Sensitivity to initial conditions of a d-dimensional long-range-interacting quartic Fermi-Pasta-Ulam model: Universal scaling

Debarshee Bagchi[1,*] and Constantino Tsallis[2,3,†]

[1]*Centro Brasileiro de Pesquisas Fisicas, Rua Xavier Sigaud 150, 22290-180 Rio de Janeiro-RJ, Brazil*

[2]*Centro Brasileiro de Pesquisas Fisicas and National Institute of Science and Technology of Complex Systems, Rua Xavier Sigaud 150, 22290-180 Rio de Janeiro-RJ, Brazil*

[3]*Santa Fe Institute, 1399 Hyde Park Road, Santa Fe, New Mexico 87501, USA*

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We introduce a generalized d-dimensional Fermi-Pasta-Ulam model in the presence of long-range interactions, and perform a first-principle study of its chaos for $d = 1,2,3$ through large-scale numerical simulations. The nonlinear interaction is assumed to decay algebraically as $d_{ij}^{-\alpha}$ ($\alpha \geqslant 0$), $\{d_{ij}\}$ being the distances between N oscillator sites. Starting from random initial conditions we compute the maximal Lyapunov exponent $\lambda_{\rm max}$ as a function of N. Our $N \gg 1$ results strongly indicate that $\lambda_{\rm max}$ remains constant and positive for $\alpha/d > 1$ (implying strong chaos, mixing, and ergodicity), and that it vanishes like $N^{-\kappa}$ for $0 \leqslant \alpha/d < 1$ (thus approaching weak chaos and opening the possibility of breakdown of ergodicity). The suitably rescaled exponent κ exhibits universal scaling, namely that $(d+2)\kappa$ depends only on α/d and, when α/d increases from zero to unity, it monotonically decreases from unity to zero, remaining so for all $\alpha/d > 1$. The value $\alpha/d = 1$ can therefore be seen as a critical point separating the ergodic regime from the anomalous one, κ playing a role analogous to that of an order parameter. This scaling law is consistent with Boltzmann-Gibbs statistics for $\alpha/d > 1$, and possibly with q statistics for $0 \leqslant \alpha/d < 1$.

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I. INTRODUCTION

Many-body systems with long-range-interacting forces are very important in nature, the primary example being gravitation. Long-ranged systems deviate significantly from the conventional "well behaved" systems in many respects. Various features like ergodicity breakdown, ensemble inequivalence, nonmixing nonlinear dynamics, partial (possibly hierarchical) occupancy of phase space, thermodynamical nonextensivity for the total energy, longstanding metastable states, phase transitions even in one dimension, and other anomalies, can be observed in systems with long-range interactions. Consistently, some of the usual premises of Boltzmann-Gibbs (BG) statistical mechanics are challenged and an alternative thermostatistical description of these systems becomes necessary in many instances. For some decades now, q statistics [1,2] has been a useful formalism to study such systems, and has led to satisfactory experimental validations for a wide variety of complex systems (see, for instance, [3–17]). The deep understanding of the microscopical nonlinear dynamics of such systems naturally constitutes a must in order to theoretically legitimize the efficiency of the q generalization of the BG theory. For classical systems such as many-body Hamiltonian ones and low-dimensional maps, a crucial aspect concerns the sensitivity to the initial conditions, which is characterized by the spectrum of Lyapunov exponents. If the maximal Lyapunov exponent $\lambda_{\rm max}$ is positive, mixing and ergodicity are essentially warranted, and we consequently expect the BG entropy and statistical mechanics to be applicable. If instead $\lambda_{\rm max}$ vanishes, the sensitivity to the initial conditions is subexponential, typically a power law with time, and we might expect nonadditive entropies such as S_q and its associated statistical mechanics to emerge, as has been observed numerically as well as experimentally in many systems (see, for instance, [16–23]).

II. MODEL AND THE NUMERICAL SCHEME

In the present paper we extend to d dimensions ($d = 1,2,3$) and numerically study from first principles (i.e., using only Newton's law $\vec{F} = m\vec{a}$) the celebrated Fermi-Pasta-Ulam (FPU) model with periodic boundary conditions; nonlinear long-range interactions between all the $N = L^d$ oscillators are allowed as well. The Hamiltonian is the following one:

$$\mathcal{H} = \sum_i \frac{\vec{p}_i^{\,2}}{2m_i} + \frac{a}{2}\sum_i (\vec{r}_{i+1} - \vec{r}_i)^2 + \frac{b}{4\tilde{N}}\sum_i \sum_{j\neq i} \frac{(\vec{r}_i - \vec{r}_j)^4}{d_{ij}^{\alpha}}, \tag{1}$$

where $\vec{r}_i$ and $\vec{p}_i$ are the displacement and momentum of the ith particle with mass $m_i \equiv m$; $a \geqslant 0$, $b > 0$, and $\alpha \geqslant 0$. Here d_{ij} is the shortest Euclidean distance between the ith and jth lattice sites ($1 \leqslant i,j \leqslant N$); this distance depends on the geometry of the lattice (ring, periodic square, or cubic lattices). Thus for $d = 1$, $d_{ij} = 1,2,3,\ldots$; for $d = 2$, $d_{ij} = 1,\sqrt{2},2,\ldots$, and, for $d = 3$, $d_{ij} = 1,\sqrt{2},\sqrt{3},2,\ldots$ If $\alpha/d > 1$ ($0 \leqslant \alpha/d \leqslant 1$) we have short-range (long-range) interactions in the sense that the potential energy per particle converges (diverges) in the thermodynamic limit $N \to \infty$; in particular, the $\alpha \to \infty$ limit corresponds to only first-neighbor interactions, and the $\alpha = 0$ value corresponds to typical mean field approaches, when the coupling constant is assumed to be independent from distance. The instance $(d,\alpha) = (1,\infty)$ recovers the original β-FPU Hamiltonian, that has been profusely studied in the literature; the $d = 1$ model and generic α has been addressed in [24].

*debarshee@cbpf.br

†tsallis@cbpf.br

Although not necessary (see [19]), we have followed the current use and have made the Hamiltonian extensive for all values of α/d by adopting the scaling factor $\tilde{N}$ in the quartic coupling, where

$$\tilde{N} \equiv \sum_{i=1}^{N} \frac{1}{d_{ij}^{\alpha}}. \tag{2}$$

Hence $\tilde{N}$ depends on α, N, d, and the geometry of the lattice. Note that for $\alpha = 0$ we have $\tilde{N} = N$, which recovers the rescaling usually introduced in mean field approaches. In the thermodynamic limit $N \to \infty$, $\tilde{N}$ remains constant for $\alpha/d > 1$, whereas $\tilde{N} \sim \frac{N^{1-\alpha/d}}{1-\alpha/d}$ for $0 \leqslant \alpha/d < 1$ ($\tilde{N} \sim \ln N$ for $\alpha/d = 1$); see details in [19] and references therein.

Let us mention that the analytical thermostatistical approach of the present model is in some sense even harder than that of coupled XY or Heisenberg rotators already addressed in [19,25–28]. Indeed, the standard BG approach of these models is analytically tractable, whereas not even that appears to be possible for the original FPU, not to say anything for the present generalization. Therefore, for this kind of many-body Hamiltonian, the numerical approach appears to be the only tractable one.

To numerically solve the equations of motion (Newton's law) we have employed the symplectic second order accurate velocity Verlet algorithm. To accelerate the computationally expensive part of the force calculation routine we have exploited the convolution theorem and used a fast Fourier transform algorithm. This yields a considerable reduction in the number of operations for force calculation from $O(N^2)$ to $O(N \ln N)$, thus facilitating computation for larger system sizes and longer times.

We choose the time step Δt (which is typically $\sim 10^{-3}$ for most of our results) such that the standard deviation of the energy density over the entire simulation time (i.e., the number of iterations required by the maximal Lyapunov exponent to saturate, which is typically $\sim 10^5$–10^6 iterations, depending on system parameters) is of the order of 10^{-4} or smaller (for the range of N considered here, $10 < N < 10^6$).

Starting from random initial displacements $\vec{r}_i$ drawn from a uniform distribution centered around zero, and momenta $\vec{p}_i$ from a Gaussian distribution with zero mean and unit variance, we evolve the system and compute the maximal Lyapunov exponent $\lambda_{\max}$ defined as follows:

$$\lambda_{\max} = \lim_{t \to \infty} \lim_{\delta(0) \to 0} \frac{1}{t} \ln \frac{\delta(t)}{\delta(0)}, \tag{3}$$

where $\delta(t) = \sum_i (\delta r_i^2 + \delta p_i^2)^{1/2}$ is the metric distance between the fiducial orbit and the reference orbit having initial displacement $\delta(0)$. We numerically compute this quantity by using the algorithm by Benettin *et al.* [29]. For typical values of the exponent α, we compute $\lambda_{\max}$ as a function of the system size N for $d = 1$, 2, and 3.

III. SIMULATION RESULTS

Let us now present the results of our numerical analysis by setting $m = 1$ (no loss of generality), and fixing the energy density $u \equiv U/N = 9.0$ and $b = 10.0$ for all d, unless stated otherwise, where U is the total energy associated with $\mathcal{H}$. Additionally, we have set the harmonic term to zero, i.e., $a = 0$, for reasons that will be elaborated later. In fact such a model, with only the quartic anharmonic nearest neighbor interactions, has been studied previously in the context of heat conduction [30].

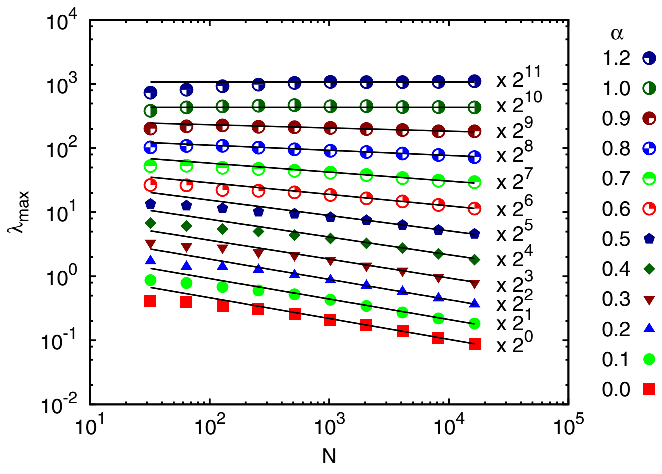

FIG. 1. Log-log plot of the dependence, for a ring ($d = 1$), of the maximal Lyapunov exponent $\lambda_{\max}$ on the number $N = L$ of oscillators for $(a,b,u) = (0,10,9)$ and typical values of the exponent α. Each individual curve has been multiplied by the number indicated next to it for visualization clarity.

In Figs. 1, 2, and 3 we present, for $d = 1$, 2, and 3, respectively, the maximal Lyapunov exponent $\lambda_{\max}$ as a function of the system size for typical values of the exponent α. We find that, for $\alpha > d$, $\lambda_{\max}$ saturates to a positive value with increasing N, which strongly suggests that it will remain so for $N \to \infty$, thus leading to ergodicity, which in turn legitimizes the BG thermostatistical theory. In contrast, for $0 \leqslant \alpha < d$, $\lambda_{\max}$ algebraically decays with $N = L^d$ as

$$\lambda_{\max} \sim N^{-\kappa}, \tag{4}$$

where $\kappa > 0$ and depends on (α, d). Assuming that it remains so for increasingly large N, we expect $\lim_{N \to \infty} \lambda_{\max} = 0$, which implies that the entire Lyapunov spectrum vanishes. This characterizes weak chaos for $0 < \alpha/d < 1$, i.e.,

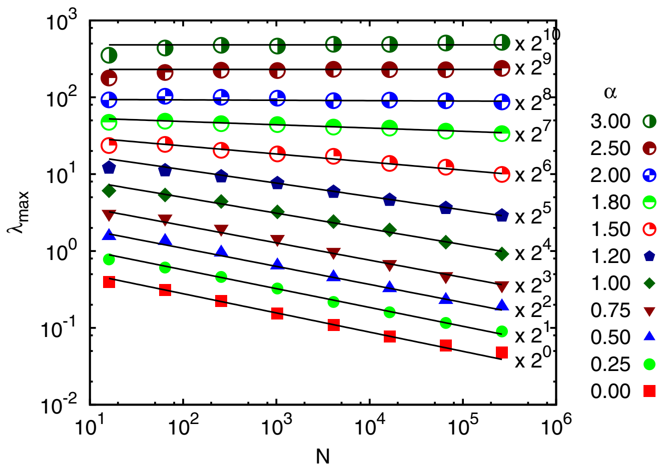

FIG. 2. Same as in Fig. 1 for a periodic square lattice ($d = 2$) with $N = L^2$ oscillators.

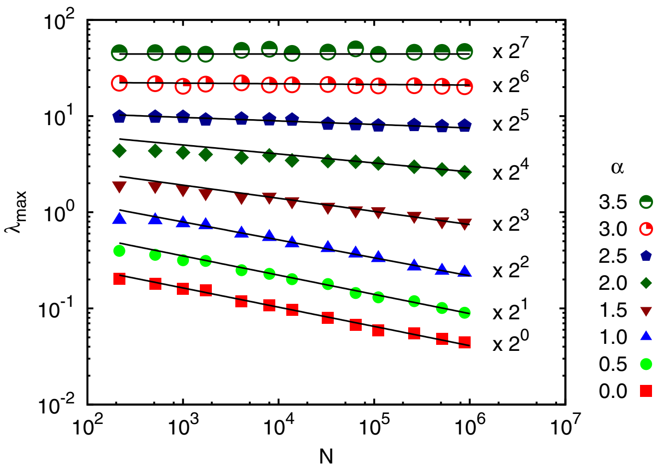

FIG. 3. Same as in Fig. 1 for a periodic cubic lattice ($d = 3$) with $N = L^3$ oscillators.

subexponential sensitivity to the initial conditions, which opens the door for breakdown of mixing, or of ergodicity, or some other nonlinear dynamical anomaly. Within this scenario, the violation of Boltzmann-Gibbs statistical mechanics in the $N \to \infty$ limit becomes strongly plausible (see, for example, [23,24]).

From the results illustrated in Figs. 1, 2, and 3 we compute the exponent $\kappa(\alpha,d)$ for $d = 1$, 2, and 3, as shown in Fig. 4, including its inset. We find that $\kappa(\alpha,d) > 0$ for $0 \leqslant \alpha < d$, and, within numerical accuracy, vanishes for $\alpha > d$. Also note that $\kappa(0,d)$ decreases for increasing d. Remarkably enough, all three curves in the inset of Fig. 4 can be made to collapse onto a single curve through the scalings $\alpha \to \alpha/d$ and $\kappa(\alpha,d) \to (d+2)\kappa(\alpha,d)$. This is shown in the main figure of Fig. 4. In other words, $(d+2)\kappa(\alpha,d) = f(\alpha/d)$, where $f(x)$ appears to be a universal function.

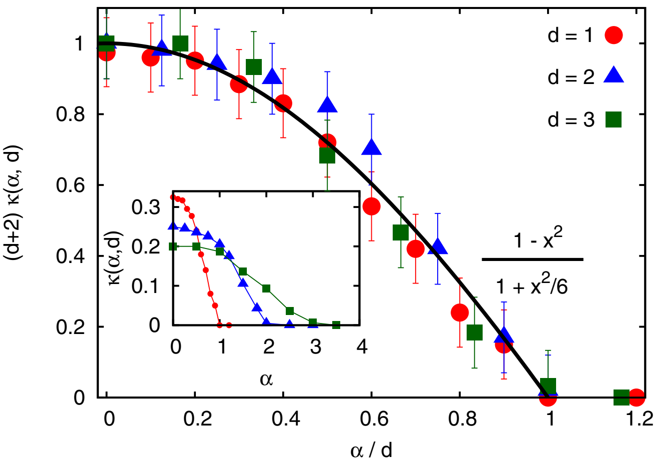

FIG. 4. Inset shows the exponent $\kappa(\alpha,d)$ as a function of α for $d = 1,2,3$. Note that $\kappa > 0$ for $0 \leqslant \alpha < d$ and $\kappa = 0$ for $\alpha > d$. The main figure exhibits the universal law obtained by appropriately rescaling the abscissas and ordinates as indicated on the axes, i.e., $(d+2)\kappa(\alpha,d) = f(\alpha/d)$. The thick continuous curve is the heuristic scaling function $f(x) = (1-x^2)/(1+x^2/6)$ [26], which, within the present precision, is a remarkably close fit to the collapsed data. The present collapse obviously implies $\kappa(0,d) = 1/(d+2)$, hence $\lim_{d\to\infty} \kappa(0,d) = 0$, thus recovering ergodicity, as intuitively expected.

A similar scaling was also verified for the classical model of long-ranged coupled rotators [19,26]. Some relevant differences exist however between the two models and their sensitivities to initial conditions. The long-range-interacting planar rotator model exhibits, for a critical energy density u_c [19,25–27], a second order phase transition from a clustered phase (ferromagnetic) to a homogeneous one (paramagnetic). Such critical phenomenon does not exist in either the short-ranged or the long-ranged FPU model. For the XY ferromagnetic model the exponent κ for $\alpha = 0$ is found to be independent from d (quite obvious since the $\alpha = 0$ model has no dimension) and given by $\kappa(0,d) = 1/3$ [26,31] (see also [32]). In contrast, our long-range model yields a value $\kappa(0,d)$ which depends on d. Indeed, for $d = 1$, 2, and 3, we respectively obtain $\kappa(0,d) \simeq 1/3$, 1/4, and 1/5.

This difference in $\kappa(0,d)$ is related to the fact that, for the XY model, the number of degrees of freedom (number of independent variables needed to specify the state of the system in phase space) for N coupled rotators in d dimensions is $2N$ ($\forall d$), whereas, for our model, there are $2Nd$ degrees of freedom; hence the dimension of the full phase space grows linearly with d. Thus there are more possible phase space dimensions for our coupled oscillator system to escape even if it gets somewhat trapped in some nonchaotic region of the phase space. Consequently, the system gets closer to ergodicity (equivalently, κ gets closer to zero) for increasing d. It is even not excluded that, because of some generic reason of this kind, $\kappa(0,d)$ ($\forall d$) for the long-ranged XY model and $\kappa(0,1)$ for the system studied here, we obtain (in the absence of the integrable term, i.e., with $a = 0$) the same value 1/3.

In this context we should mention another recent study [33] of the Hamiltonian mean field (HMF) model which is the $\alpha = 0$ particular case of the long-ranged XY model discussed above. Using numerical and analytical arguments it was suggested that the nature of chaos is quite different for this model (which has a phase transition at $u_c = 3/4$) in the homogeneous phase ($u > u_c$) where $\lambda_{max} \sim N^{-1/3}$, the ordered phase ($u < u_c$) where λ_{max} remains positive and finite, and at criticality ($u \to u_c$) where $\lambda_{max} \sim N^{-1/6}$ in the infinite size limit. However, in another earlier work [34], using scaling arguments and numerical simulations, it was observed that $\lambda_{max} \sim N^{-1/9}$ below the critical point ($u = 0.69$) in the (nonequilibrium) quasistationary regime of the HMF system.

Another class of models might also have a similar behavior. If we consider the d-dimensional long-range-interacting n-vector ferromagnet, we expect an exponent $\kappa(\alpha,n,d)$. We know that for $n = 2$ (XY symmetry) $\kappa(0,2,1) = 1/3$, for $n = 3$ (classical Heisenberg model symmetry) $\kappa(0,3,1) = 0.225 \pm 0.030$ [35], and for $n \to \infty$ (spherical model symmetry) most plausibly $\kappa(0,\infty,d) = 0$ ($\forall d$). These expressions can be simply unified through $\kappa(0,n,d) = 1/(n+1)$ ($\forall d$).

Strikingly enough, the present Fig. 4 and Fig. 2 of [26] for the d-dimensional XY model are numerically indistinguishable within error bars. This suggests the following heuristic expression:

$$\frac{\kappa(\alpha,d)}{\kappa(0,d)} = f(\alpha/d) \simeq \frac{1-(\alpha/d)^2}{1+(\alpha/d)^2/6}, \tag{5}$$

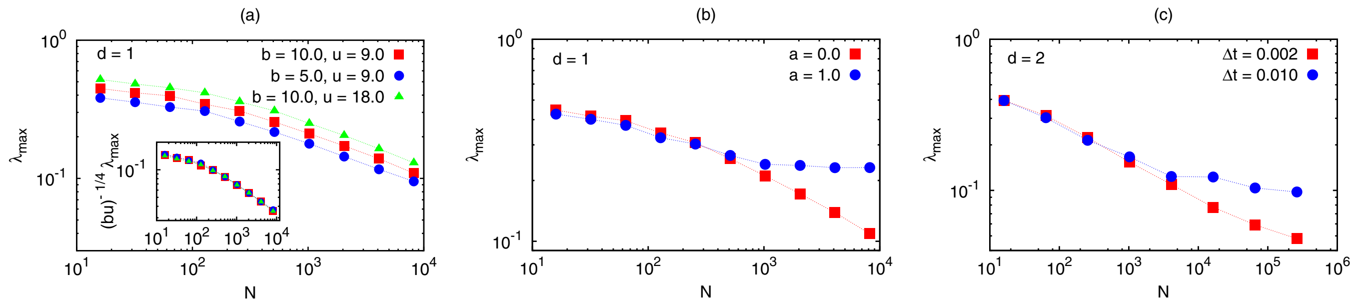

FIG. 5. Parameter dependencies of $\lambda_{\max}(N)$ with $N = L^d$: (a) for different b's and u's with $(a,\alpha,\Delta t) = (0,0,0.002)$—inset shows data collapse obtained by rescaling the y axis of the main figure as $(bu)^{-1/4}\lambda_{\max}$; (b) for different a's with $(\alpha,b,u,\Delta t) = (0,10,9,0.002)$; (c) for different Δt's with $(a,\alpha,b,u) = (0,0,10,9)$.

where this specific analytic expression for $f(x)$ has been first suggested in [26]. This or a similar universal behavior is expected to hold for d-dimensional long-range-interacting many-body models such as the present one, the XY ferromagnetic one, and others such as, for instance, the n-vector ferromagnetic one ($\forall n$).

All the numerical results presented until now are with a fixed set of parameters $(a,b,u,) = (0,10,9)$ and a fixed time step Δt. Before concluding, let us briefly mention some results concerning the influence of these parameters on $\lambda_{\max}(N)$ and $\kappa(\alpha,d)$. In Fig. 5(a) we plot $\lambda_{\max}(N)$ for $d = 1$ for three different sets of (b,u) keeping all other parameters unchanged. We find that increasing b has the same effect as increasing u—the maximum Lyapunov exponent $\lambda_{\max}$ increases with both of them but the slope of the curve κ remains practically unaltered. For $a = 0$, it is straightforward to show that the average of Hamiltonian Eq. (1) remains invariant with respect to b and u (all other parameters remaining the same) under the transformations

$$x' = (b/u)^{1/4}x, \quad t' = (bu)^{1/4}t. \tag{6}$$

The second transformation in Eq. (6) implies that the maximum Lyapunov exponent $\lambda_{\max}$ ($\sim t^{-1}$) satisfies the following scaling relation:

$$\lambda'_{\max} = (bu)^{-1/4}\lambda_{\max}. \tag{7}$$

Using the data in the main figure, we show in the inset of Fig. 5(a) the variation of $\lambda'_{\max} \equiv (bu)^{-1/4}\lambda_{\max}$ with N. As predicted by the scaling analysis, we get an excellent data collapse of the three curves. This is precisely as desired, keeping in mind the universal behavior ubiquitously found in statistical mechanics, in the sense that scaling indices, such as κ here, are generically expected to be independent of the microscopic details of the model.

For nonzero values of a, the simple scaling Eq. (7) disappears, and $\lambda_{\max}(N)$ shows a saturation to a positive value that vanishes for $a = 0$ when N is large, b being a finite positive number. This is shown in Fig. 5(b) for two values of a with the same value of b. The saturation of $\lambda_{\max}$ for $a > 0$ needs careful study to be understood properly. In Fig. 5(c) we have shown (for $d = 2$) that increasing Δt can also lead to a deviation from the $\lambda_{\max} \sim N^{-\kappa}$ behavior; this deviation is quite expected, and one should choose the time step judiciously. Note that the saturation behavior in Fig. 5(b) is not due to finiteness of the time step.

IV. SUMMARY AND DISCUSSIONS

Summarizing, we have introduced a d-dimensional generalization of the celebrated Fermi-Pasta-Ulam model which allows for long-range nonlinear interaction between the oscillators, whose coupling constant decays as $distance^{-\alpha}$. We have then focused on the sensitivity to initial conditions, more precisely on the first-principle (based on Newton's law) calculation of the maximal Lyapunov exponent $\lambda_{\max}$ as a function of the number N of oscillators using large-scale numerical simulations. Without the quadratic nearest neighbor interaction (i.e., $a = 0$), $\lambda_{\max}(N)$ appears to asymptotically behave as $N^{-\kappa}$ (with $\kappa > 0$) for $0 \leqslant \alpha/d < 1$, and approach a positive constant (i.e., $\kappa = 0$) for $\alpha/d > 1$ in the $N \to \infty$ thermodynamic limit. Our results provide strong indication that κ only depends on (α,d), and does so in a universal manner, namely $(2 + d)\kappa(\alpha,d) = f(\alpha/d)$ for $0 \leqslant \alpha/d < 1$, and $\kappa = 0$ for $\alpha/d > 1$. This universal suppression of strong chaos is well approximated by a model-independent heuristic function $f(x) \simeq (1 - x^2)/(1 + x^2/6)$, previously found [19,26] for the d-dimensional XY model of coupled rotators. Thus, in the thermodynamic limit, these systems (and plausibly others as well) have a sort of critical point at $\alpha/d = 1$, which separates the ergodic $\alpha/d > 1$ region (where the Boltzmann-Gibbs statistical mechanics is valid, and the stationary state distribution of velocities is the standard Maxwellian one), from the weakly chaotic $0 \leqslant \alpha/d < 1$ region with anomalous nonlinear dynamical behavior (where q statistics might be expected to be valid, and the one-body distribution of velocities appears to be of the q-Gaussian form, consistent with preliminary results available in the literature [24,27]). The present universality scaling for $\kappa(\alpha/d)$ enables the conjecture that the indices q of the distributions of velocities and of energies might exist and only depend on the ratio α/d. Naturally, all these observations need further and wider checking, which would be welcome. Work along this line is in progress.

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