Rényi entropy of zeta urns

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We calculate analytically the Rényi entropy for the zeta-urn model with a Gibbs measure definition of the microstate probabilities. This allows us to obtain the singularities in the Rényi entropy from those of the thermodynamic potential, which is directly related to the free-energy density of the model. We enumerate the various possible behaviors of the Rényi entropy and its singularities, which depend on both the value of the power law in the zeta urn and the order of the Rényi entropy under consideration.

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I. INTRODUCTION

Diversity, as well as how to measure it, has been a subject of fundamental interest in mathematical biology and ecology for many years [1–9]. There have been interesting contributions from numerous authors that make use of ideas from statistical mechanics and thermodynamics, specifically those related to various notions of entropy. A prototypical problem is to quantify the diversity of an ecosystem whose organisms may be divided into N distinct species, where the σth species has a relative abundance of p_σ, so that

$$p_1 + p_2 + \cdots + p_N = 1. \quad (1)$$

From a statistical mechanical perspective, p_σ is the probability of having a microstate σ in some ensemble. Given the p_σ, there are a multitude of entropylike measures of diversity that one might consider (and which have already been proposed), a small selection being species richness $\sum_\sigma p_\sigma^0$, Shannon entropy [10] $-\sum_\sigma p_\sigma \ln p_\sigma$, Gini-Simpson index [11] $1 - \sum_\sigma p_\sigma^2$, Tsallis entropy (of order λ) [12] $\frac{1-\sum_\sigma p_\sigma^\lambda}{\lambda-1}$, and Rényi entropy (of order λ) [13] $H_\lambda = \frac{1}{1-\lambda} \ln \sum_\sigma p_\sigma^\lambda$. The parameter λ is a non-negative real number. In the limit $\lambda \to 1$, the Rényi entropy H_λ [13] reproduces the Shannon entropy $H_1 = -\sum_\sigma p_\sigma \ln p_\sigma$ [10] and in the limit $\lambda \to 0$ it gives the logarithm of the species richness (i.e., logarithm of the number of microstates): $H_0 = \ln \sum_\sigma p_\sigma^0 = \ln \sum_\sigma 1$.

We focus on the Rényi entropy here. Its exponential, the diversity or Hill number [14] of order λ, is denoted by $D_\lambda = \exp(H_\lambda)$,

$$D_\lambda(\bar{p}) = \left(\sum_\sigma p_\sigma^\lambda \right)^{1/(1-\lambda)}, \quad (2)$$

where we have defined an abundance vector $\bar{p} = (p_1, p_2, p_3, \ldots, p_N)$. The Hill number is perhaps a more suitable choice than the entropy itself in an ecological setting since the resulting Hill numbers generally have a direct interpretation in terms of familiar quantities. For instance, $D_0(\bar{p})$ will be the number of distinct species and

$$D_2(\bar{p}) = \frac{1}{\sum_\sigma p_\sigma^2}$$

is the inverse participation ratio. Also, in the uniform case $D_\lambda(1/N, 1/N, \ldots, 1/N) = N \,\forall\, \lambda$, giving the number of species. In essence, the Hill numbers and their generalizations are providing an "effective number of species" for an ecosystem with some input from our prejudices on the importance of rare species determined by the parameter λ. The parameter λ can be thought of as tuning the sensitivity of the diversity measure $D_\lambda(\bar{p})$ to the occurrence of rare species. Since the summands are given by p_σ^λ, rare species (smaller p_σ) will be weighted less strongly as λ is increased. The highest sensitivity to rare species is therefore given by $\lambda = 0$.

It is possible to further refine (complicate) such models by introducing a measure of the similarity $Z_{\sigma\nu}$ between species σ and ν, with $0 \leqslant Z_{\sigma\nu} \leqslant 1$, where $Z_{\sigma\nu} = 0$ is the total dissimilarity and $Z_{\sigma\nu} = 1$ is the total similarity [5]. In this case the

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Hill numbers would be modified to

$$D^Z_\lambda(\bar{p}) = \left(\sum_\sigma p_\sigma[(Z\bar{p})_\sigma]^{\lambda-1}\right)^{1/(1-\lambda)}, \quad (3)$$

where

$$(Z\bar{p})_\sigma = \sum_\nu Z_{\sigma\nu} p_\nu. \quad (4)$$

We consider only the case $Z = I$ here.

It has been observed [15,16] that if the p_σ are given by a Gibbs measure

$$p_\sigma = \frac{\exp(-\beta E_\sigma)}{Z(\beta)}, \quad (5)$$

with the partition function defined by $Z(\beta) = \sum_\sigma \exp(-\beta E_\sigma)$, then the Rényi entropy H_λ is related to the logarithm of the ratio of partition functions

$$H_\lambda = \frac{1}{1-\lambda} \ln \frac{Z(\lambda\beta)}{Z^\lambda(\beta)}. \quad (6)$$

This may also be written as a difference of free energies $F(\beta) = -(1/\beta)\ln Z(\beta)$,

$$H_\lambda = \lambda\beta^2\left(\frac{F(\lambda\beta) - F(\beta)}{\lambda\beta - \beta}\right), \quad (7)$$

where the expression in large parentheses may be regarded as a q derivative of F defined by

$$\left(\frac{dF(x)}{dx}\right)_q = \frac{F(qx) - F(x)}{qx - x}$$

(with λ playing the role of q). We recover the usual relation between the Shannon entropy and the free energy in the limit of $\lambda \to 1$. This relation is also the basis of using the Rényi entropy and the replica trick in conformal field theory [17] and numerical [18] calculations to evaluate the entanglement entropy of various statistical mechanical systems.

II. MODEL

It is tempting to use simple explicitly solvable statistical mechanical models to investigate the properties of diversity measures such as the Rényi entropy and indeed this has already been done in [19] for the class of models, zeta urns, which we address here. However, our aims and also our notion of a "species" or microstate are rather different from those of [19], as we highlight below.

Zeta-urn models describe weighted partitions of S balls (particles) between N boxes such that each box i contains at least one particle $s_i \geqslant 1$ and $S = s_1 + s_2 + \cdots + s_N$. In our case, microstates σ in this model correspond to the particle distributions in the boxes $\sigma = (s_1, s_2, \ldots, s_N)$. The number of states for S particles in N boxes is $\mathcal{N} = \binom{S-1}{N-1}$. The abundance vector $(p_1, \ldots, p_\mathcal{N})$ is thus not the same as in [19], where the authors considered the abundance vector $(p_1, \ldots, p_S)$ in the set $\{1, 2, \ldots, S\}$ in an ensemble in which the number of boxes N was allowed to fluctuate. The geometrical picture behind this choice in [19] is of breaking a bar of length S into N segments of sizes $(s_1, s_2, \ldots, s_N)$ and maximizing the diversity (by some measure) of these, which was then applied to the general problem of partitioning a set of S elements into N components with a power-law distribution for the probabilities of the component sizes. In [19] it was found, using a phenomenological calculation based on cluster size estimation in spin models [20], that D_0 was maximized for $\beta = 2$, which is the value given by Zipf's law [21,22]. This, as well as the predicted scaling with S, agreed well with numerical simulations.

Here we would like to use (6) and (7) to investigate the singular behavior of the Rényi entropies in a zeta-urn model. To this end, the energy of the system in the state σ is taken to be logarithmic in the number of particles in each box

$$E_\sigma = \sum_{i=1}^N \ln s_i. \quad (8)$$

The corresponding partition function [23,24]

$$Z_{S,N}(\beta) = \sum_\sigma e^{-\beta E_\sigma} \quad (9)$$

may be rewritten as

$$Z_{S,N}(\beta) = \sum_{(s_1,\ldots,s_N)} w(s_1)\cdots w(s_N)\delta_{S-(s_1+\cdots+s_N)}, \quad (10)$$

with

$$w(s) = s^{-\beta} \quad (11)$$

for $s = 1, 2, 3, \ldots$. The parameter β in the power law for the weights can thus be considered as the inverse temperature: $\beta = 1/T$. Despite its simplicity, this model occurs in many problems of statistical physics, including zero-range processes [25–28] (as a nonequilibrium steady state), mass transport [29–31], random trees [32,33], lattice models of quantum gravity [34–36], emergence of the longest interval in tied-down renewal processes [37,38], wealth condensation [39], and diversity of Zipf's population [19]. The system described by the model has a phase transition which is associated with a real-space condensation [23].

We will study the Rényi entropy for this model with a given microstate being a particle distribution in the boxes $\sigma = (s_1, s_2, \ldots, s_N)$ as described above. The Rényi entropy is defined as in the Introduction,

$$H_\lambda = \frac{1}{1-\lambda} \ln \sum_\sigma p_\sigma^\lambda,$$

where p_σ is the probability of the σ state:

$$p_\sigma = \frac{1}{Z(\beta)} e^{-\beta E_\sigma}. \quad (12)$$

In Eq. (12) Z is an abbreviation for $Z_{S,N}(\beta)$. With the Gibbs measure definition of the microstates employed here, the free-energy difference or Rényi entropy relations of (6) and (7) apply. This in turn allows us to relate the singular behavior of the Rényi entropy (density) to that of the free energy (density).

Our aim is to calculate H_λ explicitly in the thermodynamic limit

$$S \to \infty, \quad \frac{N}{S} \to r, \quad (13)$$

where $r \in (0, 1)$, and then use this to obtain the singular behavior, if it exists. The parameter r is a free parameter which is equal to the inverse particle density (i.e., the average number of particles per box). In the limit (13), the free energy $F(\beta, r, S)$ is an extensive quantity, which means that it grows linearly with the system size $F(\beta, r, S) = Sf(\beta, r) + o(S)$ as S goes to infinity. We are interested in the coefficient $f(\beta, r)$ of the leading term, which can be interpreted as the free energy per particle. Only if this coefficient is zero do the next-to-leading terms denoted by $o(S)$ need to be considered. In general, we will use the convention that extensive quantities will be denoted by capital letters and the corresponding densities by lowercase letters. In particular, we will denote the Rényi entropy per particle (or the Rényi entropy density) by h_λ.

Let us introduce a thermodynamic potential

$$\phi(\beta, r) = \lim \frac{1}{S} \ln Z_{S,N}, \tag{14}$$

where lim in this equation means the thermodynamic limit as defined in (13). The function $\phi(\beta, r)$ gives the rate of exponential growth of the partition function with S in the thermodynamic limit (13) and it is directly related to the free-energy density $\phi(\beta, r) = -\beta f(\beta, r)$. Dividing both sides of (6) by S and taking the limit (13), we find a direct relationship between the Rényi entropy density and the thermodynamic potential ϕ,

$$h_\lambda(\beta, r) = \frac{\phi(\lambda\beta, r) - \lambda\phi(\beta, r)}{1 - \lambda}. \tag{15}$$

For $\lambda \to \infty$ Eq. (15) reduces to $h_\infty(\beta, r) = \phi(\beta, r)$ and for $\lambda = 0$ to $h_0(\beta, r) = \phi(0, r)$. Clearly, $h_0(\beta, r)$ is independent of β. It can be easily determined by enumeration of states, which gives

$$Z_{S,N}(0) = \sum_\sigma 1 = \binom{S-1}{N-1} = \mathcal{N}. \tag{16}$$

Substituting this into (14), we find in the thermodynamic limit (13)

$$h_0(\beta, r) = \phi(0, r) = -r \ln r - (1 - r) \ln(1 - r). \tag{17}$$

For the Shannon entropy (density) limit $\lambda \to 1$,

$$h_1(\beta, r) = \phi(\beta, r) - \partial_\beta \phi(\beta, r), \tag{18}$$

as can be seen by applying l'Hôpital's rule to (15).

The thermodynamic potential $\phi(\beta, r)$ can be found analytically using the saddle-point method. The details can be found in [23,24,34] or in the preceding paper, where results on the phase structure of the zeta-urn model have been updated and collected in one place [40]. Here we quote the result, which is expressed in terms of a generating function

$$K_\beta(\alpha) = \ln \sum_{k=1}^{\infty} w(k) e^{-\alpha k} = \ln \mathrm{Li}_\beta(e^{-\alpha}), \tag{19}$$

where $\mathrm{Li}_\beta(z)$ is the polylogarithm

$$\mathrm{Li}_\beta(z) = \sum_{k=1}^{\infty} \frac{z^k}{k^\beta}. \tag{20}$$

The middle expression in (19) is a definition of the generating function, while the last expression is just its explicit form for the power-law weights (11).

For $\alpha = 0$,

$$K_\beta(0) = \ln \zeta(\beta). \tag{21}$$

Two cases can be distinguished. For $\beta \leqslant 2$, $\phi(\beta, r)$ can be expressed as parametric equations, where both ϕ and r are parametrized by $\alpha \in (0, \infty)$:

$$r = -\frac{1}{K'_\beta(\alpha)} \tag{22}$$

and

$$\phi(\beta, r) = \alpha - \frac{K_\beta(\alpha)}{K'_\beta(\alpha)}. \tag{23}$$

These equations are valid for all values from the range $r \in (0, 1)$, which is an image of the range $\alpha \in (0, \infty)$ of the mapping (22).

For $\beta > 2$, the image of the range $\alpha \in (0, \infty)$ is $r \in (r_c, 1)$ where $r_c = r_c(\beta)$ is a critical value given by

$$r_c(\beta) = -\frac{1}{K'_\beta(0)} = \frac{\zeta(\beta)}{\zeta(\beta - 1)}. \tag{24}$$

The saddle-point solution (22) and (23) holds for $r \in (r_c, 1)$, while for $r \in (0, r_c]$ the solution is linear in r,

$$\phi(\beta, r) = r K_\beta(0) = r \ln \zeta(\beta). \tag{25}$$

For $r \in (r_c, 1)$ the system is in the fluid phase, while for $r \in (0, r_c)$ it is in the condensed phase. In the condensed phase one box captures a finite fraction of all particles S as $S \to \infty$ [23]. This is a real-space condensation. It should be noted that in the condensed phase the Rényi entropy is determined by the bulk part of the distribution, which remains in the critical state, since the contribution from the condensate in a single box vanishes in the thermodynamic limit (13). The phase transition, which the system undergoes for the given inverse temperature β at the critical inverse density $r_c(\beta)$, manifests as a singularity of the thermodynamic potential $\phi(\beta, r)$. The singularity can be seen as a discontinuity of a derivative of the thermodynamic potential

$$\lim_{r \to r_c^+} \partial_r^n \phi(\beta, r) \neq \lim_{r \to r_c^-} \partial_r^n \phi(\beta, r). \tag{26}$$

Generically, the discontinuity is infinite, as a result of the derivative divergence, but there are cases in which the discontinuity is finite, usually for the first-order phase transitions, but not only. The transition is said to be nth order when the nth derivative $\partial_r^n \phi$ is discontinuous, while all kth derivatives $\partial_r^k \phi$ for $k = 1, \ldots, n-1$ are continuous at the critical point $r_c(\beta)$.

The parametric equations (22) and (23) can be used to plot the function $\phi(\beta, r)$ and thus also $h_\lambda(\beta, r)$ (15). We show two examples in Fig. 1 for $\beta = 5/2$ and $3/2$ to illustrate the behavior for the two cases mentioned above. Here we are interested in singular points where the Rényi entropy density is singular or, more precisely, where any nth derivative is discontinuous:

$$\lim_{r \to r_c^+} \partial_r^n h_\lambda(\beta, r) \neq \lim_{r \to r_c^-} \partial_r^n h_\lambda(\beta, r). \tag{27}$$

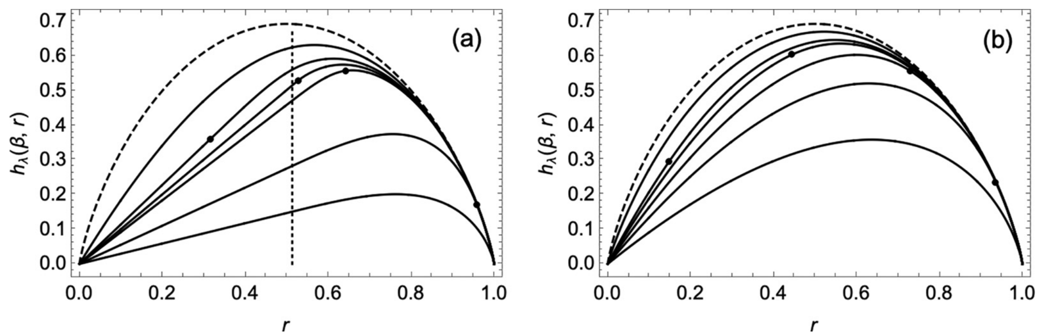

FIG. 1. (a) Rényi entropy density $h_\lambda(\beta, r)$ for $\beta = 5/2$ and, from top to bottom, $\lambda = 0$ (dashed line) and $\lambda = 0.6, 0.9, 1.01, 1.1, 2.0$, and ∞ (solid lines). The primary singular points lie on the dotted vertical line at $r_c = \zeta(5/2)/\zeta(3/2) \approx 0.5135$. The position of the secondary singular points depends on λ [see Eq. (28)]. The secondary singular points are marked by dots. For $\lambda = 1.01$ the primary and secondary singular points almost merge. For $\lambda = 0.6$ there is no secondary singular point, because $\lambda\beta \leqslant 2.0$. Note that the curves are linear in the intervals $(0, r_*)$, where $r_* = \min(r_c, r_{c,\lambda})$ (25). (b) Rényi entropy density $h_\lambda(\beta, r)$ for $\beta = 3/2$ and, from top to bottom, $\lambda = 0$ (dashed line) and $\lambda = 0.8, 1.4, 1.6, 2.0, 3.0$, and ∞ (solid lines). There are no primary singular points in this case. The secondary singular points, however, do exist for $\lambda > 4/3$ and are marked by dots. There is no secondary singular point for $\lambda = 0.8$ (the curve below the dashed line), because $\lambda < 4/3$. The singular behavior of the Rényi entropy density $h_\lambda(\beta, r)$ is not visible to the naked eye in the figure as it is associated with the discontinuity (or divergence) of higher derivatives $\partial_r^n h_\lambda(\beta, r)$ but not of the function itself. For instance, for $\lambda = 3.0$, the singular point is at $r_{c,\lambda} = \zeta(4.5)/\zeta(3.5) \approx 0.936$ (28). At this point, the second derivative $\partial_r^2 h(\beta, r)$ is discontinuous and the fourth derivative $\partial_r^4 h(\beta, r) \sim (r - r_{c,\lambda})^{-1/2}$ is divergent, as follows from Eqs. (A19) and (A20).

The Rényi entropy density $h_\lambda(\beta, r)$ inherits its singularities from $\phi(\beta, r)$. The primary singularity lies at the critical point $r_c(\beta)$ (24), but $h_\lambda(\beta, r)$ may also have a secondary singularity coming from $\phi(\lambda\beta, r)$ in (15) which is located at a different point:

$$r_{c,\lambda}(\beta) = \frac{\zeta(\lambda\beta)}{\zeta(\lambda\beta - 1)}. \tag{28}$$

In this respect, the Rényi entropy density for the zeta-urn model is behaving [unsurprisingly, given (8), (9), and (12)] as an equilibrium statistical mechanical system, with singularities at two different β values. It was found in [41] that this was not the case for the totally asymmetric exclusion process (TASEP), where H_2 was calculated by combinatorial means and found to possess no secondary singularities. It was suggested there that secondary singularities would generically be absent in such nonequilibrium systems, since they were a consequence of the relations (6) and (7), which are peculiar to equilibrium systems. Although the distribution of particles in a zeta-urn model can be considered as arising as a nonequilibrium steady state in a zero-range process with suitable jumping rates for the particles [25], we are treating it as a purely equilibrium model here.

The function $h_\lambda(\beta, r)$ has a primary singularity at r_c (24) for $\beta > 2$ and a secondary singularity at $r_{c,\lambda}$ (28) for $\lambda\beta > 2$, so there are four different cases: (a) $h_\lambda(\beta, r)$ is regular for any $r \in (0, 1)$ for $\beta \leqslant 2$ and $\lambda\beta \leqslant 2$, (b) $h_\lambda(\beta, r)$ is singular at $r_{c,\lambda}$ for $\beta \leqslant 2$ and $\lambda\beta > 2$, (c) $h_\lambda(\beta, r)$ is singular at r_c for $\beta > 2$ and $\lambda\beta \leqslant 2$, and (d) $h_\lambda(\beta, r)$ is singular at r_c and $r_{c,\lambda}$ for $\beta > 2$ and $\lambda\beta > 2$. The positions of the secondary and primary singularities merge for $\lambda \to 1$ (the Shannon entropy). The behavior is illustrated in Fig. 2. The primary singularities of $h_\lambda(\beta, r)$ at r_c (24) are directly related to the singularities of the thermodynamic potential $\phi(\beta, r)$ at the critical point $r = r_c$, while the secondary singularities of $h_\lambda(\beta, r)$ (15) are related to the singularities of $\phi(\lambda\beta, r)$ at the phantom critical point $r_{c,\lambda}$ (28). The thermodynamic potential $\phi(\lambda\beta, r)$ has a critical point $r_c(\beta)$ for $\beta > 2$ and $\phi(\lambda\beta, r)$ has a phantom critical point $r_{c,\lambda}(\beta)$ for $\lambda\beta > 2$.

The critical behavior of $\phi(\beta, r)$ is encoded in discontinuities of higher-order derivatives of $\phi(\beta, r)$ at the critical point r_c. The second derivative for $r \to r_c^+$ behaves like (see the Appendix)

$$\partial_r^2\phi(\beta, r) \sim \begin{cases} -c_1(r - r_c)^x + \cdots & \text{for } \beta \in (2, 3) \\ +c_2 \ln(r - r_c) + \cdots & \text{for } \beta = 3 \\ -c_3 + \cdots & \text{for } \beta \in (3, \infty), \end{cases} \tag{29}$$

where $x = (3 - \beta)/(\beta - 2)$ (A10) and c_1, c_2, and c_3 are positive constants. The ellipses indicate subleading terms. In contrast, $\partial_r^2\phi(\beta, r) = 0$ for $r \to r_c^-$. So we conclude that the second derivative has a finite discontinuity for $\beta \in (3, \infty)$ and it is logarithmically divergent for $\beta = 3$. It is continuous for $\beta \in (2, 3)$, but then higher derivatives diverge. Moreover, as discussed in the Appendix, for $\beta \in (3, \infty)$, the second derivative contains, among the subleading terms, a term of approximately $(r - r_c)^{\beta-3}$ for a noninteger β or a term of approximately $(r - r_c)^{\beta-3}\ln(r - r_c)$ for an integer β. This term leads to a divergence of higher derivatives for $r \to r_c^+$.

To summarize, the second derivative of the Rényi entropy density (15) inherits its singular behavior at the critical point from $\partial_r^2\phi$:

$$\partial_r^2 h_\lambda(\beta, r) = \frac{\partial_r^2\phi(\lambda\beta, r) - \lambda\partial_r^2\phi(\beta, r)}{1 - \lambda}. \tag{30}$$

This is the primary singularity. However, additionally, $\partial_r^2 h_\lambda(\beta, r)$ can acquire a secondary singularity at $r_{c,\lambda}$ (28) when $\lambda\beta > 2$. The singularity type is the same as for the primary singularity except that it corresponds to the critical behavior of the thermodynamic potential ϕ for the inverse temperature $\lambda\beta$ rather than β.

For $\lambda = 0$, $h_0(\beta, r)$ (17) is independent of β and has no singular points in the range $r \in (0, 1)$. Another exception is $\lambda \to 1$ because the resulting singularity of $h_1(\beta, r)$ comes from the

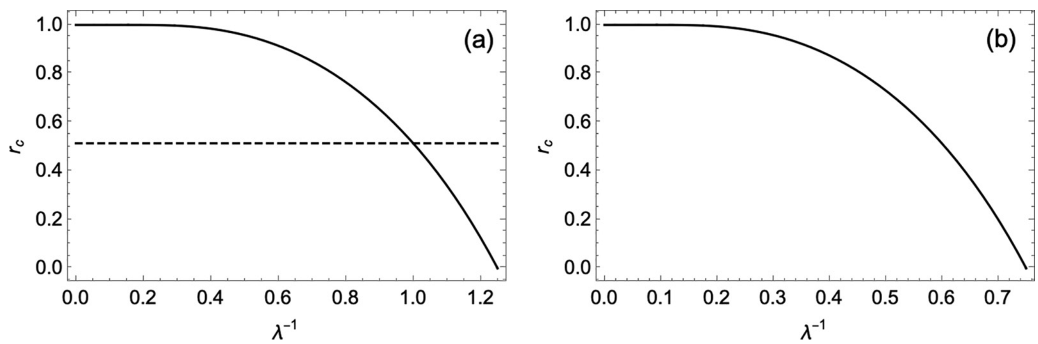

FIG. 2. (a) Position of the primary (dashed line) and secondary (solid line) singular points [Eqs. (24) and (28), respectively] for $\beta = 5/2$ and (b) position of the secondary singular point for $\beta = 3/2$ plotted as a function of λ^{-1} in the range $\lambda^{-1} \in (0, \beta/2)$. The solid curves have the same universal shape, differing mainly in their support $(0, \beta/2)$, which depends on β. There is no secondary singular point outside this range. Similarly, there is no primary singular point for $\beta \leqslant 2$.

merging of the primary and the secondary singularities. One can expect from Eq. (18) that the power-law singularities will acquire an extra logarithmic factor from the derivative of a power depending on β. For example, the second derivative has the singularity

$$\partial_r^2 h_1(\beta, r) \sim (r - r_c)^x \ln(r - r_c). \tag{31}$$

The logarithm here is generated from the derivative in the second term in (18).

III. DISCUSSION

We have calculated analytically the Rényi entropy for the abundance vector defined by the Gibbs measure for a zeta-urn model. In the thermodynamic limit for a suitable choice of parameters, the model has a (condensation) phase transition, which manifests as a singularity of the free energy at the critical point. The Rényi entropy also has a singularity at this point, but in addition to this the Rényi entropy can, depending on its order, display a secondary singularity at another point unlike the archetypal nonequilibrium model, the TASEP, as demonstrated in [41]. The secondary singularity is a phantom of the original singularity but itself is not directly related to any critical behavior in the system. The mechanism which leads to the occurrence of the secondary singularity is quite generic, following from (6) and (7), so such secondary singularities will occur in other statistical mechanical models with Gibbs weights and phase transitions. In the case of the TASEP, the weights are given by matrix products and do not have this structure. We stress, however, that these secondary singularities are rooted in the mathematical definition of the Rényi entropy rather than in physical behavior of the system. Below we illustrate this in a discussion of the secondary singularities for the Rényi divergence, where they arise from a comparison of two systems at different temperatures, so as such they cannot be a physical property of either one of the systems individually.

The Rényi divergence of order λ,

$$\Delta_\lambda(\bar{p}|\bar{q}) = \frac{1}{\lambda - 1} \ln \sum_\sigma \frac{p_\sigma^\lambda}{q_\sigma^{\lambda-1}}, \tag{32}$$

is a generalization of the Kullback-Leibler divergence [42] which is reproduced from the expression (32) in the limit $\lambda \to 1$. The Rényi divergence for two Gibbs distributions $\bar{p} = \{p_\sigma = e^{-\beta_1 E_\sigma}/Z(\beta_1), \sigma = 1, \dots, \mathcal{N}\}$ and $\bar{q} = \{q_\sigma = e^{-\beta_2 E_\sigma}/Z(\beta_2), \sigma = 1, \dots, \mathcal{N}\}$ for the same statistical system at different temperatures $T_1 = 1/\beta_1$ and $T_2 = 1/\beta_2$ is

$$\Delta_\lambda(\beta_1|\beta_2) = \frac{1}{\lambda - 1} \ln \frac{Z(\lambda\beta_1 - (\lambda - 1)\beta_2) Z^{\lambda-1}(\beta_2)}{Z^\lambda(\beta_1)}, \tag{33}$$

which should be compared with (6). For convenience, we have replaced arguments of Δ_λ by β_1 and β_2, which uniquely identify the thermal distributions $\bar{p}$ and $\bar{q}$. The divergence is proportional to the temperature difference and the heat capacity of the system

$$\Delta_\lambda(\beta|\beta + \Delta\beta) = \frac{\lambda \Delta\beta^2}{2} [\ln Z(\beta)]'' + o(\Delta\beta^2). \tag{34}$$

For the zeta-urn model, in the thermodynamic limit (13), Eq. (33) yields

$$\Delta_\lambda(\beta_1|\beta_2) = \frac{1}{\lambda - 1} [\phi(\lambda\beta_1 - (\lambda - 1)\beta_2, r) - \lambda\phi(\beta_1, r) + (\lambda - 1)\phi(\beta_2, r)]. \tag{35}$$

We see that, apart from the primary singularities at $r_{c,1} = \zeta(\beta_1)/\zeta(\beta_1 - 1)$ and $r_{c,2} = \zeta(\beta_2)/\zeta(\beta_2 - 1)$, the Rényi divergence can have a secondary singularity at $r_{c,\lambda} = \zeta(\beta_\lambda)/\zeta(\beta_\lambda - 1)$, where $\beta_\lambda = \lambda\beta_1 - (\lambda - 1)\beta_2$, if $\beta_\lambda > 2$.

Returning to the interpretation of the Rényi entropy density as a diversity measure, it is interesting to look at the behavior of h_λ as r is varied in Fig. 1. For a given β as r is decreased (i.e., as the density of particles is increased), h_λ initially increases, reaching a maximum value at

$$\partial_r h_\lambda(\beta, r) = \frac{\partial_r \phi(\lambda\beta, r) - \lambda \partial_r \phi(\beta, r)}{1 - \lambda} = 0, \tag{36}$$

with the limiting case of $\lambda = 1$ being given by

$$\partial_r h_1(\beta, r) = \partial_r \phi(\beta, r) - \partial_{\beta r}^2 \phi(\beta, r) = 0. \tag{37}$$

The values taken by $\partial_r \phi(\beta, r)$ in (36) and (37) will depend on whether a singularity has been encountered or not, giving $\ln \zeta(\beta)$ for $r \in (0, r_c]$ and $K_\beta(\alpha(r))$ for $r \in (r_c, 1)$, with similar considerations for $\partial_r \phi(\lambda\beta, r)$. Whether the maximum value of $h_\lambda(\beta, r)$ is attained as r is decreased before a singularity is encountered will depend on both λ and β. For instance, when $\beta = 5/2$ we can see in Fig. 1 that the maximum of h_λ occurs before any singularities are encountered when $\lambda \leqslant 1$, whereas it may encounter the secondary singularity at $r_{c,\lambda}(\beta)$ for sufficiently large λ before reaching its maximum. The Shannon entropy h_1 attains a maximum value in the fluid phase and then decreases linearly with r into the condensed phase after encountering the primary singularity as the density of particles is increased. In the second example in Fig. 1, $\beta = 3/2$, there is no primary singularity but the secondary one exists for $\lambda > 4/3$ and can lie on either side of the maximum of h_λ depending on the value of λ.

It is also clear that whatever the value of β, the maximum value of h_λ decreases from that of h_0 as λ is increased and shifts to larger r. The value of the maximum diversity and the density at which it occurs hence both depend on the value of λ chosen for a given β. Similarly, increasing β for a given λ decreases the maximum value of h_λ and shifts it to larger r. The task of maximizing the diversity for a zeta-urn model in the ensemble we consider thus depends on both what we mean by the diversity, e.g., the choice of λ, and what parameters we have under our control, e.g., r and/or β.

APPENDIX

In this Appendix we discuss the critical behavior of the thermodynamic potential $\phi(\beta, r)$ at $r = r_c$. We want to establish how the singularity type at the critical point r_c depends on β. We find it convenient to take the partial derivative of $\phi(\beta, r)$ with respect to r because the corresponding parametric equations for $\partial_r\phi(\beta, r)$ are simpler than those for $\phi(\beta, r)$ (22) and (23) and are therefore more useful in the analysis of critical point singularity. For $r \in (0, r_c]$ we get

$$\partial_r\phi(\beta, r) = K_\beta(0) = \ln\zeta(\beta), \tag{A1}$$

while for $r \in (r_c, 1)$,

$$r = -\frac{1}{K'_\beta(\alpha)} \tag{A2}$$

and

$$\partial_r\phi(\beta, r) = K_\beta(\alpha), \tag{A3}$$

where $\alpha \in (0, \infty)$. The equations will be used as follows. First we will expand the right-hand side of (A2) to extract the dependence of $\alpha = \alpha(r)$ on r, for r approaching r_c from above. Then we will substitute $\alpha = \alpha(r)$ into the expression on the right-hand side of (A3) to determine the type of singularity of $\partial_r\phi(\beta, r)$ for $r \to r_c$. To this end we will use the series expansion of the polylogarithm for a noninteger β [43]:

$$\mathrm{Li}_\beta(e^{-\alpha}) = \Gamma(1-\beta)\alpha^{\beta-1} + \sum_{k=0}^{\infty}\frac{(-1)^k\zeta(\beta-k)}{k!}\alpha^k. \tag{A4}$$

For $\beta \in (2, 3)$, Eqs. (A2) and (A3) can be written as

$$r = r_c + B\alpha^{\beta-2} + o(\alpha^{\beta-2}) \tag{A5}$$

and

$$\partial_r\phi(\beta, r) = \mu_c - a_1\alpha + o(\alpha) \tag{A6}$$

with coefficients r_c, μ_c, a_1, and $B > 0$, depending on β. The dependence of the coefficients on β can be easily determined [for instance, $\mu_c(\beta) = \ln\zeta(\beta)$], but will not be displayed in the analysis below because we want to concentrate on the dependence on r. From (A5) we get

$$\alpha = C(r - r_c)^{1/(\beta-2)} + o((r - r_c)^{1/(\beta-2)}), \tag{A7}$$

with $C = B^{-1/(\beta-2)}$. Substituting this into (A6) leads to

$$\partial_r\phi(\beta, r) = \mu_c - D(r - r_c)^{1/(\beta-2)} + o((r - r_c)^{1/(\beta-2)}), \tag{A8}$$

with $D = a_1C$. The coefficients μ_c and D depend only on β, so if we take the derivative of both sides with respect to r we get

$$\partial_r^2\phi(\beta, r) = -E(r - r_c)^{(3-\beta)/(\beta-2)} + o((r - r_c)^{(3-\beta)/(\beta-2)}), \tag{A9}$$

with $E = (\beta - 2)D$ a positive function of $\beta \in (2, 3)$. The second derivative $\partial_r^2\phi(\beta, r)$ is related to particle density fluctuations. For $\beta \in (2, 3)$ the exponent

$$x = \frac{3-\beta}{\beta-2} \tag{A10}$$

changes from zero to infinity when β changes from 3 to 2, so the transition is of second or higher order. For $\beta = 2$ the transition disappears and there is no phase transition for $\beta \leqslant 2$. On the other hand, for $\beta = 3$ the second derivative has a logarithmic singularity at r_c. To see this, let us use the series expansion of the polylogarithm for an integer β [43],

$$\mathrm{Li}_\beta(e^{-\alpha}) = \frac{(-1)^{\beta-1}}{(\beta-1)!}[H_{\beta-1} - \ln(\alpha)]\alpha^{\beta-1} + \sum_{k=0, k\neq\tau-1}^{\infty}\frac{(-1)^k\zeta(\beta-k)}{k!}\alpha^k, \tag{A11}$$

with $H_n = 1 + 1/2 + \cdots + 1/n$ the nth harmonic number. For $\beta = 3$, Eqs. (A2) and (A3) take the form

$$r = r_c + b_1\alpha + B\alpha\ln\alpha + o(\alpha\ln\alpha) \tag{A12}$$

and

$$\partial_r\phi(\beta, r) = \mu_c - a_1\alpha + o(\alpha), \tag{A13}$$

where again the coefficients r_c, b_1, B, μ_c, and a_1 depend only on β. Calculating α as a function of r from (A12), we get

$$\alpha = c_1(r - r_c) - C(r - r_c)\ln(r - r_c) + o((r - r_c)\ln(r - r_c)), \tag{A14}$$

with $c_1 = 1/b_1 + B/b_1^2\ln b_1$ and $C = B/b_1^2$. Substituting this into (A13), we get

$$\partial_r\phi(\beta, r) = \mu_c - d_1(r - r_c) + D(r - r_c)\ln(r - r_c) + o((r - r_c)\ln(r - r_c)), \tag{A15}$$

where $d_1 = a_1c_1$ and $D = a_1C$. As a consequence, the second derivative has a logarithmic singularity for $r \to r_c^+$,

$$\partial_r^2\phi(\beta, r) = -d_1 + D + D\ln(r - r_c) + o(\ln(r - r_c)). \tag{A16}$$

What is essential in this equation is that the second derivative diverges logarithmically when $r \to r_c^+$. This means that for $\beta = 3$ the particle density fluctuations are infinite at the critical point: $r \to r_c^+$.

For $\beta > 3$, Eqs. (A2) and (A3) take the form

$$r = r_c + b_1\alpha + \cdots + B\alpha^{\beta-2} + o(\alpha^{\beta-2}) \tag{A17}$$

and

$$\partial_r\phi(\beta, r) = \mu_c - a_1\alpha + o(\alpha), \tag{A18}$$

so for $r \to r_c^+$,

$$\partial_r\phi(\beta, r) = \mu_c - \frac{a_1}{b_1}(r - r_c) + \cdots + \frac{a_1 B}{b_1^{\beta-1}}(r - r_c)^{\beta-2} + o((r - r_c)^{\beta-2}) \tag{A19}$$

and hence

$$\lim_{r\to r_c^+} \partial_r^2\phi(\beta, r) = -\frac{a_1}{b_1} < 0. \tag{A20}$$

On the other hand,

$$\lim_{r\to r_c^-} \partial_r^2\phi(\beta, r) = 0, \tag{A21}$$

as follows from (25). Hence the second derivative has a finite discontinuity for $\beta > 3$. Additionally, we see that the first derivative contains a singular term of approximately $(r - r_c)^{\beta-2}$, and therefore the second derivative contains a term of approximately $(r - r_c)^{\beta-3}$, which makes higher derivatives diverge for $r \to r_c^+$. For an integer β this term is approximately $(r - r_c)^{\beta-3}\ln(r - r_c)$, as follows from (A11).

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