

On the derivation of power-law distributions in the canonical ensemble

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We note the possibility within classical thermodynamics to derive power-law distributions in the canonical ensemble. We do so by systematically finding a class of microcanonical distributions that allow for a separation of the total system energy from the reservoir. We demonstrate that all separable distributions are parametrized by a separation constant Q which is one to one related to the q parameter in Tsallis distributions. The power-laws obtained are formally(!) equivalent to those obtained by maximizing Tsallis entropy under q constraints. We comment on the possibility in finite systems that the equilibrium point and the expectation value do not coincide, and show that also for that case the variational principle holds after a transformation of variables. These results might help to explain the ubiquity of Tsallis distributions in nature.

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There has been a tremendous interest in a generalized definition of entropy, recently introduced by Tsallis [1].

$$S_q = \frac{1 - \int d\Gamma \rho^q}{q - 1} , \quad (1)$$

where ρ is the the normalized energy density and $d\Gamma$ indicates phase space integration. The reason why this modification has attracted so much interest is partly because of the possibility to derive power-law distributions in the canonical ensemble within the maximum entropy principle. This modification of entropy and its resulting formalism, which is sometimes referred to as non-extensive thermostatics, has triggered far more than a thousand works in the past few years [2]. However, despite its phantastic descriptive success of power-laws in physical, chemical, biological, and social systems, it has not yet been possible to derive this form of entropy from thermodynamic or statistical principles. Within the formalism suggested by Tsallis it is necessary to define expectation values of quantities depending on the energy spectrum of the system not in the standard way but with so-called q -expectations $\langle \mathcal{O} \rangle = \int d\Gamma \rho^q \mathcal{O}$ [3, 4] to recover the Legendre structure of thermodynamics [5]. The physical interpretation of these q -expectations is under heavy debate.

There have been several papers recently with the aim to derive canonical power distributions from first principles, see e.g. [6–8]. In convincing work [9, 10] it has been

beautifully noted that the expression $\frac{d}{dE} \left(\frac{1}{\beta} \right) = q - 1$ gives a physical meaning to q and that power laws in the canonical ensemble can be derived on a Hamiltonian basis.

In this work we adopt a somewhat different strategy and derive – using a mathematical theorem – power-law distributions for the canonical ensemble directly, just by the use of the variational principle, and a separation Ansatz, without touching the standard definition of entropy. We begin by noting that any thermodynamic system which can be measured in equilibrium must be *separable*, i.e., that the thermodynamic quantities of the measured system should not explicitly depend on the energy of the total system E . In the following we consider a sample (observed system) in contact with a reservoir. The energy of the sample is E_1 , the energy of the reservoir is E_2 , such that the total (isolated) system has a constant total energy $E = E_1 + E_2$. The number of microstates in the sample is $\omega_1(E_1)$ and $\omega_2(E_2)$ in the reservoir. The energy of the sample fluctuates around its equilibrium (extremal) value denoted by E_* . The Hamiltonians describing the sample and the reservoir are H_1 and H_2 , respectively. Thermal contact of the two systems means $H = H_1 + H_2$ and the partition function $Z(E)$ is the convolution of the two microcanonical densities

$$Z(E) = \int_0^E dE_1 \omega_1(E_1) \omega_2(E - E_1) , \quad (2)$$

with

$$\omega_i(E_i) = \int d\Gamma_i \delta(H_i - E_i) . \quad (3)$$

Following the usual line of thought to pass from the microcanonical to the canonical description, represented by

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ρ is given (up to a constant multiplicative factor) by

$$\rho(E_1) = \omega_1(E_1)\omega_2(E - E_1)Z^{-1}(E) \quad . \quad (4)$$

Note, that this description is dictated by the equations of motion. Assuming the existence of a unique extremal configuration at some $E_1 = E_*$ defined by $\delta\rho = 0$, leads to the well known condition

$$\frac{\omega'_1}{\omega_1}\Big|_{E_1=E_*} = \frac{\omega'_2}{\omega_2}\Big|_{E_2=E-E_*} := \frac{1}{kT} = \beta \quad , \quad (5)$$

which defines the temperature T of the system. The usual definition of entropy $S_i = k \ln(\omega_i)$ implies that the extremal configuration is found where $S = S_1 + S_2$ is extremal with its associated temperature as defined above.

Under which circumstances can one factorize the dependence of ρ on the total energy E ? We are hence looking for classes of microcanonical distributions that allow for such a separation of E into a multiplicative factor. A standard way to motivate the appearance of the Boltzmann term in the canonical ensemble can be seen as a consequence of this E -separation

$$\begin{aligned} \omega_2(E - E_1) &= \exp(\ln(\omega_2(E - E_1))) \\ &\approx \exp(\ln(\omega_2(E)) - \frac{\partial}{\partial E} \ln(\omega_2) E_1) \quad (6) \\ &\approx \omega_2(E) \exp(-\beta E_1) \quad . \end{aligned}$$

It is worthwhile to note that the approximation in Eq. (6) is exact for $\omega_2(E - E_1)$ being an exponential in E . Up to this point we have summarized textbook knowledge. It is one purpose of this work to emphasize that (6) is not the most general way of separation.

To find the most general separation, we generalize the log function in Eq. (6) to some real function f , being strictly monotonous and twice differentiable. Monotonicity is needed for a well defined inverse f^{-1} . The idea is to write $\omega(E - E_1) = f^{-1} \circ f \circ \omega((E - E_*) - (E_1 - E_*))$ and to expand $f \circ \omega$ around $E - E_*$. Suppose energy E is separable from the system, then there exist two functions g and h such that

$$\omega(E - E_1) = g(\omega(E - E_*)) h(x) \quad , \quad (7)$$

with $x := \beta(E_1 - E_*)$; to simplify notation we write $\bar{\omega} := \omega(E - E_*)$ in the following. We now use f to find the unknown functions g and h by expanding $f \circ \omega$ to first order

$$f(\omega(E - E_1)) = f(g(\bar{\omega})h(x)) \sim f(\bar{\omega}) - \bar{\omega} x f'(\bar{\omega}) \quad , \quad (8)$$

which is justified for small x , i.e., the system being near equilibrium. The most general solution to this separation Ansatz is given by the family of equations $(f, g, h)_Q$, parametrized by a separation constant Q , and C and C_2 being real constants

$$\begin{aligned} f(\omega) &= C \omega^{1-Q} + C_2 \\ g(\omega) &= \omega \\ h(x) &= [1 - (1 - Q)x]^{1/(1-Q)} \end{aligned} \quad (9)$$

To see this, first g is found by setting $x = 0$ and $h_0 = h(0)$, so that Eq. (8) yields $f(g(\bar{\omega})h_0) = f(\bar{\omega})$, which means $g(\bar{\omega}) = \frac{\bar{\omega}}{h_0}$. Without loss of generality set $h_0 = 1$ and arrive at $f(\bar{\omega}h(x)) = f(\bar{\omega}) - \bar{\omega} x f'(\bar{\omega})$. Form partial derivatives of this expression with respect to x and $\bar{\omega}$, and eliminate the $f'(\bar{\omega}h)$ term from the two resulting equations

$$\begin{aligned} f'(\bar{\omega}h)h' &= -f'(\bar{\omega}) \\ f'(\bar{\omega}h)h &= (1 - x)f' - \bar{\omega} x f'' \end{aligned} \quad (10)$$

to arrive at the separation equation

$$1 - \frac{1}{x} \left(\frac{h}{h'} + 1 \right) = -\bar{\omega} \frac{f''(\bar{\omega})}{f'(\bar{\omega})} = Q \quad (11)$$

where Q is the separation constant. The differential equation $1 - \frac{1}{x} \left(\frac{h}{h'} + 1 \right) = Q$ is straight forwardly solved to give $h(x) = [1 - (1 - Q)x]^{1/(1-Q)}$, using $h(0) = 1$ to fix the integration constant. The equation $-\bar{\omega} \frac{f''(\bar{\omega})}{f'(\bar{\omega})} = Q$ means, $f(\bar{\omega}) = C_1 \frac{1}{1-Q} \bar{\omega}^{1-Q} + C_2$, with C_1 and C_2 integration constants. f is strictly monotonous except for $Q = 1$, where it is constant. It is straight forward to test that Eqs. (9) solve Eq. (8). The term of interest in the canonical distribution can now be written as a generalized Boltzmann factor

$$\omega_2(E - E_1) = \omega_2(E - E_*) [1 - (1 - Q)\beta(E_1 - E_*)]^{1/(1-Q)} \quad . \quad (12)$$

The separation constant is not specified at this level. As we will see below the choice of a particular physical system will determine Q . The usual Boltzmann factor Eq. (6) is recovered as a special case in the limit $Q \rightarrow 1$. Note, that if ω_2 is of the form $\omega_2 \propto E^{1/1-Q}$, then Eq. (12) holds exactly and not only to the first order approximation in Eq. (8). The best way to prove this is to write $\beta = \frac{\omega'_2}{\omega_2}\Big|_{E-E_*} = \frac{1}{(1-Q)(E-E_*)}$ and to compute straight forwardly

$$\begin{aligned} \omega_2(E - E_1) &= (E - E_*)^{1/(1-Q)} \left(1 - \frac{E_1 - E_*}{E - E_*}\right)^{1/(1-Q)} \\ &= \omega_2(E - E_*) [1 - (1 - Q)\beta(E_1 - E_*)]^{1/(1-Q)} \quad , \end{aligned} \quad (13)$$

see also [11]. As we will see below, $\omega_2 \propto E^{1/1-Q}$ covers classical (homogenous) Hamiltonians with pair-potentials.

Having derived the principal form $(f, g, h)_Q$ to first order it is easy to see that with the same family of functions we can expand ω_2 to all orders. Repeated differentiation of ρ at its extremum leads to a hierarchy of equations relating properties of the ω densities to properties of ρ at its extremum. With the definitions

$$r_n := \beta^{-n} \frac{\rho^{[n]}}{\rho}\Big|_{E=E_*} \quad \text{and} \quad \phi_n^i := \beta^{1-n} \frac{\omega_i^{[n]}}{\omega_i^{[1]}}\Big|_{E=E_i^*} \quad (14)$$

$[n]$ being the n th derivative, and $i = 1, 2$ indicating system 1 and 2 ($E_{1*} = E_*$, $E_{2*} = E - E_*$). We successively construct the whole hierarchy to find

$$\begin{aligned} r_2 &= \phi_2^1 + \phi_2^2 - 2 \\ r_3 &= (\phi_3^1 - 3\phi_2^1) - (\phi_3^2 - 3\phi_2^2) \\ r_4 &= (\phi_4^1 - 4\phi_3^1 + 3\phi_2^1(r_2 + 2 - \phi_2^1)) \\ &\quad + (\phi_4^2 - 4\phi_3^2 + 3\phi_2^2(r_2 + 2 - \phi_2^2)) \\ &\quad \vdots \end{aligned} \quad (15)$$

Using these equations we can re-express the ϕ_n^2 terms in terms of ϕ_n^1 and r_n , so that all we know about system 2 is encoded in local properties of ρ at the equilibrium. To fourth order the general expansion reads

$$\begin{aligned} \omega(E - E_1) &= \omega(E - E_*) \{ 1 + (1 - Q) [-x \\ &\quad + \frac{1}{2!}(\phi_2^2 - Q)x^2 - \frac{1}{3!}(-3Q\phi_2^2 + \phi_3^2 + (Q + 1)Q)x^3 \\ &\quad + \frac{1}{4!}(\phi_4^2 - 4Q\phi_3^2 - 3Q(\phi_2^2)^2 + 6Q(Q + 1)\phi_2^2 \\ &\quad - (Q + 2)(Q + 1)Q)x^4 + \dots] \}^{\frac{1}{1-Q}}, \end{aligned} \quad (16)$$

which in the limit $Q \rightarrow 1$ is

$$\begin{aligned} \omega(E - E_1) &= \omega(E - E_*) \exp \left\{ -x + \frac{1}{2!}(\phi_2^2 - 1)x^2 \right. \\ &\quad \left. - \frac{1}{3!}(-3\phi_2^2 + \phi_3^2 + 2)x^3 + \frac{1}{4!}(\phi_4^2 - 4\phi_3^2 - 3(\phi_2^2)^2 \right. \\ &\quad \left. + 12\phi_2^2 - 6)x^4 + \dots \right\} \end{aligned} \quad (17)$$

Note, that for $\omega_2 \propto \exp(\beta E)$ all $\phi_n^2 = 1$, and all higher order terms vanish and the standard Boltzmann result becomes exact.

We now proceed to show how a physical meaning can be given to the separation constant Q in Eq. (12). Let us specify, as an example, the following N particle Hamiltonian for pair-potentials, governing the sample in D space dimensions. We use $n = DN$.

$$H(x, p) = \sum_i^N \frac{p_i^2}{2m} + \sum_{i < j}^N |x_i - x_j|^\alpha. \quad (18)$$

The energy density is given by the phase space integral

$$\begin{aligned} \omega(E) &= \int d^n p d^n x \delta \left(\sum_i \frac{p_i^2}{2m} + \sum_{i < j} |x_i - x_j|^\alpha - E \right) \\ &= \int_0^E dE_1 \int d^n p d^n x \delta \left(\sum_i \frac{p_i^2}{2m} - E_1 \right) \\ &\quad \times \delta \left(\sum_{i < j} |x_i - x_j|^\alpha - (E - E_1) \right). \end{aligned} \quad (19)$$

We compute the kinetic term

$$\begin{aligned} \int d^n p \delta \left(\sum_{i=1}^N \frac{|\vec{p}_i|^2}{2m} - E \right) &= \int_{\vec{p}^2 = E} d\mathcal{O}_n \left| \frac{\vec{p}^2}{2m} \right|^{-1} \\ &= \int_{|\vec{p}| = \sqrt{2mE}} d\mathcal{O}_n \frac{m}{|\vec{p}|} = \sqrt{\frac{m}{2E}} \int_{|\vec{p}| = \sqrt{2mE}} d\mathcal{O}_n \\ &= \mathcal{O}_n \sqrt{\frac{m}{2E}} (2mE)^{\frac{n-1}{2}} \propto E^{\frac{n}{2}-1} \end{aligned} \quad (20)$$

and the potential contribution

$$\begin{aligned} &\int d^n x \delta \left(\sum_{i < j} |x_i - x_j|^\alpha - E \right) \\ &= \int d^n x \delta \left(\sum_{j=2}^N \sum_{i=1}^{j-1} \left| \sum_{k=1}^D (x_i^k - x_j^k)^2 \right|^{\frac{\alpha}{2}} - E \right) \\ &= \int d^n x \delta \left(E \left[\sum_{j=2}^N \sum_{i=1}^{j-1} \left| \sum_{k=1}^D \left(\frac{x_i^k - x_j^k}{E^{\frac{1}{\alpha}}} \right)^2 \right|^{\frac{\alpha}{2}} - 1 \right] \right) \\ &= E^{\frac{n}{\alpha}} \int d^n y \delta \left(E \left[\sum_{j=2}^N \sum_{i=1}^{j-1} \left| \sum_{k=1}^D (y_i^k - y_j^k)^2 \right|^{\frac{\alpha}{2}} - 1 \right] \right) \\ &= E^{\frac{n}{\alpha}-1} \cdot \text{const.} \end{aligned} \quad (21)$$

where we used the substitution $y_i = x_i/E^{\frac{1}{\alpha}}$ and the fact $\int dx \delta(\lambda x) = \int dx \lambda^{-1} \delta(x)$. We finally get for Eq. (19)

$$\omega(E) \propto \int_0^E dE_1 E_1^{\frac{n}{2}-1} (E - E_1)^{\frac{n}{\alpha}-1} \propto E^{\frac{(\alpha+2)n}{2\alpha}-1}. \quad (22)$$

This allows us now to compare exponents (and coefficients) in Eq. (22) and Eq. (12) to arrive at the relation

$$\frac{1}{1-Q} = \frac{(\alpha+2)n}{2\alpha} - 1, \quad (23)$$

which fixes the separation constant. This equation establishes the connection between the interaction term in the Hamiltonian α , the dimensionality of the phase space $n = DN$, and the separation constant Q . From Eq. (23) it is immediately clear that for large systems the separation constant is always $Q \rightarrow 1$, i.e. the classical Boltzmann term (6) is recovered. For small systems, with a fixed number of particles Q depends on the interaction between the particles. For an ideal gas $\alpha \rightarrow -\infty$ the separation constant is $Q = \frac{4-n}{2-n}$. Nontrivial $Q \neq 1$ should be expected is for strongly interacting and/or small systems, i.e., $|\alpha|/|\alpha+2| \sim n$ and systems with $-2 < \alpha < 0$, where the limit $n \rightarrow \infty$ implies $n(\alpha+2)/(2\alpha) - 1 \rightarrow -\infty$ so that BG is not obtained. We should also remark that although q-exponentials e_Q^x may have complex phases $(-1)^{1/(1-Q)}$ for $1 - (1-Q)x < 0$, these are irrelevant for expectations since they always cancel each other.

Let us assume that for a system $Q \neq 1$ is due to its finite size. Here the standard argument in BG thermodynamics of extremely sharp peaks of the distribution at equilibrium is not necessarily valid, and E_* and the expected energy $\mathcal{U} = \langle H \rangle$ may significantly differ. Assuming $\omega_i(E_i) \propto E_i^{n_i}$ and the validity of the variational principle $\delta\rho = \left(\frac{n_1}{E_1} - \frac{n_2}{E-E_1} \right) \rho \delta E_1 = 0$ yields $E_1 = E_* = \frac{E}{1 + \frac{n_2}{n_1}}$. With this we can write $\int_0^E dE_1 E_1^A (E - E_1)^B = \left(\frac{E_*}{n_1} \right)^{A+B+1} \int_{-n_1}^{n_2} dx (n_1 + x)^A (n_2 - x)^B$ and compute

$$\mathcal{U} = \langle H_1 \rangle_E = \frac{\int_0^E dE_1 E_1 \rho(E_1)}{\int_0^E dE_1 \rho(E_1)} = E_* \left(1 + \frac{\langle x \rangle_{12}}{n_1} \right) \quad (24)$$

with $\langle x \rangle_{12} = \frac{\int_{-n_1}^{n_2} dx x (n_1 + x)^{n_1} (n_2 - x)^{n_2}}{\int_{-n_1}^{n_2} dx (n_1 + x)^{n_1} (n_2 - x)^{n_2}}$. Rewriting leads

to

$$\mathcal{U} = \frac{E}{1 + \frac{n_2 - \langle x \rangle_{12}}{n_1 + \langle x \rangle_{12}}} . \quad (25)$$

One can therefore apply the same equilibrium argumentation also to the (measurable) expectation values by substituting $\tilde{n}_1 = n_1 + \langle x \rangle_{12}$, $\tilde{n}_2 = n_2 - \langle x \rangle_{12}$ and $\tilde{\rho} \propto E_1^{\tilde{n}_1} (E - E_1)^{\tilde{n}_2}$ so that $\delta\tilde{\rho} = 0$ with $\delta E = 0$. The Q of the observable canonical ensemble is then

$$\frac{1}{1 - \tilde{Q}} = \frac{(\alpha + 2)\tilde{n}_2}{2\alpha} - 1 , \quad (26)$$

for the above example of a pair potential Hamiltonian for the reservoir.

Equation (12) is without doubt formally equivalent to the Tsallis q form of the Boltzmann term. Our result (12) appears as a consequence of the separability of the total system energy E from the microcanonical density of the sample system with the parameter Q being nothing but a separation constant not further specified at this stage. Q is fixed and a physical meaning is obtained as soon as a particular Hamiltonian is specified. Equation (12) is not exactly what Tsallis gets by extremization of S_q , with his constraints for the canonical ensemble: $\sum_i p_i = 1$, and $U_q = \frac{\sum_i p_i^q \epsilon_i}{\sum_i p_i^q} = \text{const.}$ In our derivation we get E_* and the classical β (real temperatures), where Tsallis gets the terms U_q and $\beta / \sum_i p_i^q$, respectively.

We have computed higher order terms and found that if the canonical distribution is a power, all higher terms in the expansion vanish and our result (12) holds exactly and not only as a first order approximation as we started out with in (8). This might be an interesting finding since many physically interesting microcanonical densities behave like powers in E_1 , at least for finite size systems [12].

An important aspect in our work is that all our arguments are strictly based on Hamiltonians and on the vari-

ational principle. At no point we are forced to take the thermodynamic limit. For that case we had some discussion if the equilibrium point is different from the expectation value. In case that mean and equilibrium do not coincide, our result would of course not be observable, since measurements take place at the expectations whereas we have developed our results around the extremal configuration. We can however show that for microcanonical distributions characterized by $\omega_1(E_1) \propto E^{\kappa_1}$ and $\omega_2(E_2) \propto E^{\kappa_2}$, mean and extremum coincide for $\kappa_1 = \kappa_2$. In the thermodynamic limit the difference is of course completely irrelevant.

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