Chaos suppression in the large size limit for long-range systems

LETTER TO THE EDITOR

Chaos suppression in the large size limit for long-range systems

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Abstract
We consider the class of long-range Hamiltonian systems first introduced by Anteneodo and Tsallis and called the α-XY model. This involves N classical rotators on a d-dimensional periodic lattice interacting all to all with an attractive coupling whose strength decays as $r^{-\alpha}$, r being the distance between sites. Using a recent geometrical approach, we estimate for any d-dimensional lattice the scaling of the largest Lyapunov exponent (LLE) with N as a function of α in the large energy regime where rotators behave almost freely. We find that the LLE vanishes as $N^{-\kappa}$, with $\kappa = 1/3$ for $0 \leqslant \alpha/d \leqslant 1/2$ and $\kappa = 2/3(1-\alpha/d)$ for $1/2 \leqslant \alpha/d < 1$. These analytical results present a nice agreement with numerical results obtained by Campa *et al*, including deviations at small N.

PACS numbers: 05.45.+b, 05.70.Fh, 02.40.-k

It is well known that systems interacting via long-range interactions may exhibit pathological thermodynamical as well as dynamical behaviours. This issue has been very much debated recently. In particular, for systems governed by sufficiently long-range interactions decaying as $r^{-\alpha}$, with $\alpha \leqslant d$ the Euclidean space dimension and r the interparticle distance, the Hamiltonian comes out to be *non-extensive*, that is the energy per particle diverges in the thermodynamic limit $N \to \infty$. In order to study issues related to the links between non-extensivity and long-range interactions, Anteneodo and Tsallis introduced in [1] a generalization of the Hamiltonian mean-field (HMF) [2] ferromagnetic-like X–Y model in the form

$$H = \frac{1}{2}\sum_{i=1}^{N} L_i^2 + \frac{1}{2\tilde{N}} \sum_{i,j=1,i\neq j}^{N} \frac{1 - \cos(\theta_i - \theta_j)}{r_{ij}^{\alpha}} = K(\boldsymbol{L}) + V(\boldsymbol{\theta}) \tag{1}$$

with $d \geqslant \alpha \geqslant 0$. This is a Hamiltonian model of rotators placed at the sites of a d-dimensional lattice with indices i, j and r_{ij} is the shortest distance between them with periodic boundary

conditions, so that the interaction between rotators i and j decays as the inverse of their distance to the power α. Here, the $\tilde{N}$ rescaling function is introduced in order to get an *extensive* (i.e. of order N) potential V. This trick was not adopted in [1], but then the authors had to conveniently rescale thermodynamical potentials by $\tilde{N}$. In the large-N limit [3]

$$\tilde{N} \equiv 1 + d \int_1^{N^{1/d}} r^{d-1-\alpha}\, \mathrm{d}r \sim \begin{cases} N^{1-\alpha/d} & \text{if } \alpha \neq d \\ \ln(N) & \text{if } \alpha = d. \end{cases} \tag{2}$$

As remarked in [4] this does not entail energy *additivity*. In the one-dimensional case, Tamarit and Anteneodo [5] have shown numerically that the canonical caloric and magnetization curves for model (1) could be derived from the curves of the HMF model (recovered for $\alpha = 0, d = 1$), and this result has been later derived analytically by Campa *et al* [13].

Recently, the stochasticity exhibited by system (1) has been investigated numerically through the computation of the largest Lyapunov exponent (LLE) as a function of the energy density $\varepsilon = H/N$ [1, 14, 15]. In the phase where particles behave almost freely, i.e. for ε above the critical energy density ε_c, where the system exhibits a second-order phase transition, the LLE has been found to scale with the number of rotators as $N^{-\kappa}$ where κ is a so-called 'universal' function of the ratio α/d with no dependence on the energy ε nor on d. In the past, the LLE had been studied for the HMF model [6–8].

For Hamiltonian models having a large number of degrees of freedom like (1) and using a geometric reformulation of the dynamics that associates trajectories to geodesics, Casetti, Pettini and coworkers [9–11] have proposed an expression of the LLE in terms of the ensemble-averaged curvature and fluctuations of curvature of the mechanical manifold associated to the Hamiltonian. This geometrical approach has proved to give very accurate estimates in a large number of Hamiltonian physical systems for which chaos mainly originates from parametric instability [12], that is systems for which the curvature is mainly positive but fluctuating. The method was originally applied to derive estimates of the LLE in the thermodynamic limit $N \to \infty$. Later on, this approach enabled the analytical computation [8] of the LLE for the HMF model as a function of ε. In the homogeneous phase ($\varepsilon > \varepsilon_c$) in which the LLE, denoted hereafter λ_1, vanishes in the limit $N \to \infty$, it was shown that keeping the leading order in N in the ensemble averages of geometric quantities enabled one to derive the scaling of λ_1 as a function of N. In this way, the LLE was predicted to scale as $N^{-1/3}$ for $\varepsilon > \varepsilon_c$. The aim of this calculation was to relate the behaviour of the dynamical indicator λ_1 to the occurrence of a second-order phase transition at ε_c in the system.

In this letter we wish to apply the same approach to the generalized model (1) in order to give an analytical prediction for the exponent κ. We shall use the derivation of the canonical thermodynamics for the system (1) presented in [13].

Let us first recall the expression for the LLE derived from the geometric approach [9–11]. The effective curvature felt by a geodesic is modelled as a Gaussian stochastic process whose mean is the average Ricci curvature and the variance its fluctuations. Under the ergodic hypothesis, these quantities may be replaced by their microcanonical ensemble-averages, denoted respectively κ_0 for the curvature and σ_κ^2 for its fluctuations. Then [9]

$$\lambda_1 = \frac{1}{2}\left(\Lambda - \frac{4\kappa_0}{3\Lambda}\right) \tag{3}$$

where

$$\Lambda = \left(\sigma_\kappa^2 \tau + \sqrt{(4\kappa_0/3)^3 + \sigma_\kappa^4 \tau^2}\right)^{1/3} \tag{4}$$

and where τ is a time scale for the stochastic process estimated as

$$\tau = \frac{1}{2} \left[\frac{2\sqrt{\kappa_0 + \sigma_\kappa}}{\pi} + \frac{\sigma_\kappa}{\sqrt{\kappa_0}} \right]^{-1}. \tag{5}$$

Using Eisenhart metric, the microcanonical average κ_0 of the mean Ricci curvature k_R reads $\kappa_0 = \langle k_R(\theta) \rangle_\mu$ where

$$k_R(\theta) \equiv \frac{K_R(\theta)}{N-1} = \frac{1}{N-1} \sum_{i=1}^{N} \frac{\partial^2 V}{\partial \theta_i^2} \tag{6}$$

and

$$\sigma_\kappa^2 \equiv \langle \delta^2 k_R \rangle_\mu = \frac{1}{N} \langle (K_R - \langle K_R \rangle_\mu)^2 \rangle_\mu. \tag{7}$$

As explained in [8, 10, 11] we shall assume the equivalence of microcanonical and canonical ensembles, leading to identical values of both ensemble-averages of observables in the limit $N \to \infty$, but to different values of their fluctuations with the formula [16]

$$\langle \delta^2 f \rangle_\mu = \langle \delta^2 f \rangle_c + \left(\frac{\partial \langle \varepsilon \rangle_c}{\partial \beta} \right)^{-1} \left[\frac{\partial \langle f \rangle_c}{\partial \beta} \right]^2 \tag{8}$$

where $\beta \equiv 1/T$ and $k_B = 1$. This assumption is fully justified by the recent achievement that ensemble inequivalence for averages in long-range systems is to be expected only close to first-order phase transitions [4, 17, 18]. Therefore, the first step is to express the canonical thermodynamics of system (1) following [13]. The constraint $i \neq j$ in the potential can be removed for free by defining $r_{ii}^{-\alpha} = b$, that is for the time being an arbitrary constant. Then the symmetric distance matrix $R_{ij}' = r_{ij}^{-\alpha}$ may be diagonalized, which enables one to use the Hubbard–Stratonovitch transform to evaluate the potential part Z_{Vc} of the canonical partition function. Using then the saddle-point method, one obtains from equations (12) and (20) of [13] in the long-range case ($\alpha \leqslant d$) and for $\varepsilon > \varepsilon_c$ (zero magnetization phase)

$$\ln Z_{Vc} = -\frac{\beta}{2\tilde{N}} \sum_{j=1}^{N} r_{ij}^{-\alpha} - \frac{1}{2} \sum_{n=1}^{N} \ln \left[1 - \beta \frac{s_n}{\tilde{N}} \right] \tag{9}$$

The eigenvalues s_n of the R' matrix can be easily derived following [19].

Let us first consider the $d = 1$ case for the sake of simplicity. We remind that

$$R_{ij}' = \begin{cases} r_{ij}^{-\alpha} & \text{if } i \neq j \\ b & \text{if } i = j \end{cases} \tag{10}$$

where

$$r_{ij} = \min_{l \in \mathbb{Z}} |i - j + lN|. \tag{11}$$

Therefore $R_{ij}' = R'(i - j) = R'(m)$ where R' is a N-periodic function. This periodicity of the lattice enables one to diagonalize R' in Fourier space. Its Fourier transform is

$$\tilde{R}'(n) = \sum_{m=1}^{N} \exp\left(-i\frac{2\pi}{N} nm \right) R'(m)$$

with the inversion formula

$$R'(j) = \frac{1}{N} \sum_{k=1}^{N} \exp\left(-i\frac{2\pi}{N} jk \right) \tilde{R}'(k).$$

Then it can be easily shown that $R'(i-j) = \sum_{k=1}^{N} u_{ik}^{\dagger} s_l u_{jk}$ where $u_{jk} := N^{-1/2} \exp(-i\frac{2\pi}{N} jk)$ is an element of the unitary matrix of eigenvectors with the following expression for the eigenvalues ($1 \leqslant k \leqslant N$)

$$s_k = \sum_{m=1}^{N} \exp\left(-i\frac{2\pi}{N} km\right) R'(m). \tag{12}$$

For any d-dimensional lattice, one would get the generalized expression for $s_n = s(n_1, \ldots, n_d)$ with $1 \leqslant n_1, \ldots, n_d \leqslant N^{1/d}$ as

$$s_n = \sum_{m_1=1}^{N^{1/d}} \cdots \sum_{m_d=1}^{N^{1/d}} \exp\left(-i\frac{2\pi}{N^{1/d}} \sum_{i,j=1}^{d} n_i m_j\right) R'(m). \tag{13}$$

Coming back to the $d=1$ case, we shall take N even in the following and put $N = 2p$. As R' is an even function, this implies, for $1 \leqslant k \leqslant N = 2p$,

$$s_k = b + \tilde{s}_k \tag{14}$$

with

$$\tilde{s}_k := \frac{(-1)^k}{p^\alpha} + 2 \sum_{m=1}^{p-1} \frac{\cos(\pi km/p)}{m^\alpha}. \tag{15}$$

$\tilde{s}_p$ is the smallest of the $\tilde{s}_k$ and is negative. In order to get a fully positive spectrum that enables one to apply the Hubbard–Stratonovitch transform, we can now shift the spectrum by *fixing*

$$b := -\tilde{s}_p = -\frac{(-1)^p}{p^\alpha} - 2 \sum_{m=1}^{p-1} \frac{(-1)^m}{m^\alpha}. \tag{16}$$

$\tilde{N}$ is then defined as the maximal eigenvalue

$$\tilde{N} = s_{2p} = b + \frac{1}{p^\alpha} + 2 \sum_{m=1}^{p-1} \frac{1}{m^\alpha} \tag{17}$$

and it can be easily checked that

$$\sum_{k=1}^{N=2p} \tilde{s}_k = 0. \tag{18}$$

We can now go on with the derivation of the LLE. Using expression (6), one gets

$$k_R(\theta) = \frac{1}{N-1} \frac{1}{\tilde{N}} \sum_{i \neq j}^{N} \frac{\cos(\theta_i - \theta_j)}{r_{ij}^\alpha} = \frac{1}{N-1} \left[\frac{1}{\tilde{N}} \sum_{i \neq j}^{N} r_{ij}^{-\alpha} - 2V(\theta)\right]. \tag{19}$$

Thus

$$\langle k_R(\theta)\rangle_c = \frac{1}{N-1} \left[\frac{1}{\tilde{N}} \sum_{i \neq j}^{N} r_{ij}^{-\alpha} + 2\frac{\partial \ln Z_{Vc}}{\partial \beta}\right]. \tag{20}$$

That is

$$\langle k_R(\theta)\rangle_c = \frac{1}{N-1} \left[-\frac{N}{\tilde{N}} b + \sum_{n=1}^{N} \frac{s_n}{\tilde{N} - \beta s_n}\right]. \tag{21}$$

Let us now consider the fluctuations of the curvature. Their canonical average is

$$\langle \delta^2 k_R\rangle_c = \frac{4}{N-1} \frac{\partial^2 \ln Z_{Vc}}{\partial \beta^2} = \frac{2}{N-1} \sum_{n=1}^{N} \left(\frac{s_n}{\tilde{N} - \beta s_n}\right)^2 \tag{22}$$

while the corrective term (8), needed to get the fluctuations in the microcanonical ensemble, is

$$\left(\frac{\partial \langle \varepsilon \rangle_c}{\partial \beta}\right)^{-1} \left[\frac{\partial \langle k_R \rangle_c}{\partial \beta}\right]^2 = -\frac{1}{2}\beta^2 \langle \delta^2 k_R \rangle_c^2. \tag{23}$$

Actually, the energy density above the critical point is intensive and equal to $1/(2\beta)$ (up to a constant term). And one obtains

$$\sigma_\kappa = (1 - \tfrac{1}{2}\beta^2 \langle \delta^2 k_R \rangle_c)^{1/2} \langle \delta^2 k_R \rangle_c^{1/2}. \tag{24}$$

We shall focus on the high-temperature regime and derive the scaling of λ_1 with N under both the limits of large N and small β. We will show later the validity of this scaling of λ_1 with N in a wider range of β. The results will be compared with the numerical results of [14,15] for which $\beta = 1/9$. We shall also compute a numerical estimate of the scaling of λ_1 for $\beta = 1/9$ using directly equations (3), (4) with the full expressions (21), (22), (24).

Using (21), one gets

$$\langle k_R(\theta) \rangle_c \sim_{\beta \to 0^+} \frac{\beta}{(N-1)\tilde{N}^2} \sum_{n=1}^{N} s_n^2 \tag{25}$$

where $\sum_{n=1}^{N} s_n^2 = \sum_{n=1}^{N} \tilde{s}_n^2 + Nb^2$. Using (15), one obtains $\sum_{n=1}^{N} \tilde{s}_n^2 = Np^{-2\alpha} + 2N \sum_{m=1}^{p-1} m^{-2\alpha}$. If $2\alpha \neq 1$, the sum of the $\tilde{s}_n^2$ is of the order $N^{2-2\alpha}$. Therefore, using (2) and (17), the scaling of κ_0 with N depends on the value of α as

$$\kappa_0 \propto_{\beta \to 0^+} \begin{cases} \beta N^{-1} & \text{for} \quad 0 \leqslant \alpha < 1/2 \\ \beta N^{-2+2\alpha} & \text{for} \quad 1/2 \leqslant \alpha < 1 \\ \beta (\ln N)^{-2} & \text{for} \quad \alpha = 1. \end{cases} \tag{26}$$

Let us now estimate the order of the fluctuations. From (22), (24) and in the limit of vanishing β, σ_κ^2 is equivalent to $2(N-1)^{-1}\tilde{N}^{-2} \sum_{n=1}^{N} s_n^2$, so that

$$\sigma_\kappa^2 \propto_{\beta \to 0^+} \begin{cases} N^{-1} & \text{for} \quad 0 \leqslant \alpha < 1/2 \\ N^{-2+2\alpha} & \text{for} \quad 1/2 \leqslant \alpha < 1 \\ (\ln N)^{-2} & \text{for} \quad \alpha = 1. \end{cases} \tag{27}$$

At this stage we can check that the results presented in [8] are effectively recovered for the HMF case in the high-energy regime where the curvature and fluctuations of the curvature were predicted to be of order N^{-1}. Now, considering the timescale estimated as (5), one obtains $\sqrt{\kappa_0 + \sigma_\kappa} \sim \sqrt{\sigma_\kappa}$ that vanishes in the limit of large-N while $\sigma_\kappa/\sqrt{\kappa_0} \sim \beta^{-1/2} = \mathcal{O}(1)$. This last estimate is interpreted in [10, 11] as the relevant timescale when the fluctuations are of the same order as the curvature and does not require the positivity of the curvature, which is effectively the case here. It then emerges that τ is of order one. Putting this together with estimates (26) and (27) in equations (4) and (3) leads to the expression of the LLE, in the limit of large N and at the leading order in N, as

$$\lambda_1(N, \beta \ll 1) \propto_{\beta \to 0^+} \beta^{1/6} \times \begin{cases} N^{-1/3} & \text{for} \quad 0 \leqslant \alpha < 1/2 \\ N^{-2/3+2\alpha/3} & \text{for} \quad 1/2 \leqslant \alpha < 1 \\ (\ln N)^{-2/3} & \text{for} \quad \alpha = 1. \end{cases} \tag{28}$$

where one can also check the integrability of the model in the large temperature $\beta \to 0^+$ limit for all[1] N. If one develops the curvature at higher orders in β, one obtains a power series of the type $\beta \sum_{n=1}^{N} (s_n/\tilde{N})^2 + \beta^2 \sum_{n=1}^{N} (s_n/\tilde{N})^3 + \cdots$ where it can be checked that all the sums

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[1] We have to remark that there is a mistake in equation (23) of [8] for the HMF ($\alpha = 0$) model. It should read $\lambda_1 \sim 4^{1/3} c^{3/2} \beta^{1/6} (2 - \beta c)^{-1/2} N^{-1/3}$, which is actually of order $\beta^{1/6}$ in the small-β limit.
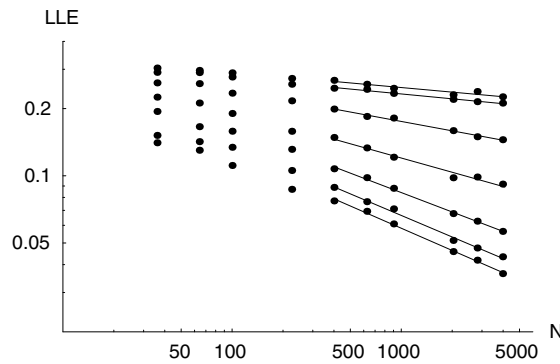
Figure 1. Log–log plot of the LLE as a function of N for different values of α with $d = 2$. The data have been communicated by the authors of [14]. At each value of α/d, the best linear fit of the logarithm of the LLE as a function of the logarithm of N is plotted for N between 400 and 4000. The values of α/d are, from top to bottom, 1, 0.95, 0.8, 0.6, 0.4, 0.2 and 0.

of the successive powers of $s_n/\tilde{N}$ are equivalent in the large-N limit. Similar expansions are obtained for the fluctuations of curvature. In the large-N limit, one can thus conclude that equation (28) is valid for small β, and not only in the $\beta \to 0^+$ limit. Formula (28) is hence still valid after replacing $\beta^{1/6}$ with a function of β whose power series development in β is in principle calculable. Moreover, coming back to the general d-dimensional case, the previous procedure can be followed replacing (12) by (13). The sum (25) then involves

$$\sum_{n=1}^{N} \tilde{s}_n^2 \sim N \sum_{m_1=1}^{N^{1/d}} \cdots \sum_{m_d=1}^{N^{1/d}} (m_1^2 + \cdots + m_d^2)^{-\alpha} \sim N N^{1-2\alpha/d}$$

if $2\alpha/d \neq 1$. Therefore we can replace α by α/d in all the previous scalings. This analysis then predicts the universal exponent κ as

$$\kappa = \kappa(\alpha/d) = \begin{cases} 1/3 & \text{if} \quad 0 \leqslant \alpha/d < 1/2 \\ \frac{2}{3}(1 - \alpha/d) & \text{if} \quad 1/2 \leqslant \alpha/d < 1. \end{cases} \tag{29}$$

Hence κ is a function of α/d which is equal to $1/3$ for $\alpha/d = 0$, consistently with numerical and analytical results obtained for the HMF model [6–8]. It vanishes in the limit $\alpha/d \to 1$ consistently with the intensivity of the LLE for short-range ($\alpha \geqslant d$) potentials predicted from thermodynamics [13]. Moreover we predict that for $\alpha = d$ the LLE should scale as $(\ln N)^{-2/3}$ in the limit of large N and energy density. This agrees with the intuitive statement made in [14] that the LLE should scale as some power of $1/\ln N$ for $\alpha = d$.

We shall now compare these estimates with the numerical results presented in [1] for $d = 1$ and in [14, 15] for $d = 1, 2$ and 3. In these papers, the LLE has been computed numerically for values of N ranging from 5 to 1000 for $d = 1$ and from 36 to 3969 for $d = 2, 3$. In [1, 14, 15], the curves giving the LLE as a function of N in a log–log scale were fitted by the functional form $aN^{-\kappa} + bN^{-\kappa-c}$ with $c = 1$. We do not agree that this form is the correct second-order approximation for any value of α/d between 0 and 1, nor that c should be equal to 1. Moreover, due to obvious numerical constraints, the values of N used are not sufficiently large to discard additional finite-N effects. For the values used in [14, 15] for $d = 2$ and 3 we instead performed a linear fit retaining only the highest values of N, with N between 500 and 4000, as shown in figures 1 and 2 and got the numerical values of κ plotted in figure 3. On the other hand, using (3)–(5) together with (21), (22), (24), we can
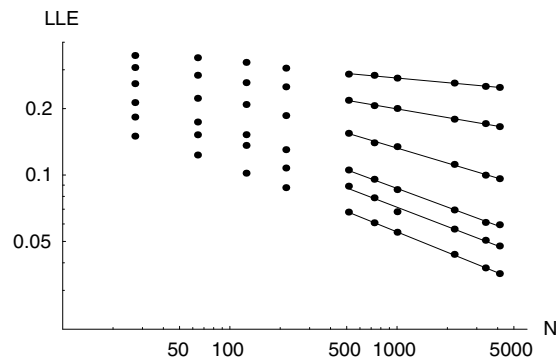
Figure 2. Same plot as in figure 1 with $d = 3$. The values of α/d are, from top to bottom, 0.95, 0.8, 0.6, 0.4, 0.2 and 0.
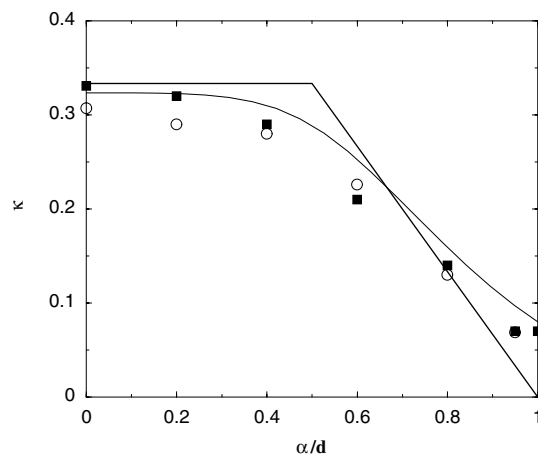

Figure 3. Plot of the exponent κ as a function of α/d. The bold line corresponds to the analytical prediction obtained in the infinite-N limit. The thinner curve gives the exponent obtained by fitting the logarithm of the analytical prediction of the LLE as a function of the logarithm of N for N between 500 and 4000. This is to be compared with the values of κ as a function of α/d deduced from the fits shown in figures 1 (with filled squares) and 2 (with empty circles).

compute the LLE for different values of α and N and obtain the theoretical curves associated with the numerical ones in figures 1 and 2. In log–log scale, we have derived the best linear fits from the theoretical curves giving the LLE as a function of N for different values of α. It should be mentioned that the results so far obtained for κ benefit from a better statistics for the largest values of N compared to the numerical results of [14, 15], which explains why the theoretical curve is slightly above the numerical points in figure 3. Nevertheless in this figure we observe a good agreement between the theoretical and numerical finite-N derivation of κ as a function of α/d. The agreement is worse for $d = 3$, compared with the $d = 2$ case; this may be related to more important finite-N effects as d increases for a given value of N. This supports the validity of our theoretical predictions. Consequently, we suggest that the so-called 'universal curves' published in [1] and [14, 15] are plagued by finite-N effects. In the asymptotic limit in N, we claim that the correct universal scaling of the LLE with N is

given by (29)[1]. This means that there is a sharp change in the dynamical behaviour of the model for $\alpha/d = 1/2$. For $0 \leqslant \alpha/d \leqslant 1/2$, the suppression of chaos scales like in the HMF model, which then provides a universal law in this range, with a universal exponent $\kappa = 1/3$.

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[1] Completing the proofs, we note that this asymptotic scaling (24) has also been obtained by C Anteneodo and R O Vallejos, using a random matrix approach, in a preprint very recently submitted for publication.