-N)}} & \text{if} \quad 2N-s < k \leq 2N \end{cases}$$

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

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

Regular motion:

$GALI_k \rightarrow \text{constant} \neq 0$ or $GALI_k \rightarrow 0$ power law decay

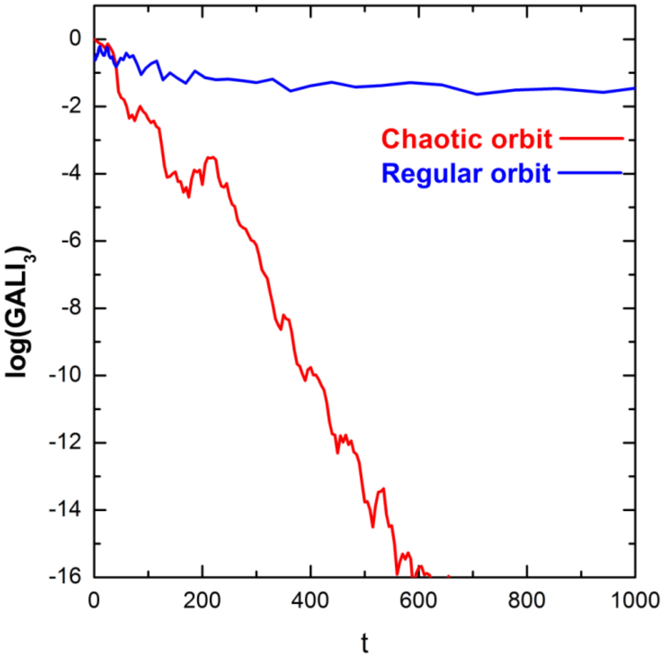
$$GALI_k(t) \propto \begin{cases} \text{constant} & \text{if} \quad 2 \leq k \leq s \\ \dfrac{1}{t^{k-s}} & \text{if} \quad s < k \leq 2N-s \\ \dfrac{1}{t^{2(k-N)}} & \text{if} \quad 2N-s < k \leq 2N \end{cases}$$

Global dynamics

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

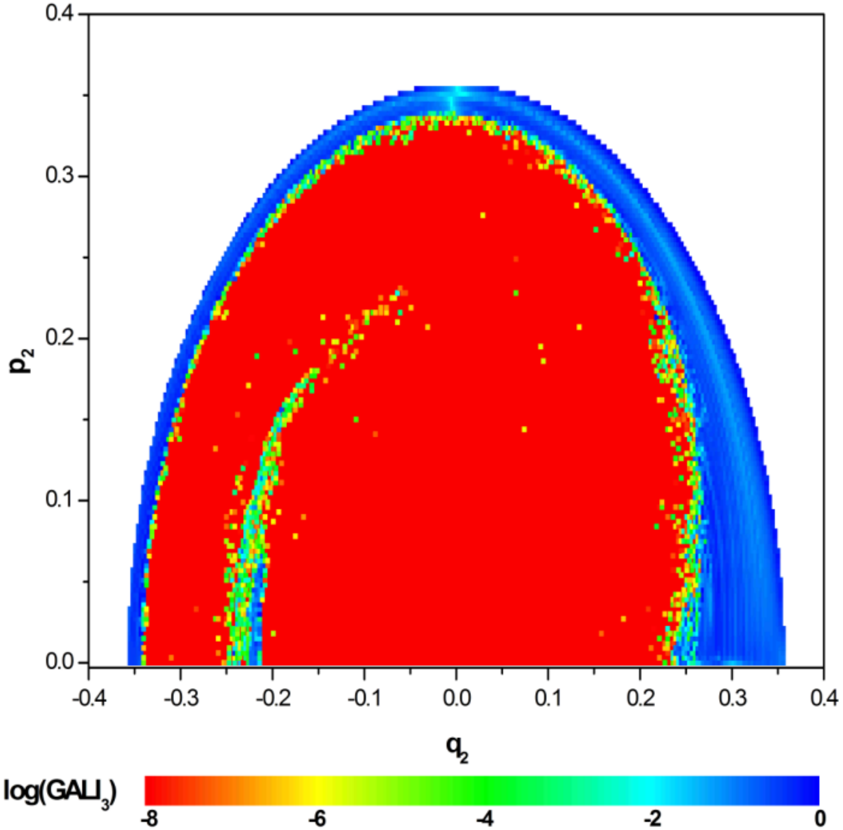
Chaotic motion: GALI$_N \rightarrow 0$ (exponential decay)

Regular motion: GALI$_N \rightarrow$constant$\neq 0$



3D Hamiltonian

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



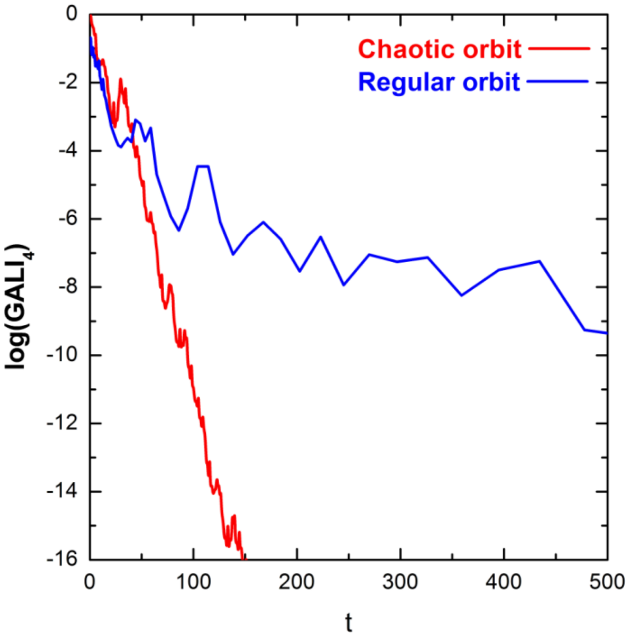
Global dynamics

GALI$_k$ with k>N

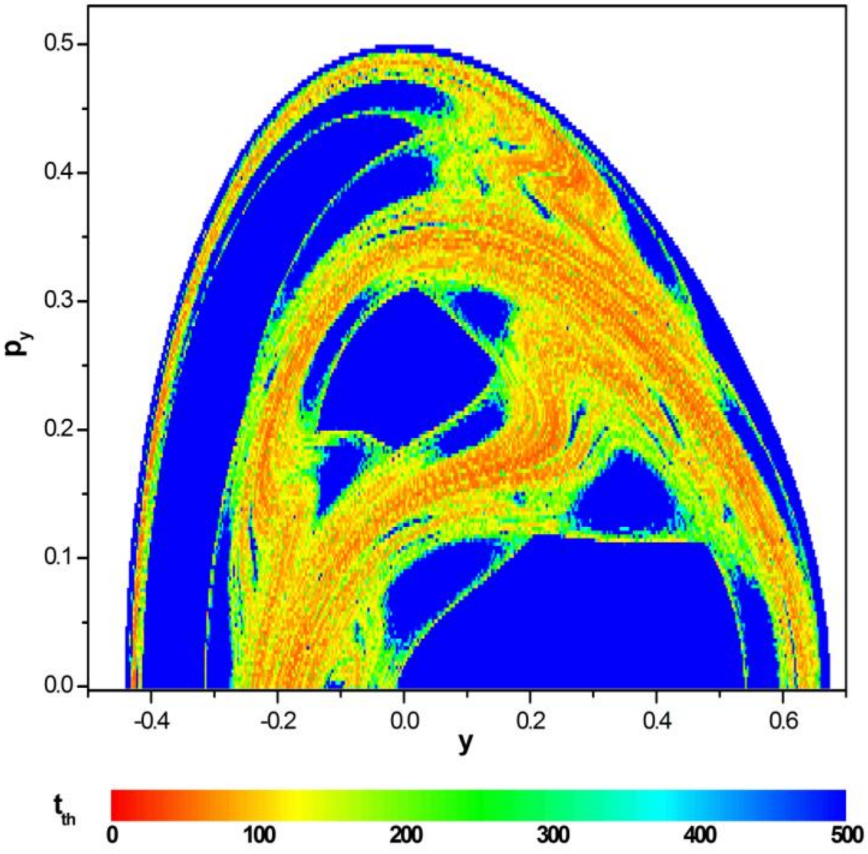
The index tends to zero both for regular and chaotic orbits but with completely different time rates:

Chaotic motion: exponential decay

Regular motion: power law



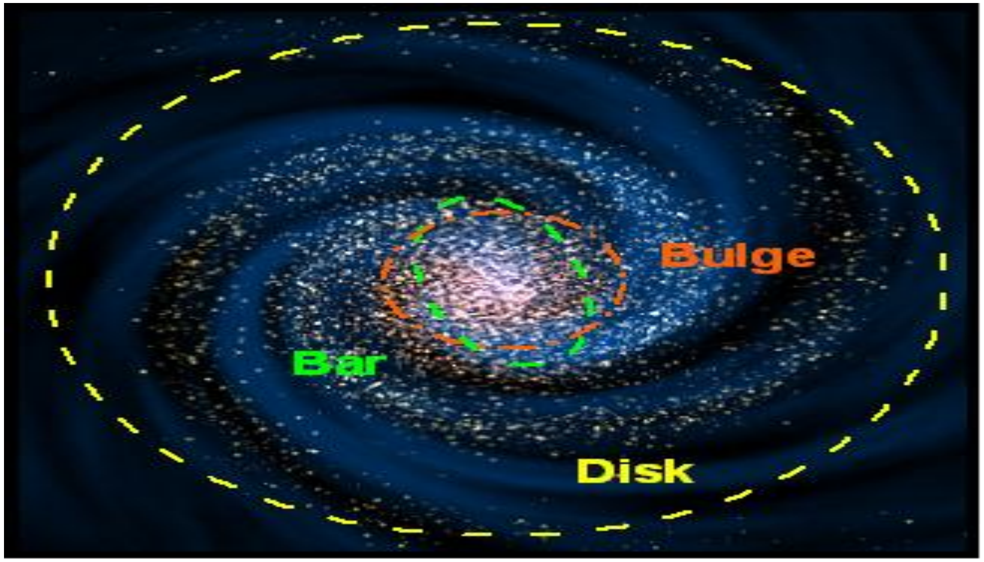
2D Hamiltonian (Hénon-Heiles)
Time needed for GALI$_4$<10^{-12}



Barred galaxies

NGC 1433

NGC 2217



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:

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

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:

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

(Ferrers bar)

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

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

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 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:

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

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:

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

i) Plummer sphere:

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

ii) Miyamoto–Nagai disc:

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

b) Bar component:

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

(Ferrers bar)

$$\rho_c = \frac{105}{32\pi} \frac{G M_B(t)}{abc}$$

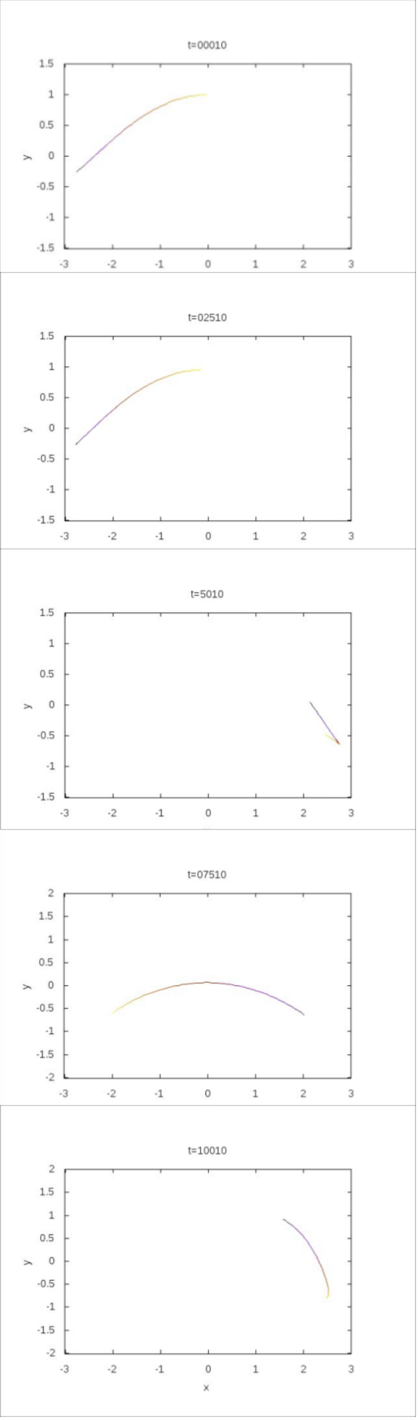
$$\text{where } m^2(u) = \frac{x^2}{a^2+u} + \frac{y^2}{b^2+u} + \frac{z^2}{c^2+u}, \quad \Delta^2(u) = (a^2+u)(b^2+u)(c^2+u),$$

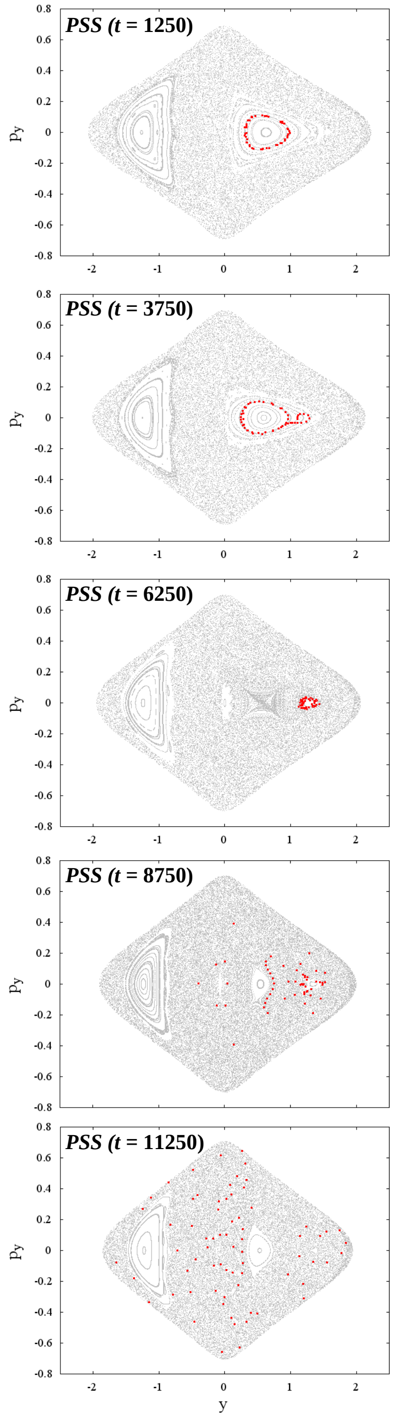
n: positive integer ($n = 2$ for our model), λ: the unique positive solution of $m^2(\lambda) = 1$

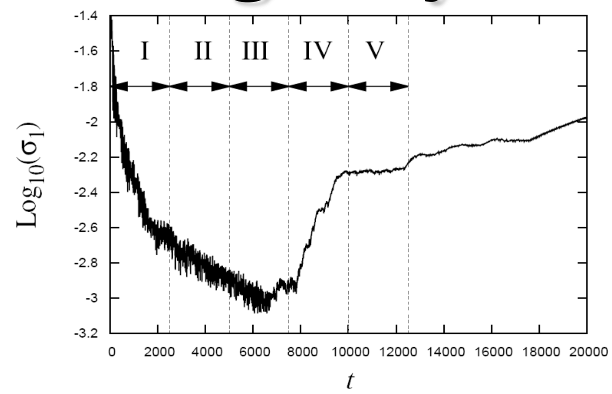
Its density is:

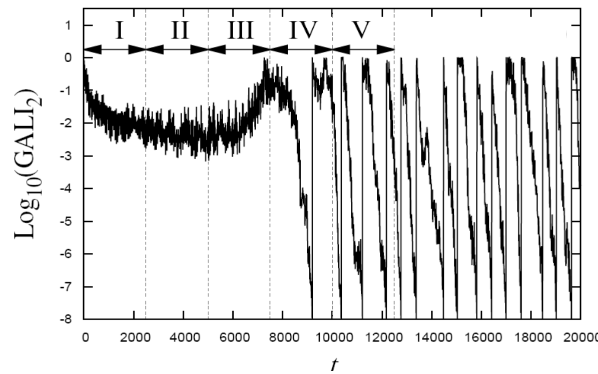
$$\rho = \begin{cases} \rho_c (1 - m^2)^n, & \text{for } m \le 1 \\ 0, & \text{for } m > 1 \end{cases}, \quad \text{where } m^2 = \frac{x^2}{a^2} + \frac{y^2}{b^2} + \frac{z^2}{c^2}, \quad a > b > c \text{ and } n = 2.$$

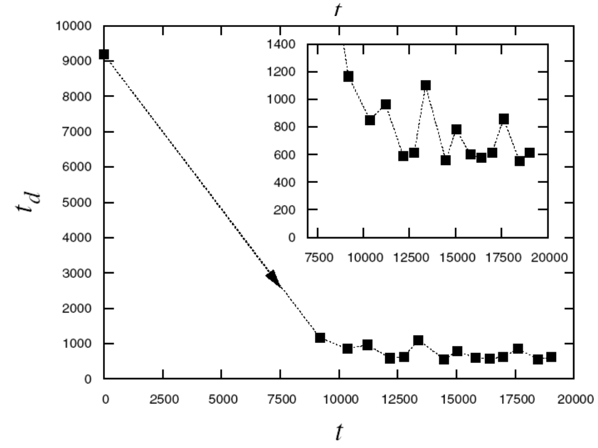
Time-dependent 2D barred galaxy model





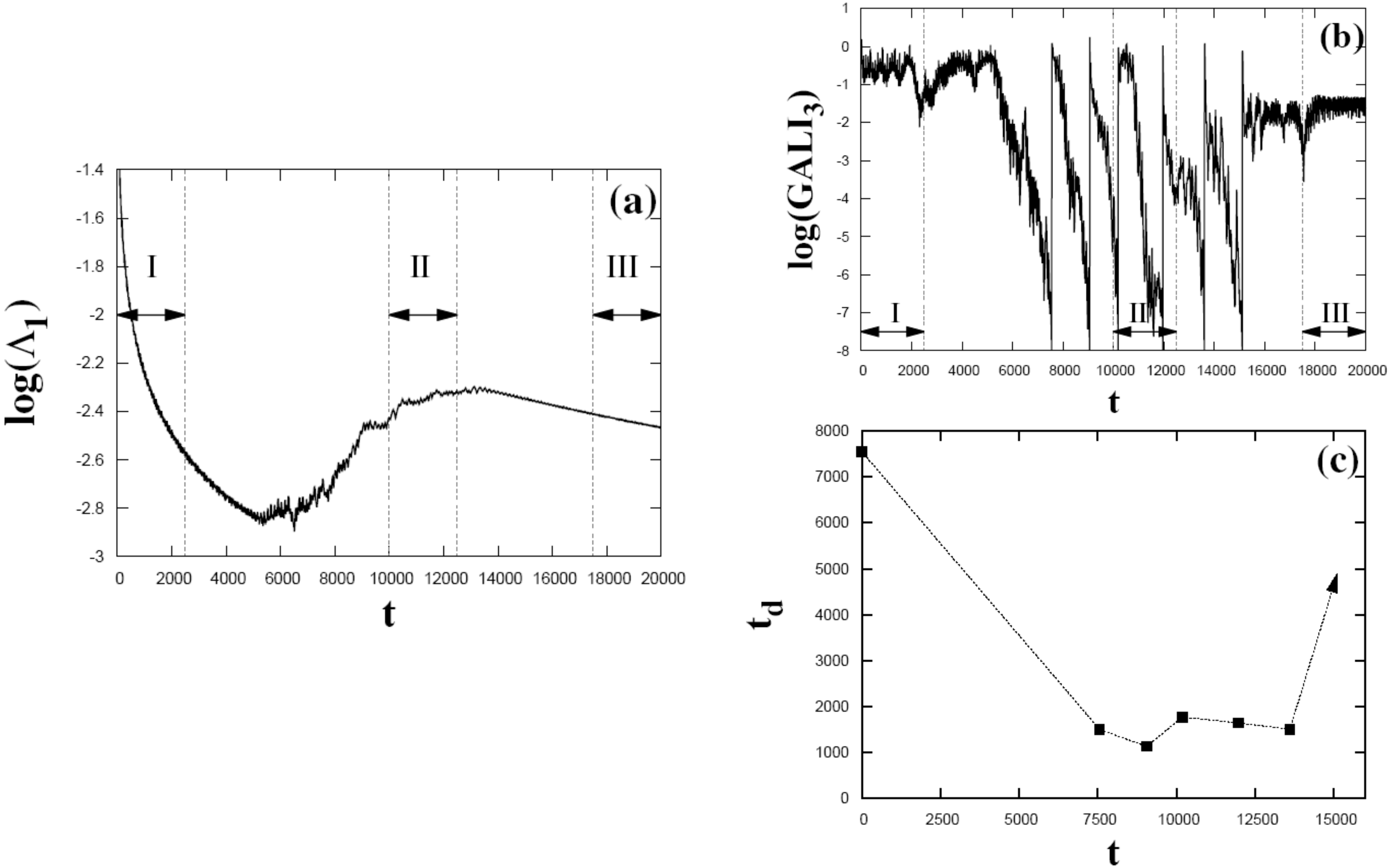






Time-dependent 3D barred galaxy model

Interplay between chaotic and regular motion



Symplectic Integrators (SIs)

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

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

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+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.

<u>So the dynamics over an integration time step τ is described by a series of successive acts of Hamiltonians A and B.</u>

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.

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

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 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 $S = \sum_l |\psi_l|^2$ of the wave packet.

Distribution characterization

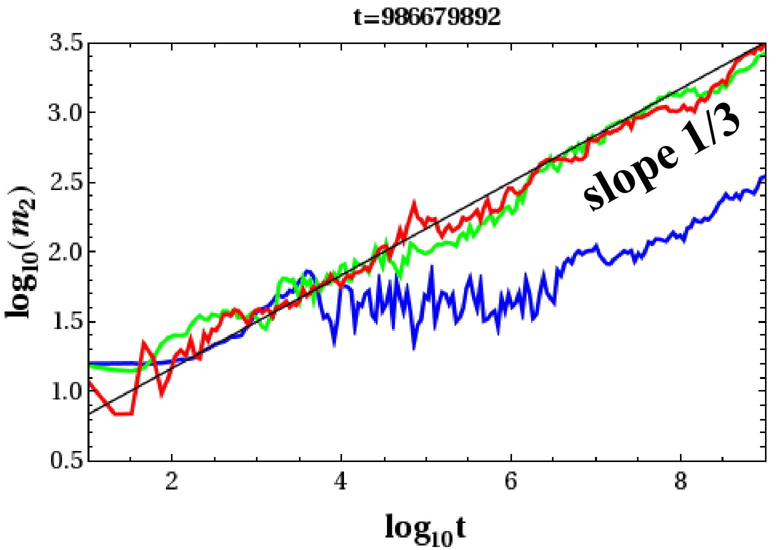
We consider normalized energy distributions in normal mode (NM) space

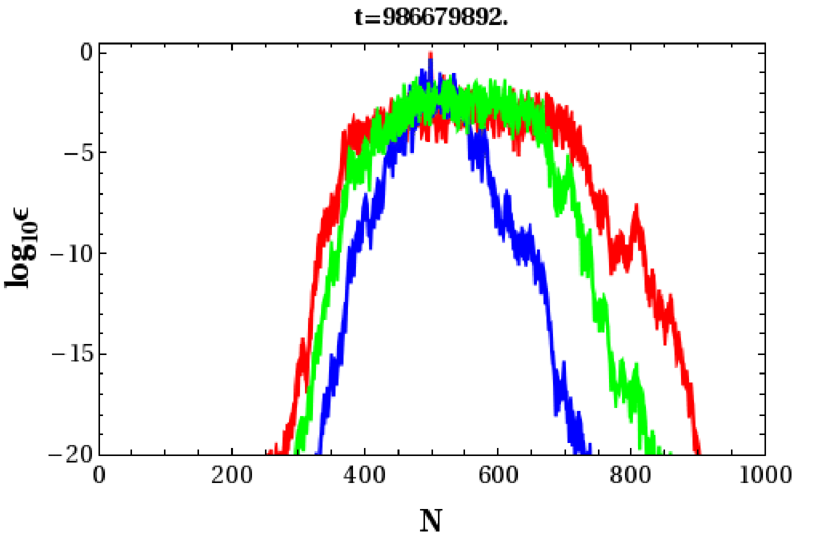
$$z_\nu \equiv \frac{E_\nu}{\sum_m E_m} \quad \text{with} \quad E_\nu = \frac{1}{2}\left(\dot{A}_\nu^2 + \omega_\nu^2 A_\nu^2\right)$$

, where A_ν is the amplitude of the νth 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





The KG model

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

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

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

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

with a corrector term which corresponds to the Hamiltonian function:

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

The DNLS model

How can we use Symplectic Integrators for the DNLS model?

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

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

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

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

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

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)** $LF(\tau) = e^{\frac{\tau}{2}L_{\mathcal{A}}} e^{\tau L_{\mathcal{B}}} e^{\frac{\tau}{2}L_{\mathcal{A}}}$

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

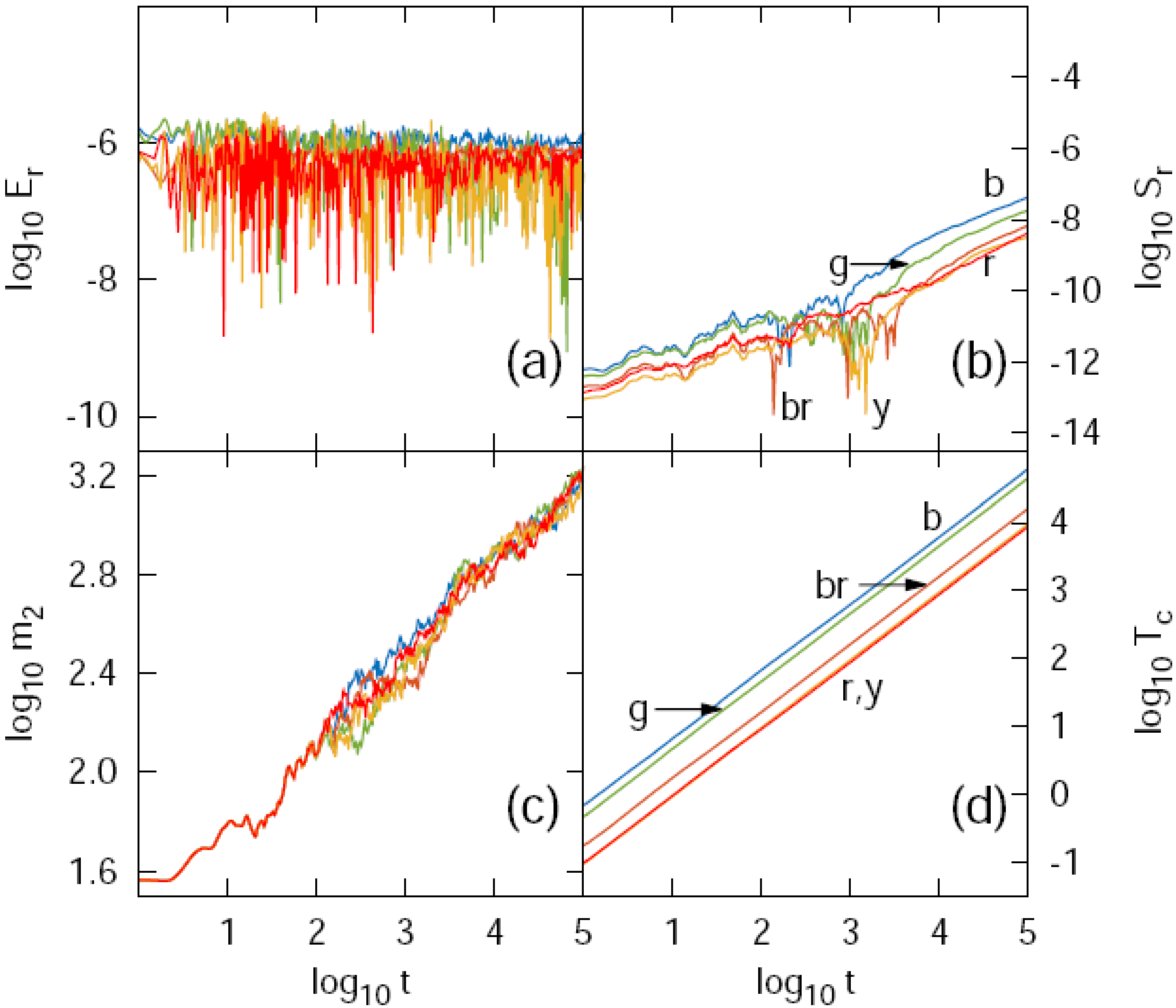
ABA864 **[Blanes et al., 2013, App. Num. Math.] (15 steps)**

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



N=1000, W=4, β=0.72, H_D=-28.5

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.

DNLS model: 3 part split SIs

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

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

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_1: $\begin{cases} q_l' = q_l, \\ p_l' = p_l + (q_{l-1} + q_{l+1})\tau \end{cases}$

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^2:

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

$\tau' = \tau / 2$

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

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

DNLS model: 3 part split SIs

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

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

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

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

DNLS model: 3 part split SIs

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

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

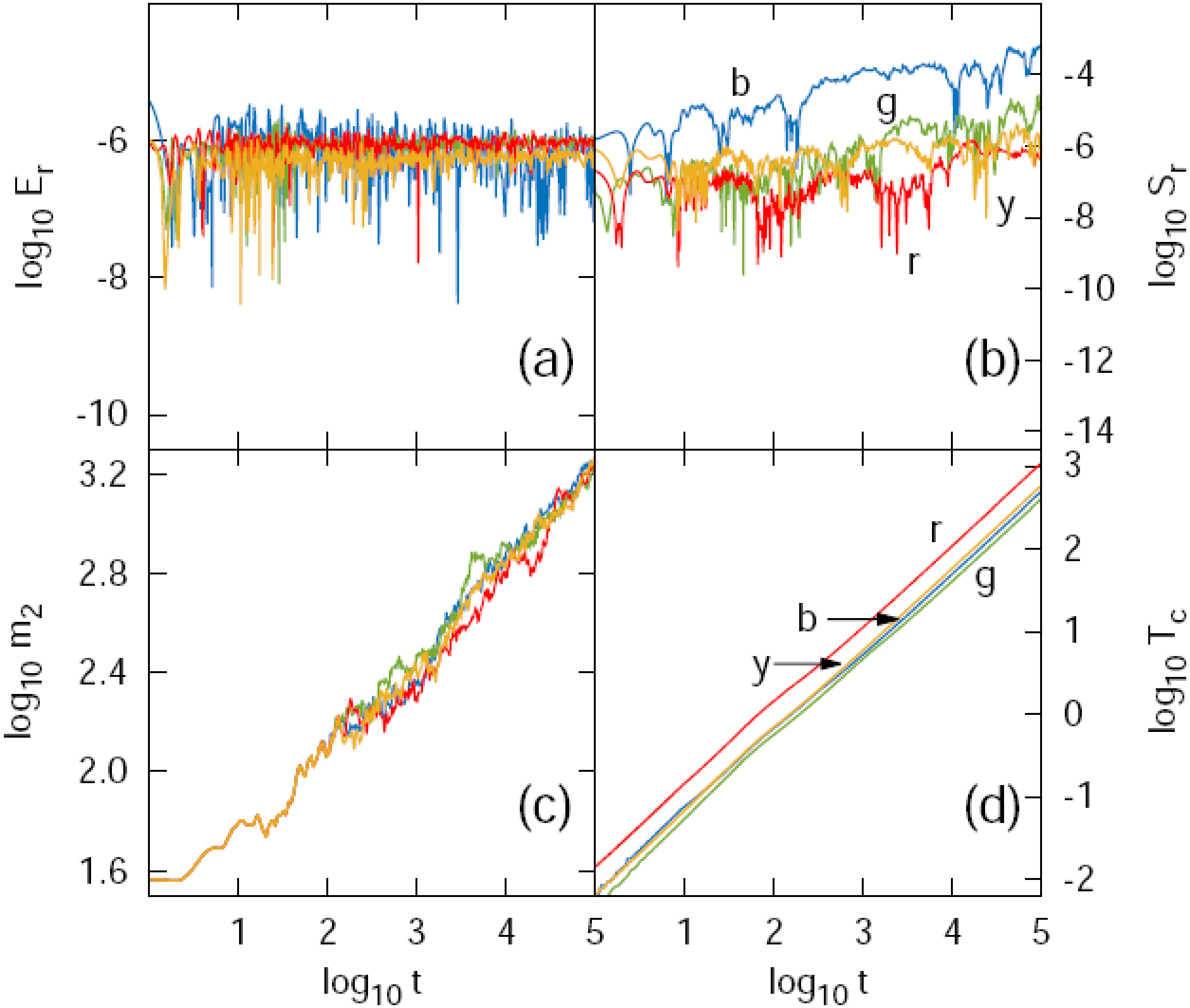
In this way, starting with the 2^{nd} order integrators SS^2 and ABC^2 we construct the 4^{th} order integrators:

SS^4 with 37 steps $\qquad$ $ABC^4_{[Y]}$ 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, β=0.72, H_D=-28.5

$ABC^4_{[Y]}$ τ=0.05

SS^4 τ=0.05

SS^4_{864} τ=0.125

$ABC^6_{[SS]}$ τ=0.225

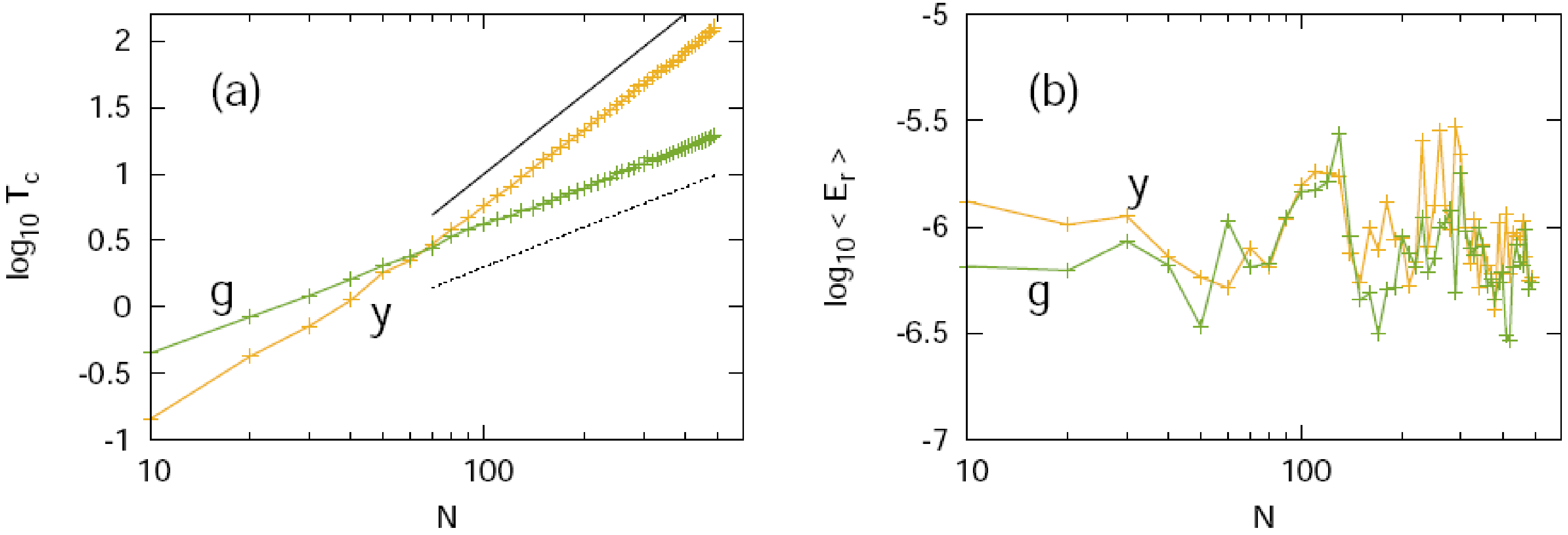
E_r: relative energy error

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 τ=0.125

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

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

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

Summary

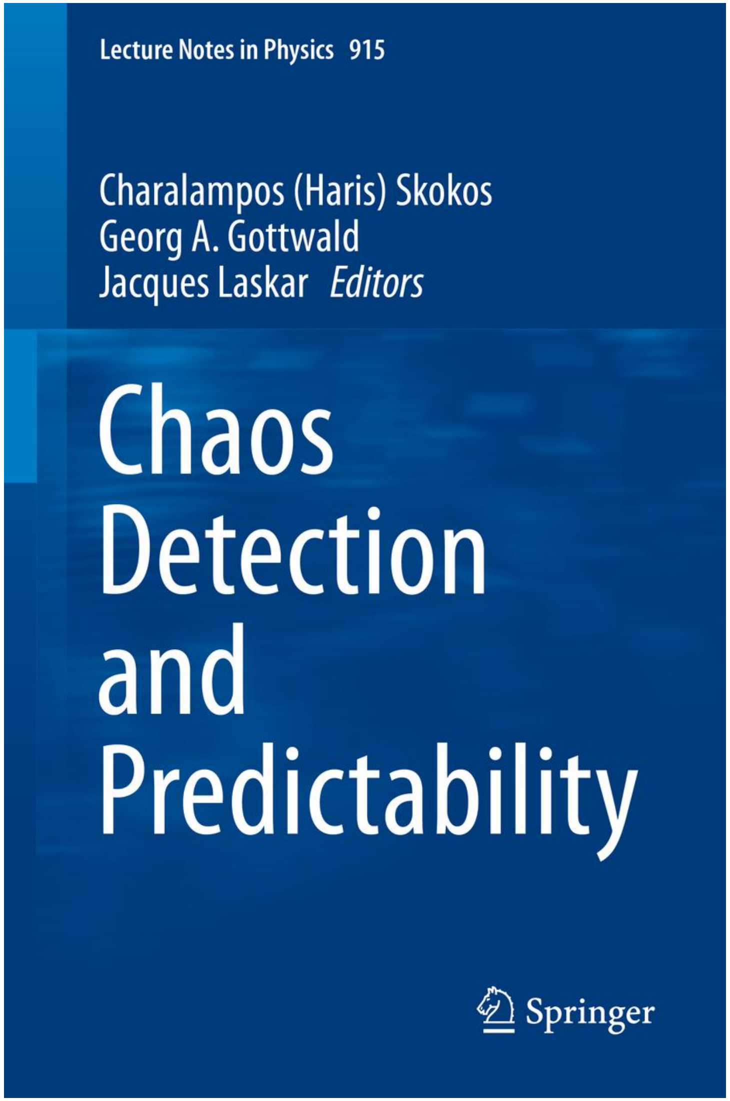
- **GALI$_k$ indices are perfectly suited for studying the dynamics of time-dependent models as they able to capture subtle changes in the nature of an orbit even for relatively small time intervals.**
- **We presented several efficient symplectic integration methods suitable for the integration of the 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.**

References

•Manos T., Bountis T. & Ch.S. (2013) J. Phys. A, 46, 254017

•Gerlach, Meichsner, Ch.S. (2016) Eur. Phys. J. Sp. Top. - in press, arXiv: physics.comp-ph/1512.07778

A …shameless promotion



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