On the derivation of power-law distributions within classical statistical mechanics far from the thermodynamic limit

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Abstract

We show that within classical statistical mechanics without taking the thermodynamic limit, the most general Boltzmann factor for the canonical ensemble is a $q$-exponential function. The only assumption here is that microcanonical distributions have to be separable from the total system energy, which is the prerequisite for any sensible measurement. We derive that all separable distributions are parametrized by a mathematical separation constant $Q$ which can be related to the non-extensivity $q$-parameter in Tsallis distributions. We further demonstrate that nature fixes the separation constant $Q$ to 1 for large dimensionality of Gibbs $\Gamma$-phase space. Our results will be relevant for systems with a low-dimensional $\Gamma$-space, for example nanosystems, comprised of a small number of particles or for systems with a dimensionally collapsed phase space, which might be the case for a large class of complex systems.

Keywords: Boltzmann distribution, power laws, non-extensive thermodynamics, Tsallis distribution, extremal principle

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INTRODUCTION

There is a certain need in the physical, chemical, biological, social and economical sciences to understand the origin and ubiquity of power law-distributions. Many of these distributions appear to be $q$-exponentials upon closer inspection, which are defined as

$$e^x_q \equiv [1 + (1 - q)x]^{1/(1-q)} ,$$

for $1 + (1-q)x \geq 0$. An appealing attempt for a general approach to the matter is to construct a thermostatistics, where with the use of classical principles, such as the variational principle and the second fundamental theorem of thermodynamics, one would be able to naturally derive these distributions. The canonical entropy associated to $q$-exponential distribution functions is the so-called Tsallis entropy $\[1, 2\]$,

$$S_q \equiv \frac{1 - \int d\Gamma \rho^q}{q - 1} ,$$

where $\rho$ is the normalized energy density and $d\Gamma$ indicates phase space integration. Tsallis entropy which is a generalization of Boltzmann-Gibbs (BG) entropy is in principle non-additive and non-extensive. Classical BG entropy is recovered in the limit $q \to 1$.

In contrast to the vast amount of papers in non-extensive statistical physics, there has been relatively little effort to derive power-law distributions, in particular $q$-exponential distributions, from first statistical mechanics principles. To mention some fruitful work in this direction, in \[3\] it was shown that if phase space volumes are not covered in a Poissonian manner, the resulting entropy functional can be of Tsallis type. Within the framework of superstatistics \[4\] the inverse temperatures $\beta$ are considered to fluctuate, such that a generalized Boltzmann factor, $B = \int d\beta f(\beta)e^{-\beta E}$ arises. If $f$ is a $\chi^2$ distribution, the natural distribution functions are $q$-exponentials. An other approach was taken in \[5\], where the non-uniqueness of counting rules are discussed. It is shown that a proper modification of the log-counting rule yields Tsallis entropy instead of the usual BG entropy. In a recent paper \[6\], we could show that a more general view is possible, in the sense that the most general Boltzmann factor that can be derived for the canonical ensemble is exactly a $q$-exponential. This result might be of relevance for systems with a low dimensionality of $\Gamma$ phase space (Gibbs). Examples for such systems are nanosystems, which have gained recent interest due to being at the edge of technical accessibility, and for systems, whose phase...
space has effectively collapsed in dimensions (like a fractal), due to long range interactions, aging, synchronization, as is the case in many complex systems.

DERIVATION OF THE GENERAL BOLTZMANN FACTOR

The following argument is solely based on the observation that any thermodynamic system which can be measured in equilibrium must be *energy separable*, i.e. thermodynamic quantities of the measured system must not explicitly depend on the energy of the total system, $E$. We consider a sample (observed system) in contact with a reservoir (bath). The energy of the sample is $E_1$, the energy of the reservoir is $E_2$, such that the total system has a constant total energy $E = E_1 + E_2$. The number of microstates are $\omega_1(E_1)$ and $\omega_2(E_2)$ for the sample and the bath, respectively. The energy of the sample fluctuates around its equilibrium (extremal) value denoted by $E_*$. Thermal contact of the two systems means that the Hamiltonian of the total system is $H = H_1 + H_2$ and the partition function $Z(E)$ is the convolution of the two microcanonical densities

$$Z(E) = \int_0^E dE_1 \omega_1(E_1) \omega_2(E - E_1) \quad \text{with} \quad \omega_i(E_i) = \int d\Gamma_i \delta(H_i - E_i).$$

Following usual reasoning, we pass from the microcanonical to the canonical description. Its density $\rho$ is given (up to a constant multiplicative factor) by

$$\rho(E_1) = \frac{\omega_1(E_1)}{Z} = \frac{\omega_1(E_1) \omega_2(E - E_1)}{Z}.$$

(4)

Note, that this description is entirely 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 definition of inverse temperature

$$\frac{\omega'_1}{\omega_1}
\bigg|_{E_1=E_*} = \frac{\omega'_2}{\omega_2}
\bigg|_{E_2=E-E_*} \equiv \beta \frac{1}{k_BT}.$$

(5)

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 $\rho$ on the total energy $E$, i.e. which microcanonical distributions allow for a separation of $E$ into a multiplicative factor? The standard way to motivate the appearance of the Boltzmann term in the canonical ensemble
is a consequence of this $E$-separation

$$
\omega_2(E - E_1) = \exp(\ln(\omega_2(E - E_1)))
\approx \exp(\ln(\omega_2(E)) - \frac{\partial}{\partial E}\ln(\omega_2) E_1)
\approx \omega_2(E) \exp(-\beta E_1)
.$$  

The approximation in Eq. (6) is exact for $\omega_2(E - E_1)$ being an exponential in $E$. However, this is not the most general way of separation.

Now, to find the most general separation, we generalize the log function in Eq. (6) to some real function $f$, being twice differentiable and with 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 $E - E_*$. If the energy $E$ is separable from the system into a factor, then there must exist two functions $g$ (factor) and $h$ (general Boltzmann term) such that

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

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

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

which is justified for small $x$, i.e., the system being at or 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

$$
f(\omega) = C \omega^{1-Q} + C_2
\quad g(\omega) = \omega
\quad h(x) = \left[1 - (1 - Q)x\right]^\frac{1}{1-Q}
.$$  

To prove this, set $x = 0$ and $h_0 = h(0)$, so that Eq. (9) 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

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

4
to arrive at the separation equation

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

where $Q$ is a mathematically necessary separation constant. The differential equation $1 - \frac{1}{x} (\frac{h}{h'} + 1) = Q$ is straightforwardly solved to give the general Boltzmann term, $h(x) = [1 - (1 - Q)x]^{-\frac{1}{2\alpha}}$, using $h(0) = 1$ to fix the integration constant. 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. The term of interest in the canonical distribution can now be written as the generalized Boltzmann factor

$$\omega_2(E - E_1) = \omega_2(E - E_v) \left[ 1 - (1 - Q)\beta(E_1 - E_v) \right]^{\frac{1}{1 - Q}} .$$

The usual Boltzmann factor Eq. (6) is recovered as the special case in the limit $Q \to 1$. If $\omega_2$ is of power-form, $\omega_2 \propto E^{1/1 - Q}$, as is the case for a huge class of physical systems, Eq. (12) holds exactly.

The separation constant $Q$ is not specified at this level. What fixes $Q$? The choice of the physical system (Hamiltonian and characteristics of phase space) does. As an example, in Eq. (6) we have shown that for a $N$-particle Hamiltonian with pair-potentials, in $D$ space dimensions

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

the following relation, fixing the separation constant, holds exactly,

$$\frac{1}{1 - Q} = \frac{(\alpha + 2)n}{2\alpha} - 1 .$$

This equation establishes the connection between the interaction term in the Hamiltonian $\alpha$, the dimensionality of phase space, $n = DN$, and the separation constant $Q$. From Eq. (14) it is immediately clear that for large systems the separation constant is always $Q \to 1$, i.e. the classical Boltzmann term (6) is recovered. For small systems, either due to low particle numbers or due to an effectively collapsed phase space dimensionality, a non-trivial $Q \neq 1$ is expected.

**ON THE DEFINITION OF TEMPERATURE IN LOW-DIMENSIONAL SYSTEMS**

For large systems, the notion of equilibrium is well defined. However, for systems where we would expect $Q \neq 1$ the definition of temperature is not necessarily unique. In Eq. (6)
the definition of $\beta$ or the inverse temperature was based on the extremal value of $\rho$, but this is not what is going on in a measurement. A measurement of temperature yields an *expected* value (due to averages of kinetic energy taken in the measurement process) and not the *extremal* value, i.e. the most likely one. To construct a theory which is consistent with the measured temperature of the sample system, and by – at the same time – keep the extremal principle, one can now ask to modify the definition of $\rho \rightarrow \bar{\rho}$, such that the extremal value is obtained at the measured temperature. Effectively this amounts to an energy shift from equilibrium energy to expected energy, $E^* \rightarrow \bar{E}$. Such a modification could look like

$$\bar{\rho}(E_1) \equiv \bar{\omega}_1(E_1)\bar{\omega}_2(E - E_1) \quad ,$$

at $E_1 = \bar{E}_1$ and where $\bar{\omega}_i(E_i) \sim E_i^{\bar{\lambda}_i}$. The idea is to identify $\bar{E}_1$ with the measured energy $\bar{\omega}_1(E_1) = \int_0^{E_1} d\epsilon \rho(\epsilon)$, and not with the equilibrium $E_*$ as before. The variation $\delta \bar{\rho} = 0$ leads to the relation

$$\frac{\bar{\lambda}_1}{\bar{\lambda}_2} = \frac{\bar{E}_1}{E - E_1} \quad ,$$

which establishes the relation of the $\bar{\lambda}$s, which are of course not independent. Now we note that

$$\bar{E}_1 = \int_0^{E_1} d\epsilon \omega_1(\epsilon)\omega_2(E - \epsilon)Z(E)^{-1} = E\beta(\lambda_1 + 1, \lambda_2)/\beta(\lambda_1, \lambda_2) \quad ,$$

with the usual beta functions, $\beta(a, b) \equiv \int_0^1 dx x^a(1 - x)^b$. Substituting $\bar{E}_1$ into Eq. (16) allows to compare the $\lambda$ exponents from the original system, Eq. (4), with those of the energy shifted system, $\bar{\lambda}$,

$$\frac{\bar{\lambda}_1}{\lambda_2} = \frac{1}{\beta(\lambda_1, \lambda_2)/\beta(\lambda_1 + 1, \lambda_2) - 1} \quad .$$

If we now assume that the exponent of the sample system is known (for example from a Hamiltonian), and unchanged in the shifted system, $\lambda_1 = \bar{\lambda}_1$, we observe that the shift from $E_* \rightarrow \bar{E}$, has as a consequence for the bath density, $\omega(E_2) \rightarrow \omega(E_2)^z$, where $z = \frac{\lambda_1 \beta(\lambda_1, \lambda_2 + 1)}{\lambda_2 \beta(\lambda_1 + 1, \lambda_2)}$. For the usual entropies this means

$$S_1 = \ln(\omega_1) \quad S_2 = \ln(\omega_2^z)$$

with the temperatures ($k_B \equiv 1$) $1/T_i = \partial S_i/\partial E$ so that equi-temperature is assumed when both systems contain the expected energy, i.e. $T_1 = T_2 \leftrightarrow \delta S = 0$. Here we obtain non-additivity of entropies as a result of harmonizing the concept of temperature for small systems.
In order to see that this gives consistent results we compute the expected temperature of both systems $\langle T_1 \rangle$ and $\langle T_2 \rangle$ in both, the most-probable state temperature interpretation and in the expected-state temperature interpretation. Let us think of the sample system (1) as the thermometer then the above definition implies that our thermometer shows the same average temperature obtained by multiple measurements whether we use the maximal or expected energy interpretation and $\langle T_1 \rangle = (E/\lambda_1)\beta(\lambda_1 + 1, \lambda_2)/\beta(\lambda_1, \lambda_2)$ since we have chosen to modify only the exponent of the bath system. Now the bath shows the expectation of temperature, $\langle T_2 \rangle = (E/\lambda_2 w)\beta(\lambda_1, \lambda_2+1)/\beta(\lambda_1, \lambda_2)$ with $w = 1$ for the most-probable and $w = z$ for the expected-state temperature interpretation. Consequently, the expected-state temperature interpretation is consistent with the BG expectation, 

$$\frac{\langle T_1 \rangle}{\langle T_2 \rangle} = \frac{\lambda_1 z \beta(\lambda_1 + 1, \lambda_2)}{\lambda_2 \beta(\lambda_1, \lambda_2+1)} = 1$$

Note that the expected-temperature definition involves knowledge about sample and bath system. On the other hand the most-probable-state temperature interpretation gives

$$\frac{\langle T_1 \rangle}{\langle T_2 \rangle} = \frac{\lambda_2 \beta(\lambda_1 + 1, \lambda_2)}{\lambda_1 \beta(\lambda_1, \lambda_2+1)}$$

which in general will not equal unity. The corresponding notion of equilibrium allows to define the most-probable entropy merely upon the knowledge of the particular micro-systems separately. Since we only actually measure the sample system this temperature difference can not be observed. Averaging over multiple temperature measurements does not converge to an equilibrium temperature. The way of how to average multiple temperature measurements in order to obtain the equilibrium temperature in terms of the most-probable state therefore is dual to the manipulation of the bath entropy, constructed to match the expected-state interpretation.

It becomes evident that the usage of expected and most probable energies can both be consistently used in order to define the macroscopic notion of equilibrium. Which of the two possibilities is realized experimentally is defined by the choice of the experimentator. Intuitively we would think that in terms of keeping records of repeated experiments the expected-state temperature interpretation seems more natural since we can directly identify averages on multiple measurements of the temperature with the equilibrium temperature itself. Whatever procedure we fix, we can not escape modifying either, the average on the replicas, i.e. multiple measurements, or the definition of the bath entropy. The asymmetric
definition of the entropy does not appear explicitly in the canonical variational principle, based on single particle entropies where the same mechanisms are controlled by constraints.

CONCLUSION

Based on very general assumptions we have derived that the most general Boltzmann factor in the canonical ensemble is a $q$-exponential. We have shown that this result might be relevant for systems of relatively small phase space, which might be realized for several types of complex systems. We comment on the temperature definition in small systems and discuss its consequences. Let us stress again, that all presented arguments are strictly based on Hamiltonians and on the variational principle, we never leave the field of classical statistical mechanics, except for not taking the thermodynamic limit.

[1] C. Tsallis, J. Stat. Phys. 52, (1988) 479.
[2] M. Gell-Mann and C. Tsallis, Nonextensive Entropy – Interdisciplinary Applications, (Oxford University Press, New York, 2004).
[3] A. Carati, cond-mat/0407768.
[4] C. Beck and E. G. D. Cohen, Physica A 322 267-275 (2003).
[5] S. Abe and A.K. Rajagopal, Phys. Lett. A 272, 341 (2000).
[6] R. Hanel and S. Thurner, Physica A 351, 260-268 (2005).