Detecting chaos and determining the dimensions of tori in Fermi-Pasta-Ulam lattices by the GALI method

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Abstract

The recently introduced Generalized Alignment Index (GALI) method of chaos detection [1] is applied to distinguish efficiently between regular and chaotic orbits of multi–dimensional Hamiltonian systems. The GALI of order k (GALI_k) is proportional to volume elements formed by k initially linearly independent unit deviation vectors whose magnitude is normalized to unity from time to time. **For chaotic orbits, GALI_k tends exponentially to zero with exponents that involve the values of several Lyapunov exponents**, while in the case of **regular orbits, GALI_k fluctuates around nonzero values or goes to zero following particular power laws that depend on the dimension of the torus and on the order k**. We apply these indices to rapidly detect chaotic motion and identify low–dimensional tori of Fermi-Pasta-Ulam (FPU) lattices [2]. We also present an efficient computation scheme of the GALI's, based on the Singular Value Decomposition (SVD) algorithm.

1 The GALI method

1.1 Definition

Following [1] we consider **a Hamiltonian system of N degrees of freedom** having a Hamiltonian $H(q_1,\ldots,q_N,p_1,\ldots,p_N)$ where q_i and p_i, $i=1,\ldots,N$ are the generalized coordinates and momenta respectively. An orbit of this system is defined by a vector $\vec{x}(t)=(x_1(t),\ldots,x_{2N}(t))$, with $x_i=q_i$, $x_{i+N}=p_i$, $i=1,\ldots,N$. This orbit is a solution of Hamilton's equations $d\vec{x}/dt=\vec{\mathcal{V}}(\vec{x})=(\partial H/\partial\vec{p},-\partial H/\partial\vec{q})$, while the evolution of a deviation vector $\vec{w}(t)$ from $\vec{x}(t)$ obeys **the variational equations** $d\vec{w}/dt=\mathbf{M}(\vec{x}(t))\,\vec{w}$, where $\mathbf{M}=\partial\vec{\mathcal{V}}/\partial\vec{x}$ is the Jacobian matrix of $\vec{\mathcal{V}}$.

We follow k normalized deviation vectors $\hat{w}_1,\ldots,\hat{w}_k$ (with $2\le k\le 2N$) in time, and determine whether they become linearly dependent, by checking if the volume of the corresponding k–parallelogram goes to zero. This volume is equal to the norm of the wedge or exterior product of these vectors. Hence we are led to define the following 'volume' element:

$$\text{GALI}_k(t)=\|\hat{w}_1(t)\wedge\hat{w}_2(t)\wedge\cdots\wedge\hat{w}_k(t)\|\ , \tag{1}$$

which we call the **Generalized Alignment Index (GALI) of order k**. We note that the hat ($\hat{}$) over a vector denotes that it is of unit magnitude. Clearly, if at least two of these vectors become linearly dependent, the wedge product in (1) becomes zero and the volume element vanishes.

1.2 Behavior

In the case of a **chaotic orbit** all deviation vectors tend to become linearly dependent, aligning in the direction which corresponds to the maximal Lyapunov exponent and **GALI_k tends to zero exponentially** following the law [1]:

$$\text{GALI}_k(t)\sim e^{-[(\sigma_1-\sigma_2)+(\sigma_1-\sigma_3)+\cdots+(\sigma_1-\sigma_k)]t}, \tag{2}$$

where $\sigma_1,\ldots,\sigma_k$ are approximations of the first k largest Lyapunov exponents.

In the case of regular motion on the other hand, all deviation vectors tend to fall on the N–dimensional tangent space of the torus on which the motion lies. So, the generic behavior of GALI_k for regular orbits lying on N–dimensional tori is given by [1]:

$$\text{GALI}_k(t)\sim\begin{cases}\text{constant} & \text{if } 2\le k\le N\\ \frac{1}{t^{2(k-N)}} & \text{if } N<k\le 2N\end{cases}, \tag{3}$$

while for **regular orbits lying on an s–dimensional torus, with $s\le N$**, GALI_k behaves as [2]:

$$\text{GALI}_k(t)\sim\begin{cases}\text{constant} & \text{if } 2\le k\le s\\ \frac{1}{t^{k-s}} & \text{if } s<k\le 2N-s\\ \frac{1}{t^{2(k-N)}} & \text{if } 2N-s<k\le 2N\end{cases}. \tag{4}$$

Note that from (4) we deduce that for $s=N$, GALI_k remains constant for $2\le k\le N$ and decreases to zero as $\sim 1/t^{2(k-N)}$ for $N<k\le 2N$ in accordance with (3).

1.3 Numerical computation

In order to numerically compute GALI_k we perform the **Singular Value Decomposition** (SVD) of the $2N\times k$ matrix $\mathbf{A}$ having as columns the coordinates of the k normalized deviation vectors $\hat{w}_1,\ldots,\hat{w}_k$. Then **$\text{GALI}_k$ is equal to the product of the singular values** z_i, $i=1,\ldots,k$ of matrix $\mathbf{A}$ [2], so that

$$\log(\text{GALI}_k)=\sum_{i=1}^{k}\log(z_i)\,. \tag{5}$$

2 Numerical application to the FPU system

We apply the GALI method to study chaotic and quasiperiodic motion in a multi–dimensional Hamiltonian system. In particular, we consider the **FPU β–lattice** of N particles with Hamiltonian

$$H=\sum_{i=1}^{N}\frac{p_i^2}{2}+\sum_{i=0}^{N}\left[\frac{(q_{i+1}-q_i)^2}{2}+\frac{\beta(q_{i+1}-q_i)^4}{4}\right], \tag{6}$$

with $q_1,\ldots,q_N$ being the displacements of the particles with respect to their equilibrium positions, and $p_1,\ldots,p_N$ the corresponding momenta. It is well known that if we define normal mode variables by

$$Q_k=\sqrt{\frac{2}{N+1}}\sum_{i=1}^{N}q_i\sin\left(\frac{ki\pi}{N+1}\right)\ ,\ P_k=\sqrt{\frac{2}{N+1}}\sum_{i=1}^{N}p_i\sin\left(\frac{ki\pi}{N+1}\right)\ ,\ k=1,\ldots,N, \tag{7}$$

the unperturbed Hamiltonian (Eq. (6) for $\beta=0$) is written as the sum of the so–called **harmonic energies E_i** having the form:

$$E_i=\frac{1}{2}\left(P_i^2+\omega_i^2Q_i^2\right)\ ,\ \omega_i=2\sin\left(\frac{i\pi}{2(N+1)}\right)\ i=1,\ldots,N, \tag{8}$$

with ω_i being the corresponding harmonic frequencies. In our study we impose fixed boundary conditions $q_0(t)=q_{N+1}(t)=p_0(t)=p_{N+1}(t)=0$, $\forall t$ and fix the number of particles to $N=8$ and the system's parameter to $\beta=1.5$.

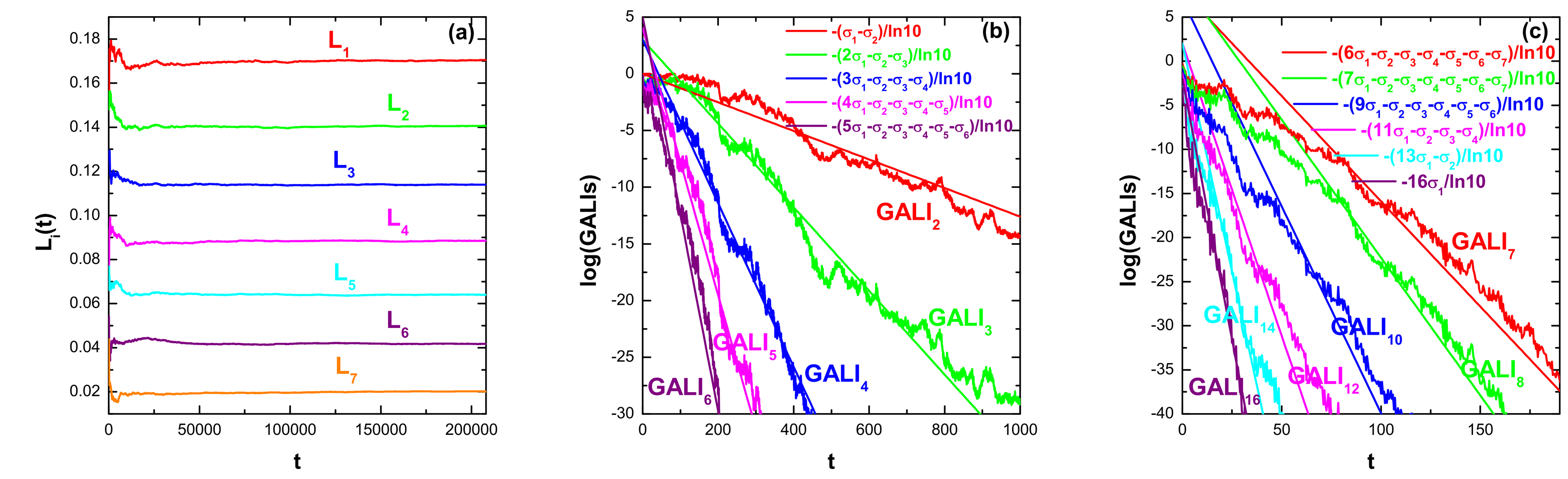

Figure 1. *(a) The time evolution of quantities L_i, $i=1,\ldots,7$, having as limits for $t\to\infty$ the seven positive Lyapunov exponents σ_i, $i=1,\ldots,7$, for a **chaotic orbit** with initial conditions $Q_1=Q_4=2$, $Q_2=Q_5=1$, $Q_3=Q_6=0.5$, $Q_7=Q_8=0.1$, $P_i=0$, $i=1,\ldots,8$ of the $N=8$ particle FPU lattice (6). The time evolution of the corresponding GALI_k is plotted in (b) for $k=2,\ldots,6$ and in (c) for $k=7,8,10,12,14,16$. The plotted lines in (b) and (c) correspond to exponentials that follow the asymptotic laws (2) for $\sigma_1=0.170$, $\sigma_2=0.141$, $\sigma_3=0.114$, $\sigma_4=0.089$, $\sigma_5=0.064$, $\sigma_6=0.042$, $\sigma_7=0.020$. Note that t–axis is linear and that the slope of each line is written explicitly in (b) and (c).*

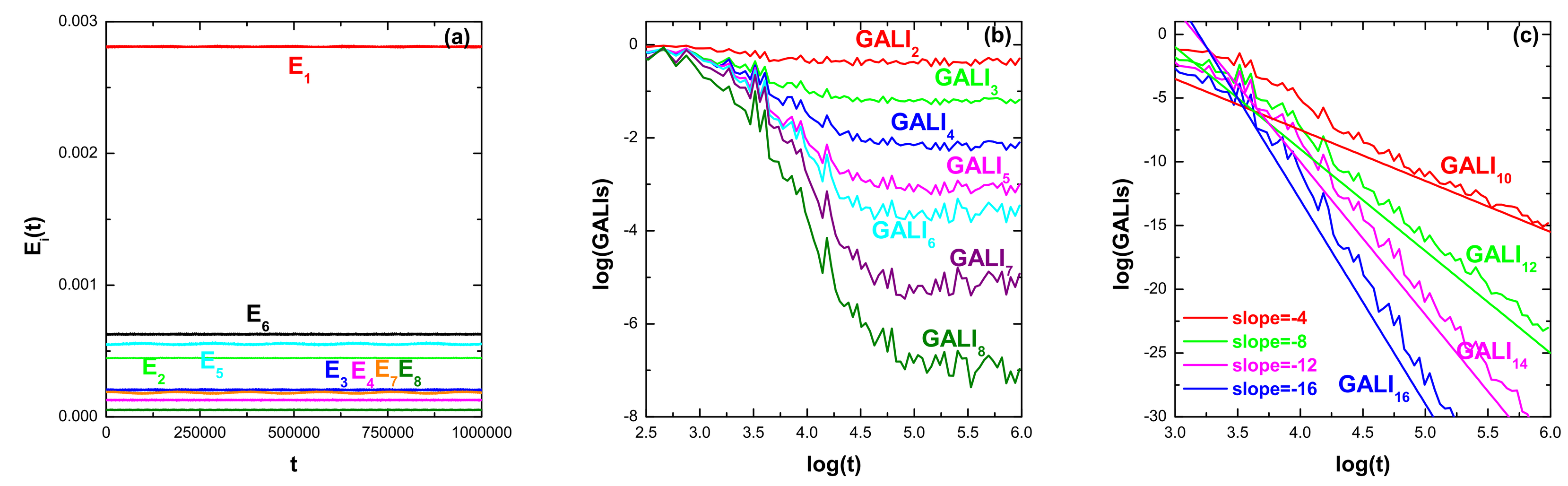

Figure 2. *(a) The time evolution of harmonic energies E_i, $i=1,\ldots,8$, for a **regular orbit** with initial conditions $q_1=q_2=q_3=q_8=0.05$, $q_4=q_5=q_6=q_7=0.1$, $p_i=0$, $i=1,\ldots,8$ of the $N=8$ particle FPU lattice (6). The time evolution of the corresponding GALI_k is plotted in (b) for $k=2,\ldots,8$ and in (c) for $k=10,12,14,16$. The plotted lines in (c) correspond to functions proportional to t^{-4}, t^{-8}, t^{-12} and t^{-16}, as predicted in (3).*

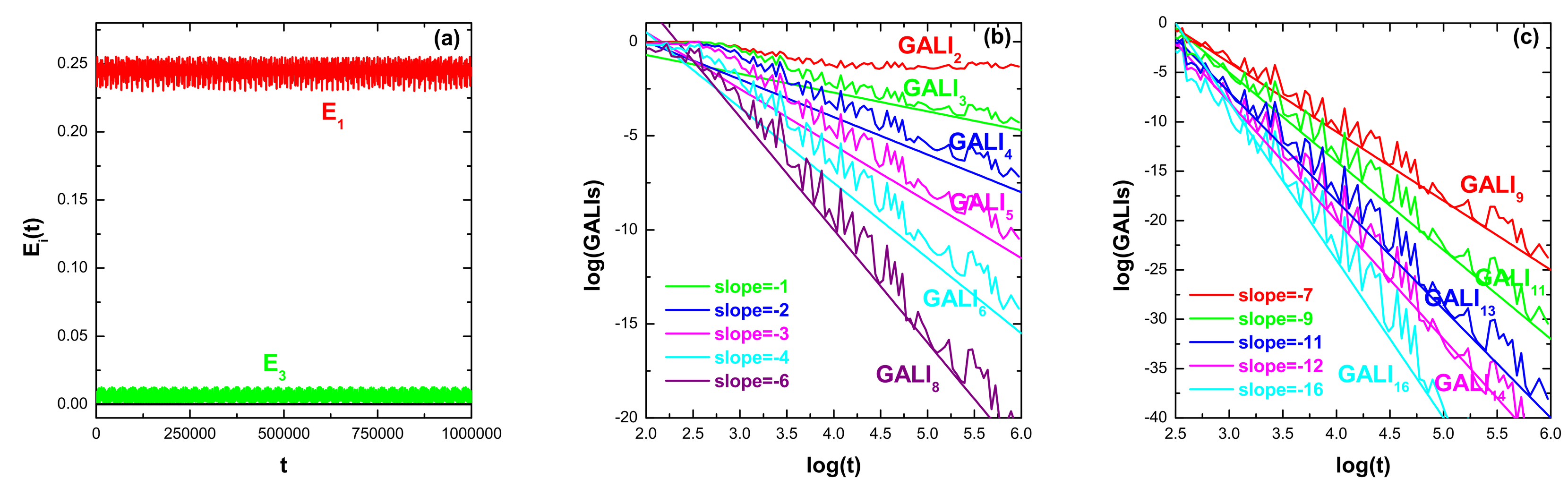

Figure 3. *(a) The time evolution of harmonic energies for a **regular orbit lying on a 2–dimensional torus** of the $N=8$ particle FPU lattice (6). Recurrences occur between E_1 and E_3, while all other harmonic energies remain practically zero. The time evolution of the corresponding GALI_k is plotted in (b) for $k=2,\ldots,6,8$ and in (c) for $k=9,11,13,14,16$. The plotted lines in (b) and (c) correspond to precisely the power laws predicted in (4) for $s=2$.*

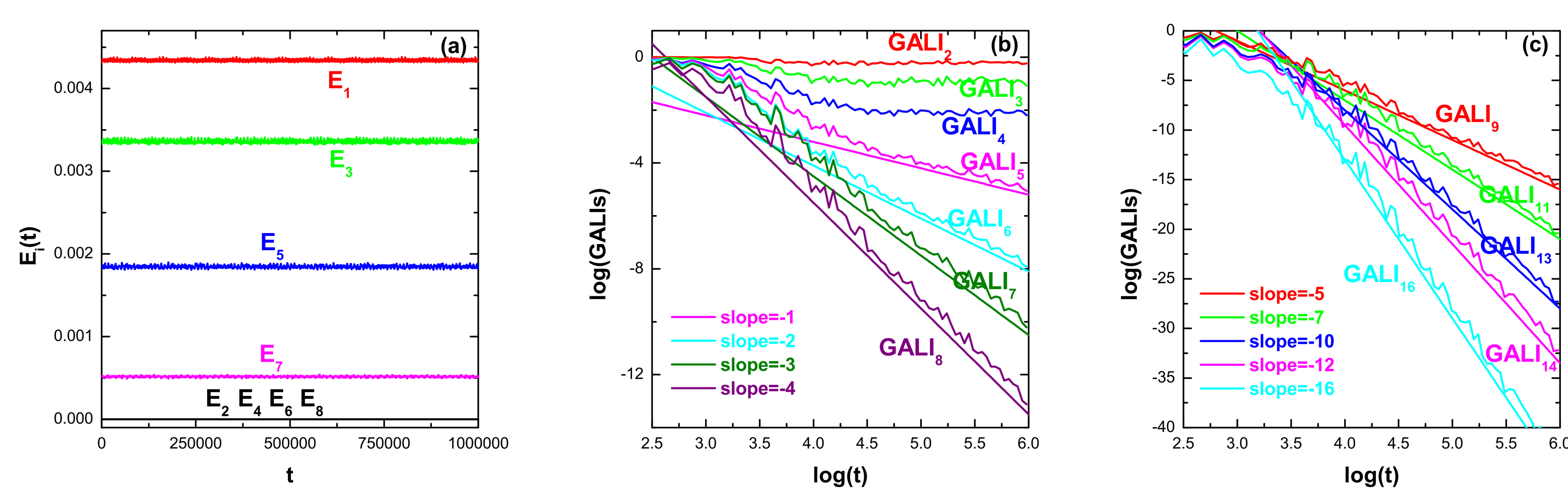

Figure 4. *(a) The time evolution of harmonic energies for a **regular orbit lying on a 4–dimensional torus** of the $N=8$ particle FPU lattice (6). Recurrences occur between E_1, E_3, E_5 and E_7, while all other harmonic energies remain practically zero. The time evolution of the corresponding GALI_k is plotted in (b) for $k=2,\ldots,8$ and in (c) for $k=9,11,13,14,16$. The plotted lines in (b) and (c) correspond to the precise power laws predicted in (4) for $s=4$.*

References

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[2] Ch. Skokos, T. C. Bountis and Ch. Antonopoulos, Eur. Phys. J. Special Topics **165**, 5 (2008)