Broken Ergodicity in classically chaotic spin systems

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A one dimensional classically chaotic spin chain with asymmetric coupling and two different inter-spin interactions, nearest neighbors and all-to-all, has been considered. Depending on the interaction range, dynamical properties, as ergodicity and chaoticity are strongly different. Indeed, even in presence of chaoticity, the model displays a lack of ergodicity only in presence of all to all interaction and below an energy threshold, that persists in the thermodynamical limit. Energy threshold can be found analytically and results can be generalized for a generic XY model with asymmetric coupling.

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I. INTRODUCTION

Systems with few degrees of freedom but good chaotic properties, can be characterized by standard statistical properties, for instance diffusive random-walk like behavior[1] or appearance of stationary distribution for single particle occupation numbers [2, 3, 4].

It is also generally assumed that, due to a sufficiently strong interaction, chaos will provide the mechanism in order to have ergodicity on the energy surface. Generally speaking, the degree of chaos will depend on the strength of the interparticle interaction and on the number of particles: typically, the larger the number of particles, the stronger is chaos, thus leading to more suitable conditions for ergodicity and statistical investigation.

This common lore is far from being satisfied by most physical systems, as explained by R.G. Palmer in his seminal paper[5] where, using his words: "The breakdown of ergodic behavior is discussed as a general phenomenon in condensed matter physics". In his paper the breakdown of ergodicity as due to an "effective" confinement of the system, respect to the observational timescale has been put forward. Nonetheless, to the best of our knowledge, there are no single examples where thresholds for broken ergodicity can be found analytically and, more important, where the relation with the interaction range has been remarked explicitly.

Only in recent years the relation between the dynamical properties, like chaos or ergodicity, and the kind of interparticle interaction has been studied [6]. Indeed, long-range interacting systems display peculiar properties from the point of view of statistical mechanics. It is well known for instance that, for such systems, the canonical and the microcanonical ensemble give different results, [7], thus questioning the validity of statistical mechanics. Moreover, chaos suppression in long-range interacting systems when the number of particles increases was recently found[8, 9, 10], and analytically investigated [11], thus leading to anomalous statistical behavior in the thermodynamical limit.

In this Paper, we investigate a one–dimensional spin chain model with two different ranges of interaction, nearest neighbors and "infinite" (all particles are interacting with all the others) and we show that, even in presence of dynamical chaos[12], a non–ergodic behavior is found, for any finite number of particles. Such non–ergodic behavior is mainly due to a unconnected phase space and the threshold for non-ergodicity can be obtained analytically. Moreover such non-ergodicity persists in the thermodynamical limit, actually the ratio between the disconnected portion of the energy range and the whole one approaches one, as the number of particles increases.

We have also found that, for all-to-all interaction, when the number of particles increases, the system dynamics becomes more regular. We also give numerical evidence that there is room for chaos in the non–ergodic region, for any finite number of particles.

For sake of comparison, we also consider the same model with short range interaction (nearest neighbor coupling) and we prove that this kind of disconnection does not exist. Of course, this does not imply that the system is ergodic, as also supported by our numerical simulations that indicate the presence of regular dynamics in some region of the energy space.

II. THE MODEL : CHAOTICITY *VS* INTERACTION RANGE

Our model is a variant of the one–dimensional Heisenberg model for N–spins. The Hamiltonian is given by:

$$H = J \sum_{\langle i,j \rangle} (s_i^x s_j^x - s_i^y s_j^y) \tag{1}$$

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where $\langle i,j\rangle$ stands for nearest neighbor ($\mathcal{N}$–interaction), or infinite range couplings (all–to–all, $\mathcal{A}$–interaction) and J is a positive constant.

Hamiltonian (1) gives rise to the standard nonlinear equations of motion:

$$\begin{cases} \dot{s}_i^x &= -J s_i^z \sum_{\langle j\rangle} s_j^y \\ \dot{s}_i^y &= -J s_i^z \sum_{\langle j\rangle} s_j^x \\ \dot{s}_i^z &= J \sum_{\langle j\rangle} (s_i^y s_j^x + s_i^x s_j^y), \end{cases} \quad (2)$$

where $\langle j\rangle$ is a shorthand notation for $j \neq i$ (in the case of $\mathcal{A}$–interaction) , and $j = i \pm 1$ when $\mathcal{N}$ interaction (without periodic boundary conditions) is assumed.

Constants of motion are the energy $H = E$, and the N squared moduli $|\vec{s}_i|^2$ (which we set equal to 1 for simplicity). For $N = 2$, an additional constant of motion, in involution with the others, is given by $s_1^z - s_2^z$, and the system becomes exactly integrable.

Let us notice that, in general, the only free parameters are the total energy E, the interaction strength J and the number of particles N. Moreover, for any finite number of particles N, the energy is bounded $|E| \leq E_{max}(J,N)$. One can also give a rough estimate for such border as $E_{max} \sim JN^2$ for $\mathcal{A}$-interaction and $E_{max} \sim JN$ for $\mathcal{N}$-interaction, even if the rigorous bound will be given below.

In order to make a fruitful comparison between $\mathcal{N}$ and $\mathcal{A}$ interaction and according to a general prescription [13] we rescale, for $\mathcal{A}$ interaction, the strength J to the number of particles N, setting $J = 2I/N$. In this way the energy of $\mathcal{A}$ systems scales with the number of particles in the same way as for $\mathcal{N}$ systems.

For $N > 2$, and sufficiently strong interaction (both $\mathcal{N}$ and $\mathcal{A}$ interaction) the system is chaotic in a large energy range $|E| < |E_{ch}(j,N)| < E_{max}$, as indicated by a maximal positive Lyapunov exponent. From now on, all results will be restricted to the chaotic energy region only.

Chaotic properties of the model has been analyzed within the frame of Standard Lyapunov analysis[14, 15]. In Fig.(1) we show the maximal Lyapunov exponent as a function of the energy per particle $\epsilon = E/N$ for different number of particles and $\mathcal{A}$ (upper) and $\mathcal{N}$ (lower) interaction. As one can see, while the maximal Lyapunov exponent λ_{max} depends on the energy per particle in some peculiar way, there is a large energy region where it is appreciably different from zero for both interactions. From the same picture it is clear that while increasing the number of particles in the case of $\mathcal{N}$ interaction, does not produces an appreciable variation of λ_{max}, the same variation in N, for $\mathcal{A}$ interaction, effectively decreases the value of λ_{max}. Even if it is difficult to give an exact scaling relation of the maximal Lyapunov exponent with all the system parameters (E,N,J) the approximate relation $\lambda_{max}(E=0,I=3) \sim 1/N^\alpha$ holds, where $\alpha = 0$ for $\mathcal{N}$ interaction and $\alpha = 1$ for $\mathcal{A}$ interaction, see Fig. (2).

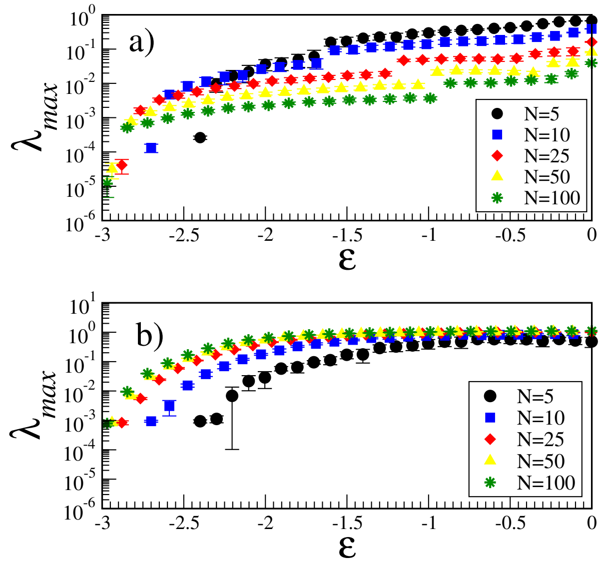

FIG. 1: a) Maximal Lyapunov exponent, λ_{max}, for different number of particles $N = 5$ (black) , $N = 10$ (blue), $N = 25$ (red), $N = 50$ (yellow) and $N = 100$ (green), as a function of the energy per particle $\epsilon = E/N$, for $\mathcal{A}$–interaction *a*), and for $\mathcal{N}$–interaction *b*). Error bars have been obtained as the standard deviation from a set of 20 initial trajectories on the same energy surface. Trajectories have been integrated for a time of 10^4. In *a*) the interaction constant has been chosen as $J = 2I/N$, with $I = 3$, while in *b*) $J = I = 3$.

The numerical results and the corresponding approximate relations are shown in Fig.(2) and indicate the absence of a chaotic dynamics for all-to-all interacting systems with a large number of particles.

The general trend where the maximal Lyapunov exponent decreases with the number of particles can be understood from the fact that in the limit $N \to \infty$ and for $\mathcal{A}$ interaction the model becomes close to an integrable one.

Indeed the Hamiltonian per particle can be written as:

$$\frac{H}{N} = I h_0 + \frac{I}{N} h_1 \quad (3)$$

where $h_0 = m_x^2 - m_y^2$ and $h_1 = \frac{1}{N}\sum_{i=1}^N \left[(s_i^y)^2 - (s_i^x)^2\right]$ where we have defined the average magnetization $m_k = \frac{1}{N}\sum_{i=1}^N s_i^k$, with $k = x, y$.

While both h_0 and h_1 remain on order 1 in the limit of large N, and fixed interaction strength I, the constant in front of h_1 goes to zero and the h_0 term dominates. A close inspection[16], and our numerical results indicate that h_0 represents an integrable model for any choice of parameters.

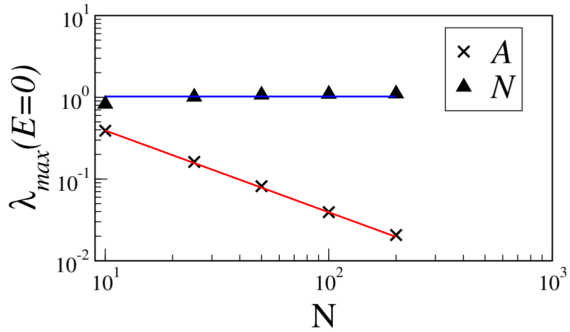

FIG. 2: Maximal Lyapunov exponent as a function of the number of particles, for the same parameters of Fig.(1) and $E = 0$. Triangles refer to $\mathcal{A}$ interaction, while crosses are for $\mathcal{N}$ interaction. Also shown the best fit lines $\lambda_N = 1.1 \pm 0.2$(blue) and $\lambda_A = (4.1 \pm 0.1)/N$ (red).

III. ERGODICITY : NUMERICAL RESULTS

While in two degrees of freedom systems the absence of ergodic motion in presence of chaos is somehow obvious (due to the presence of invariant tori), for many degrees of freedom systems the same occurrence is far from being trivial. In spite of that, we will now show that, for $\mathcal{A}$ interaction, an energy threshold exists below which one cannot have ergodic motion.

Let us first evaluate ensemble and time averages for the y magnetization and from them, respectively, the probability distributions $P^p(m_y)$ and $P^t(m_y)$.

Phase and time distributions of the mean magnetization are shown in Fig.(3) for the $\mathcal{N}$-interaction (right column) and $\mathcal{A}$-interaction (left column) with the same number of particles. All cases are characterized by a chaotic dynamics, as given by a maximal positive Lyapunov exponent, see Fig. (1).

As one can see, while for nearest neighbor interaction there is a good correspondence between the two averages (this of course does not mean ergodicity), in the case of all-to-all interaction there are strong deviations, in the lower energy case, see Fig.(3a). More precisely one trajectory with an initial $m_y > 0 (< 0)$ cannot reach a region with $m_y < 0 (> 0)$, below some energy threshold. Another difference is related to the presence of a two-peaks distribution: this indicates the presence of a phase transition and it will be the subject of a separate paper.

Strictly speaking, from these numerical results one can only infer that the time of transition from one peak to the other one is much larger than the simulation time. Nonetheless, in the next section we will show that such transition time does not exist. The origin of this deviation is that for those energy values less than the energy threshold the phase space is metrically decomposable[17] thus making the $\mathcal{A}$ system rigorously non-ergodic.

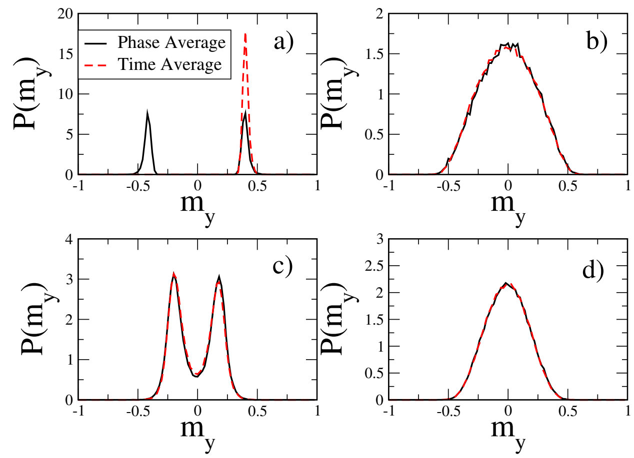

FIG. 3: Distribution of mean magnetization along the y-axis for $\mathcal{A}$ interaction (left column) and $\mathcal{N}$ interaction (right column). As black lines we show the phase distributions, $P^p(m_y)$, while red ones stand for time distributions, $P^t(m_y)$. Phase distributions have been obtained taking $M = 10^5$ different initial conditions upon the energy surface $E = -5$, a) and b) and $E = -1$, c) and d), while time averages have been obtained by computing one single trajectory in time on the same energy surface for a time $T = 10^5$ and taking values at time steps $\Delta t = 1$. Results have been checked on increasing the number of initial points upon the energy surface for the phase average, and on increasing the integration time T for the time average. Here is $N = 10$, and $I = 3$. Maximal Lyapunov exponents are positive for all the cases shown in this figure, as can be deduced from Fig.(1).

IV. NON–ERGODICITY BORDER : ANALYTICAL RESULTS

The existence of a threshold for the non ergodicity in case of $\mathcal{A}$ interaction can be proved by the following argument. Let us assume that initially the spins are oriented in such a way that $m_y(0) > 0$ with the energy E. It is clear that if we are able to prove that when $E < E_{ne}$ one cannot have the solution $m_y = 0$ on the energy surface $H = E$, it means that the trajectory should keep, for any time $m_y(t) > 0$. Since reversal of y single spin components results in change of y magnetization but not of the energy, the same argument can be applied to $m_y(0) < 0$ as well. In other words the space is metrically decomposable, since one trajectory with $m_y > 0$ cannot reach the region where $m_y < 0$ (and viceversa), although both regions belong to the same energy surface.

In order to find the explicit value of E_{ne} one should consider the problem of minimizing the value of the energy E under the constraint $m_y = (1/N) \sum_{i=1}^{N} s_i^y = 0$. In principle this task can be faced by means of the Lagrange multipliers. Nevertheless from a very simple argument we can estimate the critical energy E_{ne}.

Let us first derive the minimal energy, E_{min}, and then the non-ergodic energy, E_{ne}, for both $\mathcal{N}$ and $\mathcal{A}$ systems.

A. Minimal energy

We can find the minimal energy by minimizing the Hamiltonian (1) under the constraint:

$$(s_i^x)^2 + (s_i^y)^2 + (s_i^z)^2 = 1, \qquad i = 1, ..., N \tag{4}$$

We can take conditions (4) into account, switching to spherical coordinates:

$$\begin{cases} s_i^x &= \sin(\theta_i)\cos(\phi_i) \\ s_i^y &= \sin(\theta_i)\sin(\phi_i) \\ s_i^z &= \cos(\theta_i). \end{cases} \tag{5}$$

We can now rewrite Hamiltonian (1) as:

$$H = J \sum_{\langle i,j \rangle} \sin(\theta_i)\sin(\theta_j)\cos(\phi_i + \phi_j) \tag{6}$$

where

$$J = \begin{cases} (2I/N) & \text{for } \mathcal{A}\text{−interaction} \\ I & \text{for } \mathcal{N}\text{−interaction} \end{cases} \tag{7}$$

One absolute minimum value is obtained, for instance, setting:

$$\begin{cases} \sin(\theta_i) &= 1 \\ \cos(\phi_i + \phi_j) &= -1 \end{cases} \tag{8}$$

where $j = i + 1$ for $\mathcal{N}$ system and $j \neq i$ for $\mathcal{A}$ system.

While the first equation of (8) can be easily satisfied by both $\mathcal{N}$ and $\mathcal{A}$ system, assuming

$$\theta = \frac{\pi}{2} \tag{9}$$

some care should be taken in order to fulfill the second one.

For $\mathcal{N}$ system, we can put for instance:

$$\begin{cases} \phi_i = 0 & \text{for } i \text{ even} \\ \phi_i = \pi & \text{for } i \text{ odd} \end{cases} \tag{10}$$

On the contrary, for $\mathcal{A}$ system, we set

$$\phi_i = \pi/2 \qquad \text{for} \quad i = 1, ..., N. \tag{11}$$

Taking into account that there are $N - 1$ couplings in the $\mathcal{N}$ system and $N(N-1)/2$ in the $\mathcal{A}$ system, the minimal energy is given by (for both interactions):

$$E_{min} = -I(N - 1). \tag{12}$$

B. Non–ergodic threshold

We define the non–ergodic threshold E_{ne} in such a way that for any energy $E < E_{ne}$ the system is metrically decomposable. In order to find this non-ergodic (or disconnection) energy we have to find the minimum of Hamiltonian (1) under the additional constraint

$$m_y = 0. \tag{13}$$

For $\mathcal{A}$ system Hamiltonian (1) can be written as,

$$H = -\frac{I}{N}\sum (s_i^x)^2 + \frac{I}{N}\sum (s_i^y)^2 + INm_x^2 - INm_y^2 \tag{14}$$

Let us now search for the minimum of (14) under the constraints (4) and (13). In (14) the only term that can be negative under the given constraints is the first one, therefore,

$$E_{ne} \geq -I$$

If it is possible to minimize this term putting at the same time all the other to zero, we get the non-ergodic energy.

When N is even we can put half spins with $s_i^x = +1$, and half such that $s_i^x = -1$. In this way $m_x = 0$, $s_i^y = 0$ and $m_y = 0$, so that:

$$E_{ne} = -I, \quad \text{for } N \text{ even}$$

When N is odd we cannot minimize the first term in (14), and at the same time let the other terms to be zero, so that: $E_{ne} > -I$, for N odd.

Anyway it is easy to give an upper bound for E_{ne} which is sufficient for our scope. Indeed we can arrange $N - 1$ spins as in the previous case (N even), and for the last spin we assume $s_N^z = \pm 1$. In this way we have $m_x = 0$, $s_i^y = 0$ and $m_y = 0$, so that:

$$-I < E_{ne} \leq -I + I/N, \quad \text{for } N \text{ odd}$$

For $\mathcal{N}$ system, the non-ergodic energy, if defined as the minimum energy for which Eq.(13) holds, coincides with the minimal energy. Indeed the same values of ϕ_i (10) and θ_i (9) which minimize the Hamiltonian, satisfy condition (13) too, so that:

$$E_{ne} = E_{min} = -I(N - 1)$$

This of course does not exclude the possibility to have some other constraint that produces a disconnected phase space (even if such conclusion is not supported by our numerical simulations).

In Tables I and II we summarize the minimal and non-ergodic energies found.

As an interesting consequence of our results we note that the ratio:

$$r = \frac{|E_{ne} - E_{min}|}{|E_{min}|} \tag{15}$$

$\mathcal{A}$	E_{min}	E_{ne}
N_{even} :	$-I(N-1)$	$-I$
N_{odd} :	$-I(N-1)$	$(-I, -I + I/N]$

TABLE I: Minimal and non-ergodic energy for $\mathcal{A}$ system. Note that in the case of odd number of particles we give a lower and an upper bound for the non-ergodic energy.

$\mathcal{N}$	E_{min}	E_{ne}
	$-I(N-1)$	$-I(N-1)$

TABLE II: Minimal and non-ergodic energy for $\mathcal{N}$ system.

between the disconnected portion of the energy range and the total energy range, in the limit of a large number of particles at fixed interaction strength, goes to one for $\mathcal{A}$ interaction, and is exactly zero for $\mathcal{N}$ interaction, thus showing that in this limit the energy range is completely disconnected for $\mathcal{A}$ interaction only (note that in the positive region of the energy range the same argument used to show the existence of a non-ergodic energy can be applied considering m_x instead of m_y).

As one can see, for $\mathcal{A}$ interaction, as the number of particles increases the region of non–ergodicity does not decrease thus indicating that caution should be taken when ergodicity is tacitly assumed due to small interactions between many particles.

The presence of the non ergodic region is not related with the chaoticity of the system. Indeed, since the Lyapunov exponent increases linearly with the interaction strength, I, for any N we can find an I_c value such that there is well developed chaos for $E < E_{ne}$ and $I > I_c$, so that the system is chaotic and non-ergodic, below E_{ne}.

V. GENERALIZATION

Let us finally mention that the previous results can be easily generalized.

Let us consider a generic XY Model:

$$H = -J \sum_{\langle i,j \rangle} (s_i^y s_j^y + \eta s_i^x s_j^x) \qquad (16)$$

where $|\eta| \leq 1$ and $J > 0$. Following the same arguments given above, we can show the existence of a non-ergodic energy and roughly estimate their dependence on system parameters.

We will mainly focus on the ratio between the disconnected portion of the energy range and the total energy range, r, Eq. (15), in the limit of a large number of particles.

For $\mathcal{A}$ interaction, we can rewrite the Hamiltonian (16) as:

$$H = \frac{J}{2} \sum_i \left[\eta (s_i^x)^2 + (s_i^y)^2 \right] - \frac{J}{2} N^2 \left(\eta m_x^2 + m_y^2 \right) \qquad (17)$$

From this equation we can estimate, for large N

$$E_{min} \sim -\frac{J}{2} N^2,$$

As for the non-ergodic energy, following the same procedure described in the previous section, we have:

$$E_{ne} \simeq \begin{cases} -\frac{J}{2} N^2 \eta & \text{for} \;\; \eta > 0 \\ 0 & \text{for} \;\; \eta = 0 \\ \frac{J}{2} N \eta & \text{for} \;\; \eta < 0 \end{cases} \qquad (18)$$

so that

$$r \simeq \begin{cases} 1 - \eta & \text{for} \;\; \eta > 0 \\ 1 & \text{for} \;\; \eta \leq 0 \end{cases} \qquad (19)$$

As one can see $r = 0$ only for $\eta = 1$, while $r \neq 0$ for asymmetric coupling.

For the $\mathcal{N}$ case, we have that

$$E_{min} \sim -J(N-1),$$

while

$$-J(N-1) \leq E_{ne} \leq -J(N-3)$$

as one can see setting, for instance,

$$s_i^x = \begin{cases} 1 & \text{for} \;\; i \text{ odd} \\ -1 & \text{for} \;\; i \text{ even} \end{cases} \qquad (20)$$

Note that for $N \gg 1$, $E_{min} \simeq E_{ne}$ so that $r = 0$ for any η.

Thus, we can conclude that broken ergodicity is generic for asymmetric coupling and all-to-all interaction.

VI. CONCLUSIONS

In conclusion we have studied a spin chain model from the dynamical point of view for two different ranges of inter-spin interaction (nearest neighbor and all-to-all). Both models are mainly chaotic, in the sense that the dynamics is characterized by a positive maximal Lyapunov exponent in a wide energy region. Nevertheless, in the case of an infinite range of interaction, the motion does not explore the whole energy surface. This can be understood on the basis of a special topology of the phase space. An analytical estimate gives an energy threshold below which the system is rigorously non–ergodic: the existence of the threshold has been also confirmed by numerical simulations. Moreover, for any interaction strength, on increasing the number of particles the range of energy values characterized by such non ergodic motion spans a finite portion of the whole energy range, if the interaction has an infinite range. This could be particularly relevant in the study of multidimensional systems, where usually ergodicity is tacitly assumed for a large number of weak–interacting particles. We have also shown that this phenomenon is generic for XY model with asymmetric coupling.

Further studies about the consequences of broken ergodicity with respect to phase transitions, and the comparison with the correspondent quantum system are under current investigations[16].

VII. ACKNOWLEDGMENTS

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[1] B.V.Chirikov, Phys. Rep., **52**, 263, (1979).
[2] V. V. Flambaum and F. M. Izrailev, Phys. Rev. E **56**, 5144, (1997)
[3] F. Borgonovi and F. M. Izrailev, Phys. Rev. E **62**, 6475, (2000)
[4] F.Borgonovi, I.Guarneri, F.M.Izrailev and G.Casati, Phys. Lett. A **247** , 140 (1998)
[5] R.G. Palmer, Adv. in Phys.**31**, 669 (1982)
[6] A. Campa et al, Phys. Lett. A **286**, 251, (2001)
[7] J. Barré, D. Mukamel, S. Ruffo, Phys. Rev. Lett. **87**, 3, (2001)
[8] V. Latora, A. Rapisarda, and S. Ruffo, Phys. Rev. Lett. **80**, 692, (1998)
[9] C. Anteneodo, C. Tsallis, Phys. Rev. Lett. **80**, 24, (1998)
[10] C. Tamarit, C. Anteneodo, Phys. Rev. Lett. **84**, 208, (2000)
[11] M. C. Firpo, Phys. Rev. E **57**, 6599, (1998); M. C. Firpo and S. Ruffo, Journal of Physics A, 34, L511, (2001); C. Anteneodo, R.N.P. Maia and R. Vallejos, Phys. Rev. E **68**, 036120, (2003).
[12] According to the common lore we here call chaotic system the ones characterized in some parameters range by a positive maximal Lyapunov exponent.
[13] J. Barré, T. Dauxois, S. Ruffo, Physica A **295**, 254 (2001)
[14] G.Benettin, Physica **13D**, (1984) 211.
[15] A.J.Lichtenberg and M.A.Lieberman, *Regular and Stochastic Motion*, Applied Math. Series 38 Spinger-Verlag (1983)
[16] in preparation.
[17] A.I.Khinchin *Mathematical Foundations of Statistical Mechanics*, Dover Publications, New York (1949)
[18] F. Borgonovi, G. Celardo, F. M. Izrailev, G. Casati, Phys. Rev. Lett. **88**, 5, (2002)