# Breakdown of Exponential Sensitivity to Initial Conditions: Role of the Range of Interactions

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Within a microcanonical scenario we numerically study an $N$-sized linear chain classical inertial $XY$ model including ferromagnetic couplings which decrease with distance as $r^{-\alpha}$ ($\alpha \geq 0$). We show that for $N \to \infty$ (thermodynamic limit): (i) The energy per particle $E_N/N$ scales like $N^* \equiv (N^{1-\alpha} - 1)/(1 - \alpha)$; (ii) The properly scaled maximum Lyapunov exponent $\tilde{\lambda}_N^{\max}$ tends, for $E_N/(NN^*)$ above a threshold, to zero for and only for $\alpha \leq 1$. These results are analogous to those observed in low-dimensional and in self-organized critical dissipative systems. This entire picture suggests a connection with the nonextensive thermostatistics recently introduced by one of us. [S0031-9007(98)06314-5]

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*Ergodicity* is the basis of standard statistical mechanics and thermodynamics. The typical situation is as follows. A large Hamiltonian system with nonlinear short-range interactions has its microscopic dynamics characterized by a Lyapunov spectrum [1,2], whose largest value generically remains strictly positive *even at the thermodynamic limit* ($N \to \infty$). In other words, its sensitivity to the initial conditions is the standard one (*exponential*). Consequently, the predominant microscopic dynamical behavior is chaotic, which implies a quick occupation of practically all the allowed phase space. It is within this scenario that Boltzmann-Gibbs (BG) statistics is founded, thus yielding the usual, *extensive* thermodynamics (entropy, internal energy, free energy, and similar quantities are *extensive* functions of the *intensive* external parameters such as temperature, pressure, chemical potentials, and others). It is along these lines that the beautiful formalism referred to as statistical mechanics has proved, for well more than one century now, its power and usefulness in physics. However, more and more frequently nowadays, physical situations are identified and studied which badly accommodate this viewpoint. Within a long list we may mention Lévy anomalous diffusion (see [3,4] and references therein), stellar polytropes [5,6], anomalous phonon-electron thermalization in ion-bombarded solids [7], pure-electron plasma two-dimensional turbulence [6,8], solar neutrinos [9], inverse bremsstrahlung in plasma [10], and cosmology [11]. The main purpose of the present effort is to illustrate one of the generic mechanisms that can consistently produce both dynamical and thermodynamical anomalies; we refer to long-range interactions in a conservative (Hamiltonian) system. As supplementary bonuses we shall (i) better understand the deep meaning of the usual (artificially extensive) manner of presenting mean-field-like Hamiltonians; (ii) exhibit strong analogies with anomalous low-dimensional (edge of chaos) [12] as well as high-dimensional (self-organized criticality [13]) [14] dissipative systems; (iii) discuss the connections with the recently introduced nonextensive thermostatistics [15].

Let us consider the following $d = 1$ classical Hamiltonian (with periodic boundary conditions):

$$\mathcal{H} = \frac{1}{2}\sum_{i=1}^{N} L_i^2 + \frac{1}{2}\sum_{i \neq j} \frac{1 - \cos(\theta_i - \theta_j)}{r_{ij}^{\alpha}} \equiv E_k + E_p \quad (\alpha \geq 0; r_{ij} = 1, 2, 3, \ldots), \qquad (1)$$

where, without loss of generality, we have considered unit momenta of inertia and unit first-neighbor coupling constants, and where $\{\theta_i, L_i\}$ are conjugate canonical pairs. Since the model is essentially defined on an $N$-sized ring, every pair of (classical) spins determines, along the ring, two "distances" and not one: the $r_{ij}$ which we consider in the Hamiltonian is the *minimal* one. The model basically is a classical inertial $XY$ ferromagnet (coupled rotators), and the limiting cases $\alpha \to \infty$ and $\alpha = 0$ correspond to the first-neighbor [1,16] and mean-field-like models, respectively. The kinetic contribution $E_k$ contains $N$ different terms; the potential one $E_p$ contains $N(N-1)/2$ different terms and $\frac{E_p}{N}$ is bounded from above by a value which, for the more general, $d$-dimensional, case is asymptotically proportional to $N^* \equiv \int_1^{N^{1/d}} dr\, r^{d-1} r^{-\alpha} = \frac{N^{1-(\alpha/d)} - 1}{1 - \frac{\alpha}{d}}$. In the $N \to \infty$ limit, $N^*$ behaves, respectively, like $\frac{N^{1-(\alpha/d)}}{1-\frac{\alpha}{d}}$ (hence $N$ for $\alpha = 0$), $\ln N$, and $\frac{1}{\frac{\alpha}{d} - 1}$ for $0 \leq \alpha < d$, $\alpha = d$, and $\alpha > d$.

It is clear that the model is thermodynamically *extensive* for $\alpha > d$ and *nonextensive* otherwise. However, this model can be written in an artificially *pseudoextensive* manner as follows:

$$\mathcal{H}' = \frac{1}{2}\sum_{i=1}^{N} L_i^2 + \frac{1}{2N^*}\sum_{i \neq j} \frac{1 - \cos(\theta_i - \theta_j)}{r_{ij}^{\alpha}} \quad (\alpha \geq 0;\ r_{ij} = 1, 2, 3, \ldots). \qquad (2)$$

This presentation should be considered as very artificial indeed, since it turns the *microscopic* coupling constants $N$ dependent, i.e., modified through *macroscopic* information. At this (conceptually rather high) price, we obtain a thermodynamically (pseudo) extensive quantity for *all* values of $\alpha$ [17]. In particular, for $\alpha = 0$, we obtain the usual mean-field-like form, within which the coupling constant is renormalized by $N$. This special case has been focused by several authors [18,19]. Recently, Latora, Rapisarda, and Ruffo [19] obtained quite interesting results which we shall connect to ours later on.

Before going on let us exhibit a convenient connection between $\mathcal{H}$ and $\mathcal{H}'$. If we take into account that the variables $\{L_i\}$ involve a first derivative with respect to time $t$, we immediately verify that

$$\mathcal{H} = N^* \mathcal{H}', \tag{3}$$

where the time scales $t$ and $t'$ respectively, associated with $\mathcal{H}$ and $\mathcal{H}'$ satisfy $t' = \sqrt{N^*}\, t$. Consequently, if we recall that by definition the Lyapunov exponents appear multiplied by $t$ in all expressions concerning the sensitivity to the initial conditions, and note that $\lambda_N^{\max}$ and $\lambda_N'^{\max}$ are the largest Lyapunov exponents, respectively, associated with Hamiltonians $\mathcal{H}$ and $\mathcal{H}'$, we have that

$$\tilde{\lambda}_N^{\max} \equiv \frac{\lambda_N^{\max}}{\sqrt{N^*}} = \lambda_N'^{\max}. \tag{4}$$

This relationship will prove generically helpful later on (and very particularly in order to compare our $\alpha = 0$ results with those presented in [19]). At the present stage let us make clearer what we refer to. If we call $x$ the direction in the $2N$-dimensional phase space corresponding to the largest Lyapunov exponent and define $\xi \equiv \lim_{\Delta x(0)\to 0} \frac{\Delta x(t)}{\Delta x(0)}$, then we have $\xi = \exp(\lambda_N^{\max} t)$ for the Hamiltonian $\mathcal{H}$. It is, however, known that Lyapunov exponents, due to the fact that they carry a physical dimension (inverse time), are not mathematically fully defined in the sense that they are not *dimensionless* quantities. Consequently, either we have to restrict our considerations to *ratios* of Lyapunov exponents, or we must *refer them all to a unique conventional time unit.* We shall adopt the latter. More precisely, we can rewrite $\xi$ as follows: $\xi = \exp(\lambda_N^{\max} t) = \exp([\lambda_N^{\max}/\sqrt{N^*}][\sqrt{N^*}\, t]) \equiv \exp(\tilde{\lambda}_N^{\max} \tilde{t})$. The practical use of this transformation will become transparent on Fig. 1.

The numerical simulation we have implemented in the present work is a standard molecular dynamics one within a microcanonical scenario (applied to Hamiltonian $\mathcal{H}$ associated with $N$ spins), this is to say at fixed total energy $E_N$. As initial conditions ($t = 0$ values) we have used random values of $\theta_i$ compatible with the expected equilibrium distribution (which, for the relatively high energy region mainly focused in the present Letter, corresponds to a uniform distribution in the interval $[0, 2\pi]$), and a "water-bag" distribution (i.e., a symmetric uniform

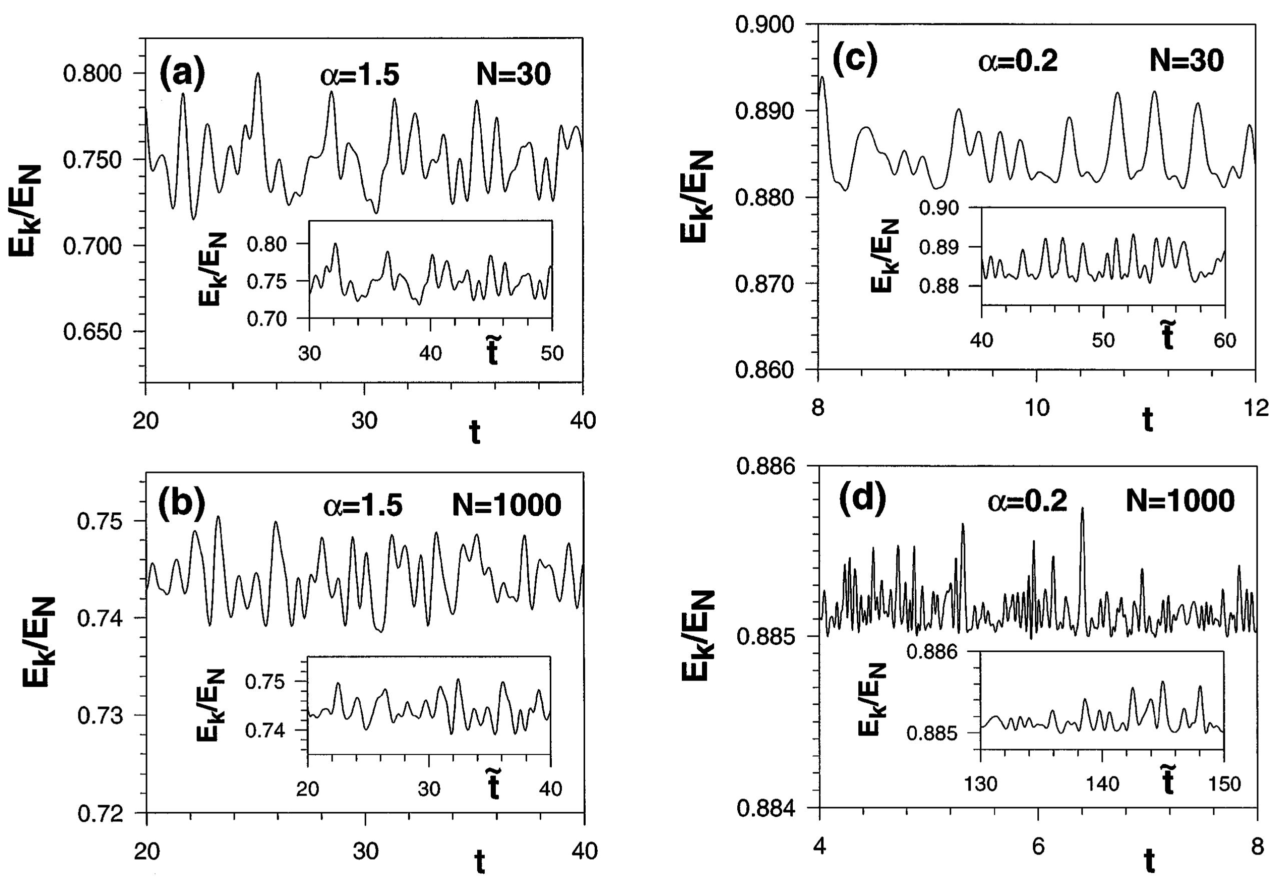


FIG. 1. Evolution of $\frac{E_k}{E_N}$ as a function of $t$, for a $\frac{E_N}{NN^*} = 5$ single realization for typical values of $(\alpha, N)$ (the insets contain the same examples as functions of $\tilde{t}$). We recall that, for $\alpha > 1$, $N^*$ is asymptotically independent from $N$, whereas, for $\alpha \leq 1$, $N^*$ strongly depends on $N$. It is remarkable that the dominating frequency, in the $\tilde{t}$ variable, of the fluctuations is $N$ independent $\forall\ \alpha$, whereas, in the $t$ variable, this occurs *only* for $\alpha > 1$.

distribution on a compact support, in such a way that the total angular momentum equals zero) for the $\{L_i\}$. The time evolution has then followed Newton's law (using a fourth-order symplectic algorithm [20] with a relative error in the total energy conservation less than $10^{-4}$). A typical evolution of $E_k$ is presented in Fig. 1. For each choice of $(\alpha, \frac{E_N}{NN^*}, N)$ we have typically run 100 realizations for small systems ($N = 5, 10$) down to a few for large systems ($N = 1000$), and then averaged, over all the realizations, the maximal Lyapunov exponents (calculated by the method of Benettin *et al.* [21]). Typical results are presented in Figs. 2 and 3. The fact that, for fixed $(\alpha, N)$, the thermodynamic variable which generically emerges [as follows from our earlier considerations concerning Eq. (1)] is $\frac{E_N}{NN^*}$ and not the usual $\frac{E_N}{N}$ one clearly reflects the possible nonextensivity of the system: only for $\alpha > 1$ (short-range interactions) is $\frac{E_N}{N}$ the convenient variable. Also, since *both* $\frac{E_N}{NN^*}$ and $\frac{E_k}{E_N}$ remain *finite* in the $N \to \infty$ limit, so does $\frac{E_k}{NN^*}$ which is $\propto \frac{k_B T}{N^*}$; hence, for $\alpha \le 1$, the correct variable to describe, say, an equation of states is *not* the usual *intensive* variable $T$ but the present renormalized one [22], i.e., $T^* \equiv \frac{T}{N^*}$ (through these transformations for $\alpha = 0$, we precisely recover Fig. 1 of [19], for instance). These facts are absolutely consistent with recent results presented in the literature for a variety of long-range interaction physical situations [22] (Lennard-Jones-like fluids, magnets).

Let us summarize our main results. We have shown, for the particular classical magnetic model herein studied, that the thermodynamics is *extensive* if and only if $\alpha > 1$ (short-range interactions); the *nonextensivity* which appears for $0 \le \alpha \le 1$ (long-range interactions) is illustrated, among others, by the fact that the *macroscopic* energy quantity which remains well defined at the thermodynamic limit ($N \to \infty$) is $\frac{E_N}{NN^*}$ and *not* the usual one $\frac{E_N}{N}$. The *microscopic* dynamical counterpart of this extensive-nonextensive critical point is very enlightening, namely, the fact that, above a ($\alpha$-dependent) threshold of $\frac{E_N}{NN^*}$ (approximately corresponding to the maxima of $\tilde{\lambda}_N^{\max}$ in the plots of Fig. 2), the largest properly scaled Lyapunov exponent ($\tilde{\lambda}_N^{\max}$) remains, at the thermodynamic limit, positive and finite for short-range interactions but *collapses to zero (and with it the entire Lyapunov spectrum) for long-range interactions* (see Fig. 3). In other words, the range of the interactions controls the type of sensitivity to the initial conditions that a *large* system will exhibit: strong chaos (exponential law) clearly is the case for short-range interactions, and weak chaos (presumably power law) for long-range interactions. The former will exhibit standard ergodicity, whereas important anomalies are to be expected for the latter. It goes without saying that the present scenario is expected to hold for large classes of Hamiltonian systems and not only for the system herein studied.

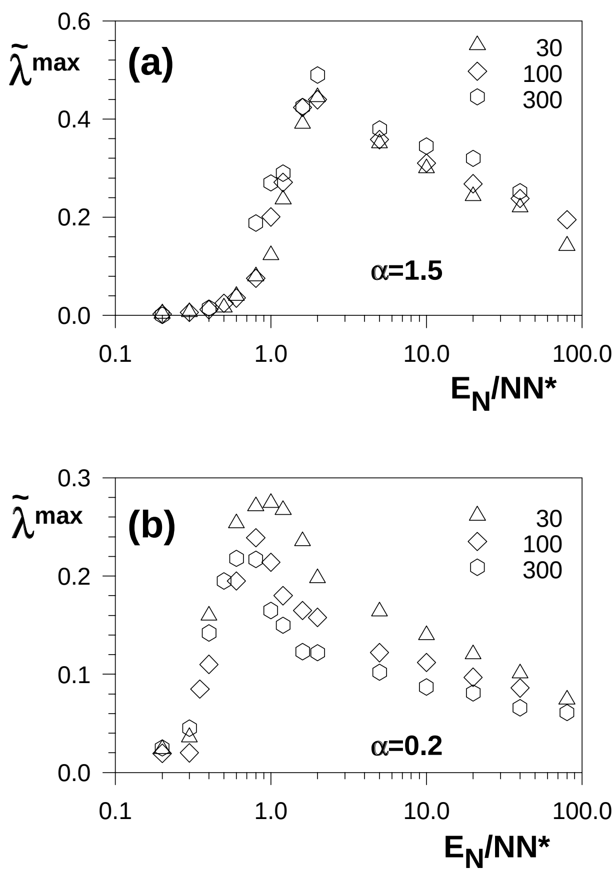


FIG. 2. The $\frac{E_N}{NN^*}$ dependence of the properly scaled Lyapunov exponent $\tilde{\lambda}_N^{\max}$ for $\alpha = 1.5$ (a) and $\alpha = 0.2$ (b) and typical values of $N$. As it is illustrated in Fig. 3, the $N \to \infty$ limit yields, for high enough energies (essentially above the para-ferro phase transition critical value), a nonvanishing (vanishing) $\tilde{\lambda}_N^{\max}$ for $\alpha > 1 (\le 1)$.

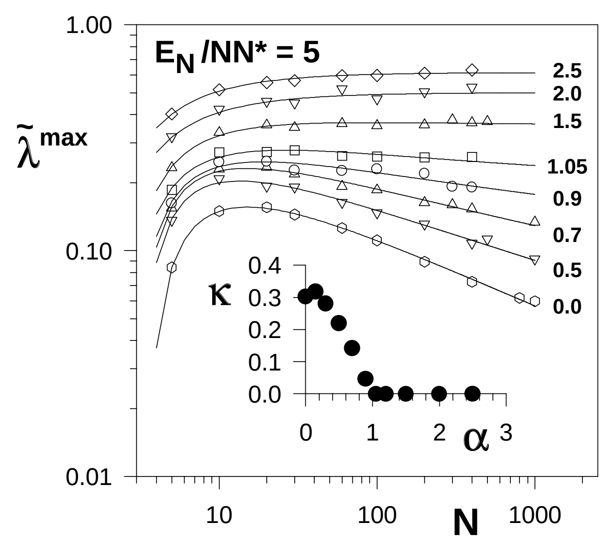


FIG. 3. $\tilde{\lambda}_N^{\max}$ versus $N$ (log-log plot) for typical values of $\alpha$ and $\frac{E_N}{NN^*} = 5$. The full lines are the best fittings with the forms $(a - \frac{b}{N})/(N^*)^c$. Consequently, $\tilde{\lambda}_N^{\max} \propto N^{-\kappa(\alpha)}$ where $\kappa(\alpha) = (1 - \alpha)c$ for $0 \le \alpha < 1$ and $\kappa(\alpha) = 0$ for $\alpha > 1$; for $\alpha = 1$, $\tilde{\lambda}_N^{\max}$ is expected to vanish as a power of $1/\ln N$. Inset: $\kappa$ versus $\alpha$ (related random matrices arguments will be detailed elsewhere).

To discuss the present (as well as other) anomalies, a generalized statistical formalism has been advanced and developed during the last few years [15]. The generalization essentially consists in considering the following entropic form: $S_q = \frac{1-\sum_i p_i^q}{q-1}$ ($\sum_i p_i = 1$; $q \in \mathcal{R}$ characterizes the degree of nonextensivity), which recovers the usual BG entropy ($-\sum_i p_i \ln p_i$) in the limit $q \to 1$; $S_q(A + B) = S_q(A) + S_q(B) + (1 - q)S_q(A)S_q(B)$, if $A$ and $B$ are *independent* systems in the sense that the probabilities of $A + B$ *factorize* into those of $A$ and of $B$. A wealth of works has shown that the above nonextensive thermostatistical prescription retains much of the formal structure of the standard theory such as Legendre thermodynamic structure, $H$ theorem, Onsager reciprocity theorem, Kramers and Wannier relations, Bogolyubov inequality, and thermodynamic stability, among others [15,23]. This formalism has proved to correctly describe a variety of *dissipative* nonlinear systems (both low [12] and high [14] dimensional cases, respectively, related to the edge of chaos and to self-organized criticality). Details can be seen in [12], but, in particular, it has been argued that the solution of $d\xi/dt = \lambda_q \xi^q$ is given by $\xi(t) = [1 + (1 - q)\lambda_q t]^{1/(1-q)}$. This solution recovers the standard, *exponential* law in the limit $q \to 1$ (extensive case), but it implies a *power-law* sensitivity when nonextensivity takes place ($q \neq 1$). Several examples of $q \neq 1$ situations have been exhibited [12] (logisticlike, periodic, and circular maps as well as in the Bak-Sneppen model for biological evolution). The attractors towards which the systems evolve are complex (multifractal) ones, a fact which implies anomalies in what concerns the validity of standard ergodicity. The present work provides evidence that Hamiltonian (i.e., conservative) long-range interaction systems might be further examples of nonextensivity along the above lines ($q \neq 1$).

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