

## Constructing a statistical mechanics for Beck-Cohen superstatistics

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The basic aspects of both Boltzmann-Gibbs (BG) and nonextensive statistical mechanics can be seen through three different stages. First, the proposal of an entropic functional ( $S_{BG} = -k \sum_i p_i \ln p_i$  for the BG formalism) with the appropriate constraints ( $\sum_i p_i = 1$  and  $\sum_i p_i E_i = U$  for the BG canonical ensemble). Second, through optimization, the equilibrium or stationary-state distribution ( $p_i = e^{-\beta E_i} / Z_{BG}$  with  $Z_{BG} = \sum_j e^{-\beta E_j}$  for BG). Third, the connection to thermodynamics (e.g.,  $F_{BG} = -(1/\beta) \ln Z_{BG}$  and  $U_{BG} = -(\partial/\partial\beta) \ln Z_{BG}$ ). Assuming temperature fluctuations, Beck and Cohen recently proposed a generalized Boltzmann factor  $B(E) = \int_0^\infty d\beta f(\beta) e^{-\beta E}$ . This corresponds to the second stage described above. In this paper, we solve the corresponding first stage, i.e., we present an entropic functional and its associated constraints which lead precisely to  $B(E)$ . We illustrate with all six admissible examples given by Beck and Cohen.

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The foundation of statistical mechanics and thermodynamics is a fascinating and subtle matter. Its far reaching consequences have attracted deep attention since more than one century ago (see, for instance, Einstein's remark on the Boltzmann principle [1]). The field remains open to new proposals focusing nonequilibrium stationary states, such as metaequilibrium and others. One of such proposals is nonextensive statistical mechanics, advanced in 1988 [2,3] (see Ref. [4] for reviews). This formalism is based on an entropic index  $q$  (which recovers usual statistical mechanics for  $q = 1$ ), and has been applied to a variety of systems, covering certain classes of both (meta)equilibrium and nonequilibrium phenomena, e.g., turbulence [5], hadronic jets produced by electron-positron annihilation [6], cosmic rays [7], motion of *Hydra viridissima* [8], quantum chaos [9], and one-dimensional [10] and two-dimensional [11] maps, among others. In addition to this, it has been noted that it could be appropriate for handling some aspects of long-range interacting Hamiltonian systems (see Ref. [12], and references therein).

Let us be more precise. Nonextensive statistical mechanics is based on the entropic form (here written for  $W$  discrete events)

$$S_q = k \frac{1 - \sum_{i=1}^w p_i^q}{q-1} \left( \sum_{i=1}^w p_i = 1; q \in \mathcal{R} \right), \quad (1)$$

with

$$S_1 = S_{BG} = -k \sum_{i=1}^w p_i \ln p_i. \quad (2)$$

If we focus on the canonical ensemble (system in contact with a thermostat), we must add the following constraint [3]:

$$\frac{\sum_{i=1}^w p_i^q E_i}{\sum_{i=1}^w p_i^q} = U_q \quad (U_1 = U_{BG}), \quad (3)$$

where  $\{E_i\}$  is the set of eigenvalues of the Hamiltonian with given boundary conditions. Optimizing  $S_q$ , we straightforwardly obtain the distribution corresponding to the equilibrium, metaequilibrium, or stationary state, namely,

$$p_i = \frac{[1 - (1-q)\beta_q(E_i - U_q)]^{1/(1-q)}}{\bar{Z}_q}, \quad (4)$$

with

$$\bar{Z}_q = \sum_{j=1}^w [1 - (1-q)\beta_q(E_j - U_q)]^{1/(1-q)}, \quad (5)$$

and

$$\beta_q = \frac{\beta}{\sum_{j=1}^w p_j^q}, \quad (6)$$

$\beta$  being the Lagrange parameter. We easily verify that, for  $q = 1$ , we recover the celebrated BG equilibrium distribution

$$p_i = \frac{e^{-\beta E_i}}{Z_{BG}}, \quad (7)$$

with

$$Z_{BG} = \sum_{j=1}^w e^{-\beta E_j}. \quad (8)$$

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Very recently, Beck and Cohen have proposed [13] a generalization of the BG factor. More precisely, assuming that the inverse temperature  $\beta$  might itself be a stochastic variable, they advance

$$B(E) = \int_0^\infty d\beta' f(\beta') e^{-\beta' E}, \quad (9)$$

where the distribution  $f(\beta')$  satisfies

$$\int_{-\infty}^\infty d\beta' f(\beta') = 1. \quad (10)$$

It is clear that  $f(\beta') = \delta(\beta' - \beta)$  recovers the usual BG factor. They have also shown that, if  $f(\beta')$  is the  $\gamma$  (or  $\chi^2$ ) distribution, then the distribution associated with nonextensive statistical mechanics is reobtained. They have also illustrated their proposal with the uniform, bimodal, log-normal, and  $F$  distributions. Moreover, they define (see also Ref. [14])

$$q_{BC} = \frac{\langle \beta^2 \rangle}{\langle \beta \rangle^2} \left( \langle \dots \rangle \equiv \int_{-\infty}^\infty d\beta f(\beta) (\dots) \right), \quad (11)$$

where we have introduced the notation  $q_{BC}$  in order to avoid confusion with the present  $q$ . Clearly, if  $f(\beta')$  is the  $\gamma$  distribution, then  $q_{BC} = q$  (see Ref. [13]). Finally, they argue that whenever  $|q_{BC} - 1| \ll 1$ , for all admissible  $f(\beta)$ , we can write the asymptotic expression  $B(E) = \langle e^{-\beta E} \rangle \simeq e^{-\langle \beta \rangle E (1 + \sigma^2 E^2 / 2)}$ , where  $\sigma^2 = \langle \beta^2 \rangle - \langle \beta \rangle^2$ . This expression coincides with the expansion of the power-law function that represents the generalized Boltzmann factor associated with nonextensive statistical mechanics if we use Eq. (11) and identify  $q_{BC} = q$ . In other words, nonextensive statistical mechanics would correspond, for this particular mechanism, where nonextensivity is driven by the fluctuations of  $\beta$ , to the *universal* behavior whenever the fluctuations are relatively small.

This is no doubt a very deep and interesting result, *but* it does not constitute by itself a statistical mechanics. The reason is that the factor  $B(E)$  has been introduced through what can, in some sense, be considered as an *ad hoc* procedure. The basic element which is missing in order to be legitimate to speak of a statistical-mechanical formalism is to be able to *derive* the factor  $B(E)$  from an entropic functional with concrete constraints (and especially the energetic constraint, which generates the concept of thermostat temperature). The purpose of the present paper is to exhibit such entropic form and constraint.

Let us first write a quite generic entropic form (from now on  $k = 1$  for simplicity), namely,

$$S = \sum_{i=1}^w s(p_i) \quad [s(x) \geq 0; s(0) = s(1) = 0]. \quad (12)$$

For the BG entropy  $S_{BG}$ , we have  $s(x) = -x \ln x$ , and for the nonextensive one  $S_q$ , we have  $s(x) = (x - x^q)/(q - 1)$ . The

function  $s(x)$  should generically have a definite concavity  $\forall x \in [0, 1]$ . Conditions (12) imply that  $S \geq 0$  and that certainty corresponds to  $S = 0$ .

Let us now address the constraint associated with the energy. We consider the following form:

$$\frac{\sum_{i=1}^w u(p_i) E_i}{\sum_{i=1}^w u(p_i)} = U \quad [0 \leq u(x) \leq 1; u(0) = 0; u(1) = 1]. \quad (13)$$

For the BG internal energy  $U_{BG}$ , we have  $u(x) = x$ , and for the nonextensive one  $U_q$ , we have  $u(x) = x^q$ . The function  $u(x)$  should generically be a monotonically increasing one. Certainty about  $E_j$  implies  $U = E_j$ . The quantity  $u(p_i) / \sum_{j=1}^w u(p_j)$  constitutes itself a probability distribution (which generalizes the escort distribution defined in Ref. [15]). The constraint associated with the energy applies, in principle, for the (meta)equilibrium state. However, its validity (either exact or approximate) has been verified in various nonequilibrium stationary states related with nonextensive statistical mechanics (e.g., turbulence [5], granular matter [18]). For example, we may interpret the energy spectrum used in the constraint in the same spirit as the temperature used by Beck and Cohen. It represents the mean value of some fluctuation distribution. The general foundational question and its possible geometrical interpretation (in phase space) remain, nevertheless, open.

Let us consider now the functional

$$\Phi \equiv S - \alpha \sum_{i=1}^w p_i - \beta \frac{\sum_{i=1}^w u(p_i) E_i}{\sum_{i=1}^w u(p_i)}, \quad (14)$$

where  $\alpha$  and  $\beta$  are Lagrange parameters. The condition  $\partial \Phi / \partial p_j = 0$  implies

$$s'(p_j) - \alpha - \frac{\beta}{\sum_{i=1}^w u(p_i)} u'(p_j) (E_j - U) = 0. \quad (15)$$

Let us now heuristically assume

$$u'(x) = \mu + \nu s'(x), \quad (16)$$

$$u(x) = \mu x + \nu s(x) + \xi. \quad (17)$$

But the condition  $s(0) = u(0) = 0$  implies  $\xi = 0$ , and the conditions  $s(1) = 0$  and  $u(1) = 1$  imply that  $\mu = 1$ , hence,

$$u(x) = x + \nu s(x) \quad (18)$$

and

$$u'(x) = 1 + \nu s'(x). \quad (19)$$

Observe that if  $\nu=0$ , we have  $u(x)=x$  and  $\sum_{j=1}^W u(p_j) = \sum_{j=1}^W p_j = 1$ .

The replacement of Eq. (19) into Eq. (15) yields

$$s'(p_i) = \frac{\alpha + \beta \frac{E_i - U}{w} \sum_{j=1}^W u(p_j)}{1 - \beta \nu \frac{E_i - U}{w} \sum_{j=1}^W u(p_j)}, \quad (20)$$

hence

$$p_i = (s')^{-1} \left( \frac{\alpha + \beta \frac{E_i - U}{w} \sum_{j=1}^W u(p_j)}{1 - \beta \nu \frac{E_i - U}{w} \sum_{j=1}^W u(p_j)} \right), \quad (21)$$

where  $(s')^{-1}(\dots)$  is the inverse function of  $s'(\dots)$ . The condition  $\sum_{i=1}^W p_i = 1$  enables the (analytical or numerical) elimination of the Lagrange parameter  $\alpha$ . The function (21) is to be identified with  $B(E)/\int_0^\infty dE' B(E')$  from Ref. [13]. In other words, if  $E(y)$  is the inverse function of  $B(E)/\int_0^\infty dE' B(E')$ , we have that

$$s(x) = \int_0^x dy \frac{\alpha + \beta \frac{E(y) - U}{w} \sum_{j=1}^W u(p_j)}{1 - \beta \nu \frac{E(y) - U}{w} \sum_{j=1}^W u(p_j)}, \quad (22)$$

which, together with Eq. (18), completely solves the problem once  $\nu$  is determined. Summarizing, given an admissible function  $B(x)$ , we have uniquely determined the functions  $s(x)$  and  $u(x)$ , which replaced into Eqs. (12) and (13) concludes the formulation of the statistical mechanics associated with the Beck-Cohen superstatistics. An important remark remains to be made, namely, *any* monotonic function of  $S$  given by Eq. (12) also is a solution at this stage. Which of those is to be retained for a possible connection with thermodynamics is a different matter, and remains an open issue at the present stage. For example, for nonextensive statistical mechanics, in what concerns the stationary distribution,  $S_q$  and the Renyi entropy  $S_q^R = \ln[1 + (1-q)S_q]/(1-q)$  are equivalent. In other words, *at this level*, we could indistinctively use  $S_q$  or  $S_q^R$ . There is, however, a variety of physical arguments which are out of scope of the present work but which nevertheless point, in that particular case,  $S_q$  as being the correct physical quantity to be used for thermodynamic

and dynamic purposes. A strong argument along this line concerns the stability of the entropy under arbitrarily small deformation of the statistical state probabilities [16]. For instance, Abe [17] and Lesche [16], respectively, showed that  $S_q$  is stable and  $S_q^R$  is unstable.

Let us now compare the  $B(E)$  factor obtained by Beck-Cohen formalism with the distribution presented here in Eq. (21). In addition to the fact that the former does not include the normalization constant whereas the latter does, we notice that the  $B(E)$  factor has parameters such as  $\beta_0 \equiv \langle \beta \rangle$ , instead of the parameters  $\alpha$ ,  $U$ ,  $\nu$ , and  $\beta/\sum_j^W u(p_j)$  [generalization of Eq. (6)] appearing in Eq. (21). This problem will be handled as follows. Since our aim is to determine the *functional forms* of  $s(x)$  and  $u(x)$ , it is enough to work with only one variable. So, we take  $\beta_0 = \beta/\sum_j^W u(p_j) = 1$  and  $U=0$ . Let us now determine  $\nu$ . Using Eqs. (15) and (19), and integrating, we obtain

$$u(x) = (1 + \alpha \nu) \int_0^x \frac{dy}{1 - \nu E(y)}. \quad (23)$$

It is physically reasonable to assume that  $u(x)$  monotonically increases with  $x$ , hence  $du/dx \geq 0$ , and  $(1 + \alpha \nu)/(1 - \nu E) \geq 0$ . We shall verify later that  $1 + \alpha \nu > 0$ , hence it must be  $\nu \leq 1/E$ . If we note  $E^*$ , the lowest admissible value of  $E$ , we are allowed to consider  $\nu = 1/E^*$ . In particular, if  $E^* \rightarrow -\infty$ , then it must be  $\nu = 0$ . An example where  $E^*$  is finite is nonextensive statistical mechanics with  $q > 1$ . In this case,  $E^* = 1/(1-q)$ , hence  $\nu = 1-q$ . We can trivially verify that this value for  $\nu$ , together with  $s(x) = (x-x^q)/(q-1)$  and  $u(x) = x^q$  precisely satisfy Eq. (18).

Summarizing, the final form of  $u(x)$  is given by

$$u(x) = (1 + \alpha/E^*) \int_0^x \frac{dy}{1 - E(y)/E^*}, \quad (24)$$

and, therefore,

$$s(x) = \int_0^x dy \frac{\alpha + E(y)}{1 - E(y)/E^*}. \quad (25)$$

In what follows, we shall illustrate the above procedure by addressing *all* the admissible examples appearing in Ref. [13]. The cases associated with the Dirac  $\delta$  and the  $\gamma$  distributions for  $f(\beta)$  (respectively corresponding to BG and non-extensive statistical mechanics) can be handled analytically. The other four cases [uniform, bimodal, log-normal, and  $F$  distributions for  $f(\beta)$ ] have been treated numerically as follows. We first choose  $f(\beta)$ , then calculate  $B(E)$ , and from this calculate  $\int_0^\infty dE' B(E')$ . By inverting the axes of the variables, we find the inverse  $E(y)$  of Beck-Cohen superstatistics. From this, we obtain  $E^*$ . Two cases are possible. The first one corresponds to  $E^* \rightarrow -\infty$ , hence  $\nu = 0$ ,  $u(x) = x$ , and  $s(x) = \alpha x + \int_0^x dy E(y)$ . The condition  $s(1) = 0$  determines  $\alpha$ , which is therefore given by  $\alpha = -\int_0^1 dy E(y)$ . The second case corresponds to a finite and known value of  $E^*$ , which determines  $\nu = 1/E^*$ . From this, we calculate  $\int_0^x dy/[1 - E(y)/E^*]$ . From the condition  $u(1) = 1$  and using

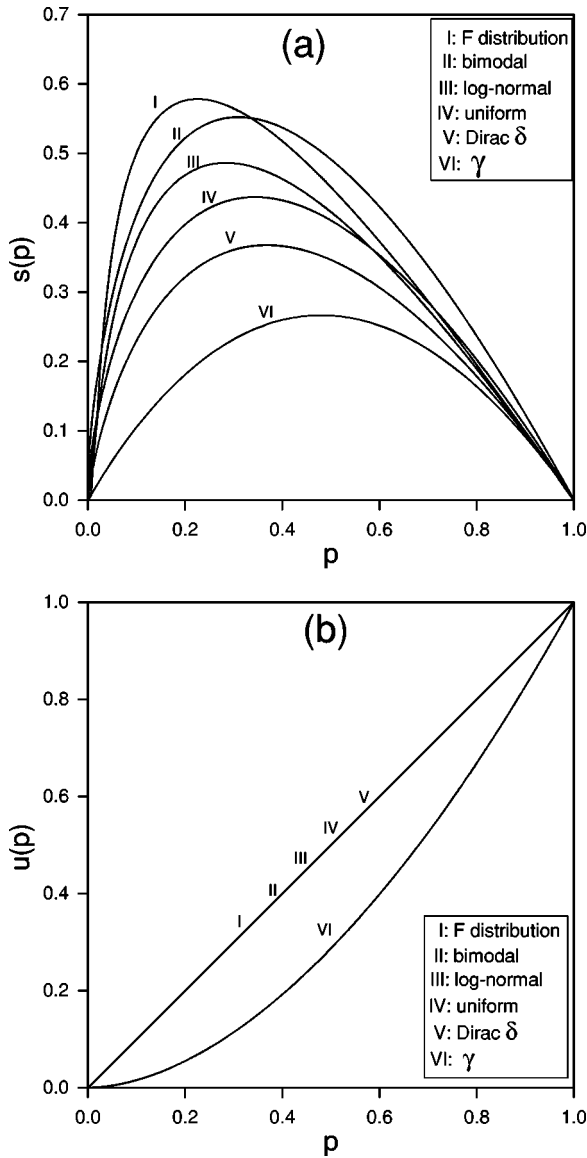


FIG. 1. Functions  $s(x)$  (a) and  $u(x)$  (b) for illustrative examples of the cases focused on in Ref. [13]. From top to bottom: (i)  $F$  distribution [ $f(\beta) = 24/(2 + \beta)^4$ ]; (ii) bimodal [ $f(\beta) = 0.5 \delta(\beta - 1/2) + 0.5 \delta(\beta - 3/2)$ ]; (iii) log normal [ $f(\beta) = (1/\beta\sqrt{2\pi})e^{-[(0.5 + \ln \beta)^2/2]}$ ]; (iv) uniform [ $f(\beta) = 1$  on the interval  $[1/2, 3/2]$ , and zero otherwise]; (v) Dirac  $\delta$  [ $f(\beta) = \delta(\beta - 1)$ ]; (vi)  $\gamma$  [ $f(\beta) = [(\beta)^{0.25}/(0.8)^{1.25}\Gamma(1.25)]e^{-1.25\beta}$ ], which corresponds to  $q = 1.8$ .

Eq. (24), it is easy to see that  $1 + \alpha\nu = 1 + \alpha/E^* = 1/\int_0^1 dy/[1 - E(y)/E^*] > 0$  and it is direct to determine  $\alpha$ , which in turn enables the calculation of  $u(x)$  using once again Eq. (24). Finally, from Eq. (18), we calculate  $s(x)$ , and the problem is solved.

In Figs. 1(a) and 1(b), typical examples of  $s(x)$  and  $u(x)$  are presented for all the cases addressed in Ref. [13]. In Fig. 2, we show the entropies associated with all these examples assuming  $W = 2$ .

Let us conclude by saying that it has been possible to find expressions for the entropy and for the energetic constraint that lead to a generic Beck-Cohen superstatistics. Of course,

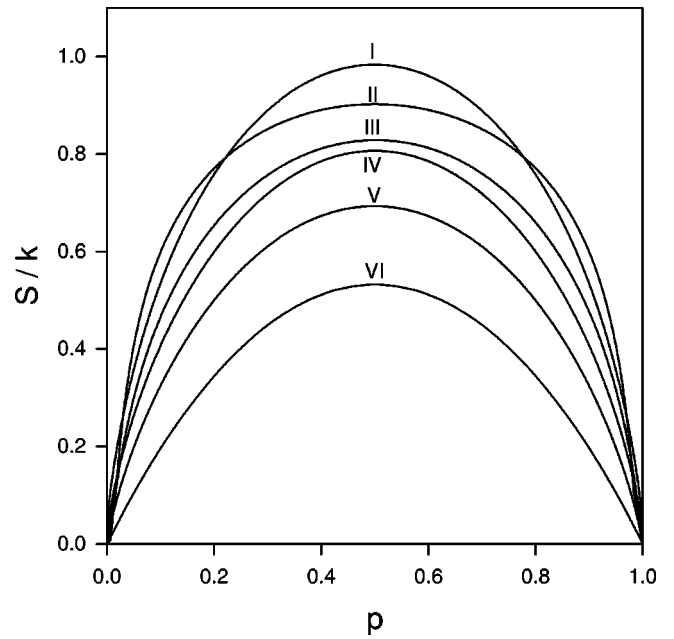


FIG. 2.  $W = 2$  entropies associated with the examples presented in Fig. 1.

similar considerations are valid for other constraints if we were focusing on say the grandcanonical ensembles. The step we have discussed is necessary for having the statistical mechanics generating these superstatistics through a variational principle. What remains to be done is the possible connection with thermodynamics. This is not a trivial task because unless we are dealing with a nonlinear power law for  $u(x)$  (which precisely is nonextensive statistical mechanics), the Lagrange parameter  $\alpha$  is *not* factorizable in Eq. (21), hence no partition function can be defined in the usual sense, i.e., a partition function which depends on  $\beta$  (and other analogous parameters), but does *not* depend on  $\alpha$ . Summarizing, nonextensive statistical mechanics not only paradigmatically represents, as shown in Ref. [13], the universal behavior of all Beck-Cohen superstatistics in the limit  $q_{BC} \approx q \approx 1$ , but it is the only one for which an  $\alpha$ -independent partition function can be defined.

Last but not least, let us emphasize that the present results strengthen the idea that the statistical-mechanical methods can be *in principle* used out of equilibrium as well. To be more specific, we can think of using them (i) in *equilibrium* (e.g., in the  $t \rightarrow \infty$  limit of noninteracting or short-range interacting Hamiltonians, as well as in the  $\lim_{N \rightarrow \infty} \lim_{t \rightarrow \infty}$  of long-range interacting many-body Hamiltonian systems; this is essentially BG statistical mechanics), (ii) in *metaequilibrium* (e.g., in the  $\lim_{t \rightarrow \infty} \lim_{N \rightarrow \infty}$  of long-range interacting many-body Hamiltonian systems; see, for instance, Ref. [12]), and (iii) for appropriate classes of *stationary states* (see, for instance, Refs. [5,18]). Further foundational work would be welcome for case (iii).

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