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BEYOND THE EXPONENTIAL STATISTICAL FACTOR

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1 Overview

In this note I shall present my personal view and path to non-extensive thermodynamics, to the realm of generalized canonical statistical factors replacing the exponential function by another, deformed exponential, and accordingly its inverse function by a deformed logarithm. The deformation can be parametrized, also by using more than one parameter, but the present discussion will be restricted to the one-parameter version.

By generalizing the familiar classical exponential weight factor, $\exp(-E/T)$, in counting the relative occurence frequency of states with energy E at temperature T one encounters primarily mathematical challenges [1]. However, it is of equal importance to built up the formalism on physical phenomena, with an ample number of special cases, realistic examples from the physical world [2–4]. Therefore I follow in this abstract the strategy of first showing simple (oversimplified) theoretical problems and then gradually generalizing the obtained results. The path of a particular understanding, outlined here, will show several similarities with the superstatistical view of non-Gibbsean thermodynamics, considering a distribution of intensity parameters, dominantly the inverse temperature, $\beta = 1/k_B T$ [5]. For the sake of simplicity we use units in which $k_B = 1$.

1.1 Simple examples in phase space filling

Let us start the discussion with some simple problem. Remembering the traditional derivation of the canonical distribution with its Boltzmann–Gibbs factor I had always wondered why should we stop at the first term. The argument, that it shall be small and negligible, is afterwards; not very convincing. And certainly false for mesoscopic or nanosize systems, or systems with too many constraints ("almost integrable systems"). The Gibbs factor needs generalization [6–8].

In our first physical example [9] we consider a very simple phase-space: the volume of all states with a given total energy, E, and n degrees of freedom (dimensionality) for ultrarelativistic particles with $E = |\vec{p}|$ is given as a hypersphere volume with radius E in dimension n: $\Omega(E) \sim E^n$. When picking up a single degree of freedom with energy ε, the phase space fraction for this partition in an ideal gas is given by the Einstein formula

$$\frac{\Omega(\varepsilon)\,\Omega(E-\varepsilon)}{\Omega(E)} = \Omega(\varepsilon)\left(1-\frac{\varepsilon}{E}\right)^n. \tag{1}$$

Here the factor $\rho_{n,E}(\varepsilon) = (1-\varepsilon/E)^n$ is the canonical weight of such configurations. In the textbook limit, $n \to \infty$ and $E \to \infty$ while $E/n = T$ constant it delivers the Boltzmann–Gibbs factor:

$$\overline{\rho}_{Gibbs} = \lim_{n\to\infty} \rho_{n,E}(\varepsilon) = \mathrm{e}^{-\varepsilon/T}. \tag{2}$$

However, this is not the only way to obtain the exponential factor and also not the only possible result in all physical situations. Consider a fluctuating number of dimensionality of the phase space at fixed total energy, with the probability P_n. Collecting results from such parallel ensembles of physical events, one measures the average environmental factor

$$\overline{\rho} := \left\langle \rho_{n,E}(\varepsilon) \right\rangle = \sum_{n=0}^{\infty} P_n \left(1-\varepsilon/E\right)^n. \tag{3}$$

In this formula no "thermodynamical limit" is taken, but an averaging (so called "superstatistics") over all possible n values with a normalized probability distribution. Also E can be small, no restriction.

Next we see what simple distributions deliver. Most notably, the very common, one-parameter distribution, the Poissonian leads to

$$\overline{\rho}_{\mathrm{POI}} := \sum_{n=0}^{\infty} \frac{\langle n\rangle^n}{n!} \mathrm{e}^{-\langle n\rangle} \left(1-\varepsilon/E\right)^n = \mathrm{e}^{-\langle n\rangle \varepsilon/E}. \tag{4}$$

This is a Boltzmann–Gibbs factor with the temperature $T = E/\langle n\rangle$. The temperature is the energy per average number of degrees of freedom [9; 10]. And this result is valid even for $\langle n\rangle < 1$!

Somewhat more general is the negative binomial distribution, utilized with respect of multi-bosonic states in high energy physics or quantum optics:

$$P_n = \binom{n+k}{n} f^n \left(1+f\right)^{-n-k-1}. \tag{5}$$

In this case $\langle n\rangle = f(k+1)$ and we obtain

$$\overline{\rho}_{\mathrm{NBD}} = \left(1+\frac{\langle n\rangle}{k+1}\,\frac{\varepsilon}{E}\right)^{-k-1}, \tag{6}$$

a Pareto distribution with the temperature parameter $T = E/\langle n\rangle$ (again) and the power law tail with the negative power $(k+1)$. This generalizes the previous result, which is re-gained in the $k \to \infty$ limit.

1.2 Connecting number of degree of freedom and temperature fluctuations

For a general P_n distribution the Pareto or Gibbs results are only approximations [10]. However, since the NBD includes the Poissonian as a limit, also the Pareto distribution includes the exponential factor as the same limit. Therefore it is expedient to compare the general result for the canonical factor $\overline{\rho}$ with the Tsallis–Pareto form. Demanding that the approximate equality

$$\overline{\rho}(\varepsilon) = \sum_{n=0}^{\infty} P_n \, (1-\varepsilon/E)^n \; = \; \left(1+(q-1)\frac{\varepsilon}{T}\right)^{-\frac{1}{q-1}}, \tag{7}$$

holds up to next to leading order, we expand for $\varepsilon \ll E$ both sides and identify the coefficients of the linear and quadratic terms:

$$\frac{\langle n \rangle}{E} \; = \; \frac{1}{T}, \qquad \text{and} \qquad \frac{\langle n(n-1) \rangle}{E^2} \; = \; \frac{q}{T^2}. \tag{8}$$

The Tsallis parameter, q, occuring in these formulas is hence given as the second scaled factorial moment:

$$q \; = \; \frac{\langle n(n-1) \rangle}{\langle n \rangle^2}. \tag{9}$$

Its deviance from the classical Boltzmann–Gibbs value, $q_{BG} = 1$, reflects the non-Poissonity of the underlying n-distribution. For the negative binomial case $q = 1 + 1/(k+1)$.

Now we consider the general phase space factor, based on Einstein's formula for the phase space volume, $\Omega(E) = \mathrm{e}^{S(E)}$. In this simplified thermodynamics solely the energy, E, determines the total entropy, $S(E)$ by its particular functional connection, the equation of state. The superstatistical average of the canonical factor becomes

$$\overline{\rho}(\varepsilon) \; = \; \left\langle \mathrm{e}^{S(E-\varepsilon)-S(E)} \right\rangle. \tag{10}$$

Expanding to second order in ε and comparing to the same expansion of the Tsallis form of the Pareto distribution given in eq.(7), we arrive at

$$\left\langle 1 - \varepsilon S'(E) + \frac{\varepsilon^2}{2}\left(S''(E) + S'(E)^2\right) + \ldots \right\rangle \; = \; 1 - \frac{\varepsilon}{T} + \frac{q\varepsilon^2}{2T^2} + \ldots \tag{11}$$

From term by term identification the following interpretation of the parameters in the Tsallis–Pareto formula emerges

$$\frac{1}{T} \; = \; \langle S'(E) \rangle \qquad \text{and} \qquad q \; = \; \frac{\langle S''(E) + S'(E)^2 \rangle}{\langle S'(E) \rangle^2}. \tag{12}$$

The interpretation of T coincides with the thermodynamical definition of the absolute temperature. For the interpretation of q one notes that $\langle S''(E) \rangle = d(1/T)/dE = -1/CT^2$, including the total heat capacity C (in extensive systems proprtional to the system size). Denoting by $\beta = S'(E)$, we have $1/T = \langle \beta \rangle$ and

$$q \; = \; 1 - \frac{1}{C} + \frac{\Delta\beta^2}{\langle \beta \rangle^2}. \tag{13}$$

One realizes that the finiteness of the system, $C < \infty$, reduces the parameter q below one, while the relative variance of the primitive (non-superstatistical) β increases it over one. In traditional textbook interpretation $q = 1$ is assumed (taken as granted) and the "Gaussian" conclusion, $\Delta\beta / \langle \beta \rangle = 1/\sqrt{C}$ is drawn. But for a general superstatisitics these two terms do not cancel each other.

Finally we establish the connection with the β-superstatistics by the equation

$$\overline{\rho}(\varepsilon) = \sum_{n=0}^{\infty} P_n (1-\varepsilon/E)^n \; = \; \int w(\beta) \, \mathrm{e}^{-\beta\varepsilon} \, d\beta. \tag{14}$$

Utilizing that $\mathrm{e}^{-\beta\varepsilon} = \mathrm{e}^{\beta E(1-\varepsilon/E)} \mathrm{e}^{-\beta E}$ and expanding the first exponential in powers of $(1-\varepsilon/E)$, it turns out that P_n is the Poisson-transform of the superstatistical factor

$$P_n \; = \; \int \frac{(\beta E)^n}{n!} \, \mathrm{e}^{-\beta E} \, w(\beta) \, d\beta. \tag{15}$$

To the Poissonian n-distribution it belongs $w = \delta(\beta - 1/T)$, to the negative binomial in n on the other hand a gamma distribution in β. A Gauss-distribution in β is unphysical, and – contrary to the folklore – never should be considered [11].

2 Non-additive composition rules

Replacing the exponential function in the statistical factor with something different also influences the well-known connection between the statistical and energetic independence. In the traditional view, using exponential probabilities, their product is also an exponential, more precisely an exponential of the sum:

$$\mathrm{e}^{S_1} \cdot \mathrm{e}^{S_2} \; = \; \mathrm{e}^{S_{12}} \tag{16}$$

leads to the additive composition rule: $S_{12} = S_1 + S_2$. On the other hand, considering e.g. the product of two Pareto distributions (as being the next to leading order approximation),

$$\left(1+(q-1)\frac{x_1}{T}\right)^{-1/(q-1)} \cdot \left(1+(q-1)\frac{x_2}{T}\right)^{-1/(q-1)} \; = \; \left(1+(q-1)\frac{x_{12}}{T}\right)^{-1/(q-1)} \tag{17}$$

leads to the Tsallis–Abe composition rule

$$x_{12} \; = \; x_1 + x_2 + (q-1) x_1 x_2. \tag{18}$$

The question arises what kind of composition rules, replacing the addition, can be compatible with basic principles of thermodynamnics [12–14].

2.1 General associative rules

A general composition rule is defined by a two-variable function [12; 13], $x_{12} = x_1 \oplus x_2 = h(x_1,x_2)$, which nevertheless has to satisfy some properties in order to describe thermodynamical systems. The triviality property reads as $h(x,0) = x$ and $h(0,y) = y$. For the repetition of the composition we require that everything is described by pairwise steps; therefore only associative functions shall be considered: $h(x,h(y,z)) = h(h(x,y),z)$. The solution of such a general requirement is given by

$$h(x,y) \;=\; K^{-1}\left(K(x)+K(y)\right), \tag{19}$$

with a strict monotonic growing real funbction $K(x)$. In this case $K(x)$ is the deformed version of the quantity x and it is additive: $K(x_{12}) = K(x_1)+K(x_2)$. We also note that a general equilibrium condition in accord with the zeroth law of thermodynamics [15] can be satisfied by using three different functions, $K_1(x), K_2(y)$ and $K_{12}(h(x,y))$, declared to be additive.

Furthermore we also want to built up large systems by small steps. Then a system with N_1 steps and another one built with N_2 steps should be composed to a system equivalent to the one built by $N_{12} = N_1+N_2$ steps. Again this procedure maps a general composition rule to the additivity. We define x_n as the quantity built up in n steps starting from zero. Then the last step obeys $x_n = h(x_{n-1},dx)$ and we can write the recursion as

$$x_n - x_{n-1} \;=\; h(x_{n-1},dx) - h(x_{n-1},0) \;=\; dx\,\left.\frac{\partial}{\partial y}h(x,y)\right|_{y=0} + O(dx^2). \tag{20}$$

In the continuous limit this leads to the differential equation

$$\frac{dx}{dt} \;=\; \frac{\partial}{\partial y}h(x,0) \tag{21}$$

with the solution

$$t = K(x) = \int \frac{dx}{\frac{\partial}{\partial y}h(x,0)}. \tag{22}$$

Due the additivity in the number of steps, $K(x)$ is the additive quantity. From the triviality condition $k(0) = 0$ and it is practical to choose $K'(0) = 1$.

2.2 Examples: Tsallis–Abe rule, Einstein velocity addition rule

By using this general formula for any composition rule the corresponding deformation function can be obtained. For example the Tswallis-Abe rule, $h(x,y) = x+y+(q-1)xy$ gives $K(x) = \frac{1}{q-1}\ln(1+(q-1)x)$. Another well-known nontrivial composition rule, Einstein's velocity addition rule in special relativity, $h(v_1,v_2) = \frac{v_1+v_2}{1+v_1v_2/c^2}$ leads to $K(v) = c\,\mathrm{Arth}(v/c)$. Indeed, the rapidity is additive in this case: by $\eta = K(v)/c$ one obtains $v/c = \mathrm{th}(\eta)$.

The general composition rule shows also the way to the deformation of the entropy. Noting that traditional formulas (Boltzmann, Gibbs, Planck, Wiener, Shannon) build the expectation value of $\ln(1/p_i) = -\ln p_i$ for entropy-additive systems, in the general case one defines

$$K(S) \;:=\; \sum_i p_i K(-\ln p_i). \tag{23}$$

Due to this definition $K(S)$ is the additive entropy for the product of individual probabilities. This takes correlations into account in a nontrivial way.

We apply this construction for the Tsallis–Abe rule. Let the non-additive entropy satisfy

$$S_{12} \;=\; S_1+S_2+(1-q)S_1S_2. \tag{24}$$

Then the additive (deformed) entropy is given by

$$S^{\mathrm{add}} \;=\; \frac{1}{1-q}\ln\left(1+(1-q)S^{\mathrm{non-add}}\right), \tag{25}$$

and the reconstruction is given by the inverse function

$$S^{\mathrm{non-add}} \;=\; \frac{1}{1-q}\left(\mathrm{e}^{(1-q)S^{\mathrm{add}}}-1\right). \tag{26}$$

In this case we obtain the Tsallis and Rényi entropies indexed by q as

$$S^{\mathrm{non-add}} \;=\; \frac{1}{1-q}\sum_i\left(p_i^q-p_i\right), \qquad \text{and} \qquad S^{\mathrm{add}} \;=\; \frac{1}{1-q}\ln\sum_i p_i^q. \tag{27}$$

3 Finite size correction of the exponential formula

What $K(S)$ deformation is optimal to use, depends on the physical situation. Natural processes may reveal the proper composition law, as in the case of the velocity addition formula of Einstein, where the constraint that the velocity of light should not be changed emerged from experimental findings in optics. In some other cases, however, the proper composition rule is not directly available, but one may have some information on the fluctuating nature of the number of relevant degrees of freedom. To shed some light onto this procedure we connect in this section the general phase space arguments with the particular non-additivity forms discussed above.

3.1 Deformed entropy for constrained phase space

The derivation of the canonical weight factor from the product of phase space sizes assumed uncorrelated subsystem and reservoir. Due to the exponential relation to the entropy it handled the entropy as an additive quantity. Generalizing this point we have to allow for non-additive entropies (correlated states between environment and a single or few selected degrees of freedom). Therefore we consider a modified canonical statistical weight factor as follows [10; 16]

$$\overline{\rho}_K(\varepsilon) = \left\langle e^{K(S(E-\varepsilon))-K(S(E))} \right\rangle \approx \left\langle e^{-\varepsilon K'S' - \frac{\varepsilon^2}{2}\left(K''S'^2+K'S''\right)} \right\rangle \approx 1-\varepsilon K'\left\langle S'\right\rangle + \frac{\varepsilon^2}{2}\left(K'^2+K''\right)\left\langle S'^2\right\rangle + K'\left\langle S''\right\rangle. \tag{28}$$

Here we assume a universal entropy deformation function, $K(S)$ and an equation of state, $S(E)$ for the thermodynamical system. Identifying the linear and quadratic term coefficients again with the corresponding factors in the Taylor expansion of the Pareto distribution (as next to leading order approximation to a general canonical distribution) we arrive at

$$q_K = \left[1+\frac{K''}{K'^2}\right]\left(1+T^2\Delta\beta^2\right) - \frac{1}{C}\frac{1}{K'}. \tag{29}$$

Requiring now $q_K = 1$, since we want to use exactly that $K(S)$ deformation which results in an additive system, we have obtained an ordinary differential equation determining the sought $K(S)$. Introducing the notations $a = T^2\Delta\beta^2$ (relative variance of the fluctuating inverse temperature β), $b = 1/C$ (the finite size, finite total heat capacity correction factor) and $F = 1/K'$ we arrive at an easily solvable equation

$$(1+a)F' + bF = a. \tag{30}$$

The "initial" condition is given by $F(0) = 1/K'(0) = 1$. Its general solution with constant (S-independent) coefficients a and b is readily given as

$$F(S) = e^{-\frac{bS}{1+a}} + \frac{a}{b}\left(e^{-\frac{bS}{1+a}} - 1\right). \tag{31}$$

From here it is straightforward to obtain

$$K(S) = \frac{1+a}{a}\ln\left[1+\frac{a}{b}\left(e^{\frac{bS}{1+a}}-1\right)\right]. \tag{32}$$

We note that here $q = 1-b+a$. Our solution can be simplified by using the core auxiliary function $h_\alpha(x) := (e^{\alpha x}-1)/\alpha$:

$$K(S) = h_\lambda^{-1}\left(h_\mu(S)\right) \quad \text{and} \quad K^{-1}(\sigma) = h_\mu^{-1}\left(h_\lambda(\sigma)\right). \tag{33}$$

with $\lambda = \frac{a}{1+a}$ and $\mu = \frac{b}{1+a}$. After all this the additive entropy formula (while $-\ln p_i$ being non-additive) is given as

$$S^{\text{add}}_{\lambda,\mu} = \frac{1}{\lambda}\sum_i p_i \ln\left[1+\frac{\lambda}{\mu}\left(p_i^{-\mu}-1\right)\right]. \tag{34}$$

The Tsallis–Pareto power index is related to the parameters of the more general entropy formula as $q = \frac{1-\mu}{1-\lambda}$.

3.2 Tsallis, Rényi and Gompertz limits

It should be enlightening to consider some limits of this general formula. The textbook case is $q = 1$, predicting $a = b$ and therefore $\mu = \lambda$. In this case we reconstruct the classical entropy formula

$$S^{\text{add}}_{\mu,\mu} = -\sum_i p_i \ln p_i. \tag{35}$$

Another possible limit is when the variance is negligible, $\Delta\beta \approx 0$, therefore $a = 0$ and $\lambda = 0$, but the finiteness of the reservoir not: $\mu = b$ and $q = 1-b = 1-1/C$. In this case we arrive at the q-entropy, promoted by Tsallis:

$$S^{\text{add}}_{0,1-q} = \frac{1}{1-q}\sum_i \left(p_i^q - p_i\right). \tag{36}$$

Finally in an interesting opposite limit we deal with a big system, approaching well the thermodynamical limit, so $b = 1/C = 0$ and therefore $\mu = 0$, but the relative fluctuations due to a distribution over similar events with varying number of degrees of freedom is important. In such a case we obtain

$$S^{\text{add}}_{\lambda,0} = \frac{1}{\lambda}\sum_i p_i \ln\left(1-\lambda \ln p_i\right). \tag{37}$$

In the extreme case of infinite variance and infinite heat capacity (this scenario is most contrary to the textbook cases usually considered) we gain a new, *parameterless* enetropy formula:

$$S^{\text{add}}_{1,0} = \sum_i p_i \ln(1-\ln p_i). \tag{38}$$

We note that energy distributions corresponding to the above entropy formulas by canonical variation (entropy maximization with constraint on the average energy) delivetr in order the Gibbs-Boltzmann, the Pareto and finally a new distribution containing the Lambert W function, with the high-energy tail looking like a Gompertz distribution ($\sim e^{-e^x}$) [16].

4 Summary

In summary we reviewed simple finite reservoir effects establishing a link to deformed entropy formulas. The cut-power law form of the Pareto distribution, in the thermodynamical limit approaching the Boltzmann–Gibbs exponential, was regarded as a next to leading order approximation to statistical weights in a finite phase space. Assuming non-additivity of the $\ln p_i$ entries in general entropy formulas, an additive deformed entropy can be constructed. Physically it contains two parameters: the relative variance in inverse temperature fluctuations and the inverse total heat capacity. The general entropy formula is a combination of nonlinear scaling functions combining these two effects. For the standard variance, $T^2\Delta\beta^2 = 1/C$, the traditional Boltzmann–Gibbs–Shannon logarithmic formula arises. For zero variance but finite total heat capacity, the Tsallis q-entropy formula, while for extreme large fluctuations in the thermodynamical limit, $C \to \infty, T^2\Delta\beta^2 \to \infty$, a **new, parameterless entropy formula** emerges.

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