Generalized thermostatistics and mean-field theory

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August 2003

Abstract

The present paper studies a large class of temperature-dependent probability distributions and shows that entropy and energy can be defined in such a way that these probability distributions are the equilibrium states of a generalized thermostatistics, which is obtained from the standard formalism by deformation of exponential and logarithmic functions. Since this procedure is non-unique, specific choices are motivated by showing that the resulting theory is well-behaved. In particular, with the choices made in the present paper, the equilibrium state of any system with a finite number of degrees of freedom is, automatically, thermodynamically stable and satisfies the variational principle.

The equilibrium probability distribution of open systems deviates generically from the Boltzmann-Gibbs distribution. If the interaction with the environment is not too strong then one can expect that a slight deformation of the exponential function, appearing in the Boltzmann-Gibbs distribution, can reproduce the observed distribution with its temperature dependence. An example of a system, where this statement holds, is a single spin of the Ising chain. However, because all systems of the present generalized thermostatistics are automatically stable, one must not expect that all open systems can be described in this way. Indeed, systems exhibiting a phase transition in their thermodynamic limit, can be unstable even when the interaction
with the environment is weak. Therefore, their equilibrium probability distribution cannot be described by a simple deformation of the Boltzmann-Gibbs distribution. In order to be able to handle such systems as well the second part of the paper discusses a further extension of the class of probability distributions using mean-field techniques.

Connections are discussed that exist between the present formalism, Tsallis’ thermostatistics, and the superstatistics formalism of Beck and Cohen. In particular, the present generalization sheds some light onto the historical development of the Tsallis formalism. It is pointed out that temperature dependence of the Tsallis distribution has hardly been verified experimentally.

Keywords Generalized thermostatistics, mean-field theory, deformed logarithmic and exponential functions, Ising chain, non-extensive thermostatistics, superstatistics

1 Introduction

Statistical physics is primarily concerned with (nearly) closed systems. A correct description of open systems, i.e. systems weakly interacting with their environment, requires that the latter is taken into account explicitly. The present paper attempts to generalize the thermostatistical formalism to open systems without the need for including the environment. Such a generalization may fill the gap between the narrow context for which the theory of statistical physics is developed and the vast domain of its applications. Indeed, often used tools, like temperature-dependent Hamiltonians and mean-field approximations, are not so well founded in the standard formalism. The main part of the paper explores how far one can go in modeling the temperature dependence of open systems. In doing so, Hamiltonians are not allowed to depend on temperature. Rather, the Boltzmann-Gibbs distribution is replaced by more general probability distributions and the microscopic definition of entropy is modified accordingly. Only the last sections include temperature-dependent Hamiltonians as a further extension of the formalism, more suited for unstable systems.

A general formalism like the one developed here helps also to improve understanding of more specific generalizations of the Boltzmann-Gibbs formalism. The present paper discusses in particular the formalism of non-extensive thermostatistics, first introduced in \[1\]. By looking from an eagle’s
point of view several peculiarities of this formalism get a new interpreta-
tion. Let me mention the role of escort probabilities, historical problems
with average energy without proper normalization and with the definition of
temperature, and the occurrence of thermodynamic instabilities. Also the
relation with the recently introduced superstatistics [2] is discussed. In this
way the present paper contributes to clarify the relation between mainstream
statistical mechanics and its generalizations.

It is of course very important that the present generalized formalism has
physical applications. Nevertheless, no such applications will be discussed.
The literature of non-extensive thermostatistics claims a large number of
applications — see e.g. [3]. It is argued below that these applications are
candidate applications of the present formalism. However, in most, if not all,
of these papers the authors verify the shape of the equilibrium probability
distribution, but not its temperature dependence. The present paper stresses
the point that in a predictive theory of thermostatistics both aspects are
equally important. Let us now explain this point.

Gibbs’ postulate implies that microstates with higher energy have a lower
probability, according to the formula

\[ p_k = \frac{1}{Z(T)} \exp(-H_k/T). \]  

In this expression \( p_k \) is the probability of the microstate labeled \( k \). It sat-
ifies \( p_k \geq 0 \) and \( \sum_k p_k = 1 \). \( H_k \) is the corresponding energy and \( T \) is the
temperature (Boltzmann’s constant is taken equal to 1).

Mathematically, it is clear that any probability distribution function (pdf)
with non-vanishing probabilities can be written in the form \( \text{(1)} \). This requires
only an appropriate definition of the notion of energy. Indeed, given \( p_k \), one
can put

\[ H_k = -T \ln(p_k). \]  

But, the Boltzmann-Gibbs distribution \( \text{(1)} \) contains more information than
the mere statement that high energy states have an exponentially small prob-
ability. It also predicts how probabilities \( p_k \) change with temperature \( T \). Once temperature is taken into account a definition of energy, like \( \text{(2)} \), is not
acceptable because in general energy levels \( H_k \), defined in such a way, are
temperature dependent. One concludes that the Boltzmann-Gibbs distribu-
tion \( \text{(1)} \) is very specific once temperature dependence is taken into account.
In the terminology of the present paper it is a temperature-dependent probability distribution.

The main tool of the paper is the notion of $\kappa$-deformed logarithmic and exponential functions, a definition of which is given in Section III. The idea of considering density functions as deformed exponential functions goes back to [4]. The name of $\kappa$-deformed functions has been used explicitly in [5]. One could of course replace the Boltzmann-Gibbs distribution (1) by an arbitrary temperature-dependent probability distribution. However, chances are small that in such a generality one could develop a complete thermostatistical theory. Therefore it is obvious to require that the function, which replaces the exponential function in (1), satisfies some additional properties. In the first place it should be an increasing function because states with a higher energy should be less probable. An additional property of the exponential function is convexity (i.e. the second derivative is positive). Functions satisfying both properties (plus some technical conditions) are called $\kappa$-deformed exponentials and are denoted $\exp_{\kappa}(x)$. Doing so has the advantage that well-known expressions from standard statistical physics are recognized on sight in the generalized formalism.

The next section starts with a discussion about the relevance of pdfs, other than that of Boltzmann-Gibbs. In the third section a new approach, based on $\kappa$-deformed logarithmic and exponential functions, is proposed. Section 4 discusses the Ising chain as an example motivating the generalized formalism following in section 5. Further examples are given in section 6. This includes a discussion of Tsallis’ thermostatistics. Generalized mean-field models are treated in section 8, using the notion of probability dependent variables introduced in section 7. Finally, a short discussion follows in section 9. The paper ends with two appendices, one about the Ising model, the other about thermodynamic stability.

2 Evidence of limited validity of the Boltzmann-Gibbs distribution

Consider an open system described by probabilities $p_{k\gamma}$, where $k$ labels the microstates of the system, and $\gamma$ the microstates of the environment. Assume these probabilities are of the form (1), i.e. there exist energy levels $H_{k\gamma}$ such
that
\[ p_{k\gamma} = \frac{1}{Z(T)} \exp(-H_{k\gamma}/T). \] (3)

Write these energies in the form
\[ H_{k\gamma} = H_k + H_\gamma^* + V_{k\gamma}. \] (4)

Then the reduced system without the environment is described by the probabilities
\[ p_k = \sum_{\gamma} p_{k\gamma} = \frac{1}{Y(T)} \exp(-(H_k + \langle V_k \rangle^*)/T), \] (5)

with the non-linear Kolmogorov-Nagumo averages \[ \langle V_k \rangle^* \] given by
\[ \langle V_k \rangle^* = -T \ln \left( \sum_{\gamma} p^*_\gamma \exp(-V_{k\gamma}/T) \right), \] (6)

with
\[ p^*_\gamma = \frac{1}{Y^*(T)} \exp(-H^*_\gamma/T), \] (7)

and with appropriate normalizations \[ Y(T) \] and \[ Y^*(T). \] Clearly, the reduced probabilities \[ p_k \] are not of the form (1), since the effective energies \[ H_k + \langle V_k \rangle^* \] depend on temperature. The only exception is when the interaction \[ V_{k\gamma} \] between system and environment vanishes. One concludes that the Boltzmann-Gibbs distribution (1) can only be universally correct in the limit that interactions of the system with its environment are negligible. Note that for systems of statistical mechanics the interactions cannot vanish because then the system is no longer open. Indeed, the dynamics of closed systems predicts conservation of energy. As a consequence, the state of the isolated system is not described by (1) but by a probability distribution concentrating on a single value of the energy.

The above reasoning shows that temperature-dependent effective Hamiltonians are rather generic. They occur in many situations and are used so frequently in applied statistical physics that it is a labor of Sisyphus to quote all occurrences. Nevertheless, they do not receive much attention in the theoretical foundation of statistical physics.
In the above discussion of open systems the assumption is made that the totality of system plus environment is correctly described by the Boltzmann-Gibbs distribution. This is not a severe limitation. Indeed, a characteristic of systems of statistical physics with many degrees of freedom is that the number of energy levels \( H_k \) in an interval \([E, E + \Delta E]\) increases exponentially with increasing energy \( E \). As a consequence, the typical equilibrium pdf \( p \) has the property that the only microstates that contribute significantly have energy levels \( E_k \) approximately equal to the average value \( U = \sum_k p_k H_k \), in the sense that the sum of \( p_k \) over these states is close to 1. This is the basis for the equivalence of ensembles — see [8, 9, 10] for a mathematical formulation of this property. In information theory [11] this property is known as equipartition theorem.

The equivalence of ensembles, when valid, implies that the actual form of the pdf is not very crucial. It is only needed for microstates with energy level \( H_k \) in the vicinity of the average energy \( U \). In particular, most systems of statistical mechanics cannot be used to test the validity of the Boltzmann-Gibbs distribution.

### 3 A new approach

The present study starts from a family of temperature-dependent probabilities, such as could be observed for an open system. If this family is of a certain form then one can construct a thermostatistic formalism that produces these probabilities as the temperature-dependent equilibrium distribution.

In order to generalize [11], the recently [12] introduced notions of \( \kappa \)-deformed exponential and logarithmic functions are used. A \( \kappa \)-deformed logarithmic function is denoted \( \ln_\kappa(x) \) and is a strictly increasing concave function defined for all positive \( x \), normalized such that \( \ln_\kappa(1) = 0 \), and with a possible divergence at \( x = 0 \), mild enough so that the integral

\[
F_\kappa(x) = \int_1^x \ln_\kappa(y) \, dy
\]

converges for \( x = 0 \). This definition is not very restrictive. A simple example of a \( \kappa \)-deformed logarithm is \( \ln_\kappa(x) = 3\sqrt{x} - 3 \). Examples of families of \( \kappa \)-deformed logarithms follow below — see [28, 47].

The inverse function of a \( \kappa \)-deformed logarithm is a \( \kappa \)-deformed exponential function and is denoted \( \exp_\kappa(x) \). If \( x \) is not in the image of the
κ-deformed logarithm then \( \exp_\kappa(x) \) is taken equal to 0 when \( x \) is too small, and equal to \( +\infty \) when \( x \) is too large.

Fix now a \( \kappa \)-deformed exponential function \( \exp_\kappa(x) \). Note that throughout the paper this function does not depend on temperature. The obvious generalization of (1) is now

\[
p_k(T) = \exp_\kappa(G(T) - H_k/T),
\]

where the function \( G(T) \) is chosen such that normalization \( \sum_k p_k = 1 \) is satisfied. The alternative of putting normalization into the partition sum \( Z(T) \), i.e.

\[
p_k(T) = \frac{1}{Z(T)} \exp_\kappa(-H_k/T)
\]

is discussed later on. Expressions (9) and (10) are of course equivalent in case the deformed exponential is replaced by the standard exponential function. In fact, the difference between the two expressions is only relevant when temperature dependence is considered. The choice (9) is the simpler one because it yields immediately an expression for the quantity \( \ln_\kappa(p_k) \), needed in the context of the definition of entropy (see below).

4 Ising example

The following example illustrates well the point of view of the present paper. The Ising chain in an external field can be solved exactly in the thermodynamic limit. The result for the occupation probability of the two levels of the spin at the origin is

\[
p_{\pm}(T) = \frac{1}{2} \left(1 \pm \frac{y(T)}{\sqrt{1 + y(T)^2}}\right),
\]

with

\[
y(T) = \sinh \left(\frac{\beta \Delta}{2}\right) e^{\beta J}.
\]

In the latter expression \( \Delta > 0 \) is the energy level splitting due to the external field, \( J \geq 0 \) is the interaction energy, and \( \beta = 1/T \) is the inverse temperature.
The question under study is whether there exists a thermodynamical formalism which reproduces the temperature-dependent probabilities $p_{\pm}(T)$ without reference to the environment, which in this example is formed by all other spins of the Ising chain. The obvious definition of internal energy $U$ is

$$U = \frac{1}{2} [p_+(T) - p_-(T)]\Delta. \quad (13)$$

If there is no interaction with the environment (i.e. $J = 0$) then the pdfs are of the Boltzmann-Gibbs form. In this case, Shannon’s measure of information

$$I^{\text{Shannon}}(p) = -\sum_{k=\pm} p_k \ln(p_k) \quad (14)$$

is an adequate expression for the entropy $S$. Indeed, it is well-known that the Boltzmann-Gibbs distribution is thermodynamically stable in the standard formalism of statistical physics based on (14). For further use let us verify that temperature $T$ corresponds with the thermodynamic notion of temperature. A short calculation using (14) and the Boltzmann-Gibbs distribution gives

$$S = \beta U + \ln \left( \cosh \left( \frac{\beta \Delta}{2} \right) \right), \quad (15)$$
so that
\[
\frac{d}{d\beta} S = U + \beta \frac{d}{d\beta} U + \frac{\Delta}{2} \tanh \left( \frac{\beta \Delta}{2} \right)
\]
\[
= \beta \frac{d}{d\beta} U.
\] 
(16)

Hence, the thermodynamic relation
\[
\frac{1}{T} = \frac{dS}{dU}
\] 
(17)
is fulfilled.

If the spin interacts with its environment (i.e. \( J \neq 0 \)) then the pdfs \( (11) \) are not of the Boltzmann-Gibbs form, but can be written in the form \( (9) \), at least when \( J/\Delta \) is not too large — see Appendix A. For the proof of this statement it is essential that inverse temperature can be written as a monotonic function of the probabilities \( p_+ \) and \( p_- \). Fig. 1 compares the deformed logarithm, used in this case, with the natural logarithm. In what follows will be shown that, with an obvious generalization of the definition of entropy \( (14) \), the thermodynamic relation \( (17) \) still holds. The definition of internal energy \( (13) \) is not modified.

5 Generalized thermostatistics

Given a temperature-dependent family of probabilities \( p_k(T) \) of the form \( (9) \), a generalized thermostatistics, which for all temperatures yields \( (9) \) as the equilibrium distribution, is formulated as follows.

Let energy as a function of temperature be defined by
\[
U(T) = \langle H \rangle_{p(T)} \text{ with } \langle H \rangle_p = \sum_k p_k H_k
\] 
(18)
and let entropy as a function of temperature be defined by
\[
S(T) = \langle \langle I \rangle \rangle_{p(T)} \text{ with }
\langle \langle I \rangle \rangle_p = \sum_k \int_0^{p_k} dx \left[ -\ln(x) - F_\kappa(x) \right].
\] 
(19)
In this expression, \( F_\kappa(0) \) is a constant defined by \( (8) \). The extended class of entropy functionals of the form \( (19) \) has been studied in \( [12, 14] \). A short calculation gives

\[
\frac{dS}{dT} = \sum_k \left[ -\ln(p_k) - F_\kappa(0) \right] \frac{dp_k}{dT} \\
= \sum_k \left[ -G(T) + H_k/T - F_\kappa(0) \right] \frac{dp_k}{dT} \\
= \frac{1}{T} \frac{dU}{dT}
\]  

(20)

— to see the latter, use that

\[
\sum_k \frac{dp_k}{dT} = 0.
\]  

(21)

This proves the thermodynamic relation \( (17) \).

Next, introduce so-called escort probabilities \( [15] \), defined by

\[
P_k(T) = Z(T)^{-1} \exp'_\kappa(G(T) - H_k/T)
\]  

(22)

with \( \exp'_\kappa(x) \) the derivative of \( \exp_\kappa(x) \) and with

\[
Z(T) = \sum_l \exp'_\kappa(G(T) - H_l/T)
\]  

(23)

These escort probabilities have been introduced in \( [16] \) for the special case of Tsallis' thermostatistics. From \( \sum_k p_k = 1 \) follows

\[
\frac{dG}{dT} = -T^{-2} \sum_k P_k(T) H_k.
\]  

(24)

Using this result one calculates

\[
\frac{dU}{dT} = \sum_k H_k \exp'_\kappa(G(T) - H_k/T) \left( \frac{dG}{dT} + T^{-2} H_k \right) \\
= Z(T)T^{-2} \sum_k P_k(T) \left[ H_k - \sum_l P_l(T) H_l \right]^2 \\
\geq 0.
\]  

(25)
Hence, energy is an increasing function of temperature, as it should be. To-gether with (17), this shows that entropy $S(U)$ as a function of energy $U$ is concave. In other words, the system is thermally stable.

There exists also a variational principle, satisfied by the probabilities $p_k$. Given any pdf $r$, consider the problem of maximizing information content $\langle I \rangle_r$ under the constraint that average energy $\sum_k r_k H_k$ equals a given value $U$. Introduce Lagrange multipliers $\alpha$ and $\beta$ and minimize the expression

$$\beta \sum_k r_k H_k - \langle I \rangle_r - \alpha \sum_k r_k. \quad (26)$$

Variation w.r.t. $r_k$ gives the condition

$$0 = \beta H_k + \ln \kappa(r_k) + F_\kappa(0) - \alpha. \quad (27)$$

Comparison with (9) shows that $r = p$, $\beta = 1/T$, and $\alpha = F_\kappa(0) + G(T)$, is a solution of this variational principle.

Assume now that $M$ is any other observable of the system, e.g., total magnetization of a spin system. Then thermodynamic stability requires not only that entropy $S$ is concave as a function of internal energy $U$ but also as a function of the average value $\langle M \rangle$. That this property holds is shown in Appendix B.

6 Examples

The example of a single spin of the Ising chain has been discussed above. The pdfs (11) are of the form (9). Therefore, the formalism developed above is applicable. One concludes that the exact equilibrium distribution of a weakly interacting Ising chain in the thermodynamic limit, when restricted to a single spin variable, is an equilibrium distribution of generalized thermostatistics.

6.1 Tsallis’ thermostatistics

Make the following specific choice of $\kappa$-deformed logarithm

$$\ln_\kappa(x) = \frac{q}{q-1} \left( x^{q-1} - 1 \right), \quad (28)$$
where \( q \) is a parameter, which for technical reasons should lie between 0 and 2. The inverse function is

\[
\exp_\kappa(x) = \left[ 1 + \frac{q - 1}{q} x \right]_{+}^{1/(q-1)}.
\]

(29)

The notation \([x]_+ = \max\{0, x\}\) is used. A short calculation shows that (19) reduces to

\[
\langle \langle I \rangle \rangle_p = \frac{1}{q-1} \left( 1 - \sum_k p_k^q \right),
\]

(30)

which is Tsallis’ \( q \)-entropy \[1\]. The temperature-dependent probabilities \( p_k \), given by equation (9), read

\[
p_k = \left[ 1 + \frac{q - 1}{q} \left( G(T) - \frac{H_k}{T} \right) \right]_{+}^{1/(q-1)}.
\]

(31)

The distribution introduced by Tsallis \[1\], in its original version, reads in the present notations

\[
p_k = \frac{1}{Z} \left[ 1 - \beta^*(q - 1) H_k \right]_{+}^{1/(q-1)},
\]

(32)

with \( Z \) a normalization constant, and \( \beta^* \) a Lagrange multiplier related to inverse temperature. It is of course possible to write (31) in the form of (32). The identification gives

\[
\beta^* = \frac{1}{T} \frac{1}{q T + (q - 1) G(T)}
\]

and

\[
Z = \left[ 1 + \frac{q - 1}{q} G(T) \right]^{1/(1-q)}.
\]

(33)

Note that \( G(T) \) can be eliminated to obtain

\[
\beta^* = \frac{1}{q T Z^{q-1}}.
\]

(34)

Clearly, the Lagrange multiplier \( \beta^* \) does not have its usual value of \( 1/T \), but depends in a rather complicated way on temperature. This difficulty was
not understood in the early days of Tsallis’ thermostatistics. In fact, it took about ten years [18] before the question of defining temperature was settled.

It is interesting to sketch briefly the evolution that the formalism has undergone. Soon after the original paper [1] appeared, it was proposed [19] to replace the constraint \( \sum_k r_k H_k = U \), used in the variational principle, with a constraint of the form

\[
\sum_k r_k^q H_k = U. \tag{35}
\]

The effect of this change is a pdf of the form (32), with \( q - 1 \) replaced by \( 1 - q \). The main advantage of the above constraint is that the usual relation \( \beta = 1/T \) between Lagrange multiplier and thermodynamic temperature \( T \), defined by (17) is restored, however, at the cost of changing the definition of thermodynamic energy \( U \). Both papers [1, 19] have been criticized [20, 21], the first because of the apparent lack of thermodynamic stability, the latter because internal energy \( U \), as given by (35), is not the average of the energy levels \( H_k \). Later attempts to cure the formalism [16, 18] (introducing escort probabilities and changing the definition of temperature) solved the problems only partly. For a recent discussion, see [22].

### 6.2 Superstatistics

In a recent proposal [23, 24, 25] the Boltzmann-Gibbs formalism is generalized by replacing the Boltzmann factor \( \exp(-\beta E) \) by an average over a range of inverse temperatures \( \beta \)

\[
B(E) = \int_0^\infty d\beta f(\beta)e^{-\beta E}. \tag{36}
\]

The resulting formalism is called superstatistics. With an appropriate choice of distribution \( f(\beta) \) the Tsallis distribution (32) is recovered as

\[
p_k = \frac{1}{Z} B(H_k) = \frac{1}{Z} \int_0^\infty d\beta f(\beta)e^{-\beta H_k} \tag{37}
\]

with \( Z = \sum_k B(H_k) \) (adapting notations to those of the present paper). The argument in favor of (36, 37) is that in non-equilibrium systems thermodynamic variables like temperature may fluctuate in space and time. This
argument is not so different from the open systems argument, given above, that due to interactions with the environment even the equilibrium distribution will deviate from Boltzmann-Gibbs.

Note that all probability distributions of superstatistics can be written as distributions of the present generalized thermostatistics. In other words, any distribution of the form \( \text{(37)} \) can be written as \( \text{(9)} \) with an appropriate choice of \( \kappa \)-deformed exponential function. Indeed, fix some positive temperature \( T \) and let

\[
\exp_\kappa(x) = \int_0^\infty d\beta g(\beta) e^{T\beta x} \tag{38}
\]

where \( g(\beta) \) is a probability distribution still to be determined. The function \( \exp_\kappa(x) \) is increasing and convex. It satisfies \( \exp_\kappa(0) = 1 \). One has

\[
\int_0^\infty dx \exp_\kappa(-x) = \int_0^\infty d\beta g(\beta) \int_0^\infty dx e^{-T\beta x} = \int_0^\infty d\beta g(\beta) \frac{1}{T\beta}. \tag{39}
\]

The latter integral is convergent if the distribution \( g(\beta) \) stays away from \( \beta = 0 \). Then \( \exp_\kappa(x) \) satisfies all requirements to be a deformed exponential function in the sense of \([12]\). Now use \( \text{(9)} \) to calculate

\[
p_k = \int_0^\infty d\beta g(\beta) e^{T\beta G(T) - \beta H_k}. \tag{40}
\]

This expression coincides with \( \text{(37)} \) provided

\[
g(\beta) = \frac{1}{Z} f(\beta) e^{-\lambda\beta} \tag{41}
\]

with \( \lambda \) the unique solution of

\[
\int_0^\infty d\beta f(\beta)e^{-\lambda\beta} = Z. \tag{42}
\]

The normalization function \( G(T) \) is then given by \( G(T) = \lambda/T \).

The above arguments show that any probability distribution produced by the formalism of superstatistics can also be produced by the present formalism of generalized thermostatistics. Is it possible to distinguish the two
formalisms by applying them to problems of physics? The obvious answer is that one should look to the temperature dependence of the equilibrium probability distributions and compare them with experimental data. However, superstatistics is meant to be valid for systems not in equilibrium, with a fluctuating temperature. It is not at all clear how the distribution of inverse temperatures $f(\beta)$ should depend on some average temperature. This point deserves further investigation.

The inverse function of $\exp_\kappa(x)$ given by (38) is denoted $\ln_\kappa(x)$, as before. It can be used to calculate an entropy functional $\langle\langle I \rangle\rangle_p$ by means of (19). Up to a prefactor, this is exactly the entropy functional introduced in [26], in the first of the two cases considered there. Indeed, the expression, found there, reads

$$S(p) = \sum_k \int_0^{p_k} dy (\alpha + E(y))$$

with $\alpha$ a constant and $E(y)$ the inverse of the function $Z^{-1}B(E)$. In the present notations is

$$\frac{1}{Z} B(E) = \exp_\kappa \left( \frac{1}{T} (\lambda - E) \right).$$

Hence the inverse function is given by

$$E(y) = \lambda - T \ln_\kappa(y).$$

One concludes that

$$S(p) = \sum_k \int_0^{p_k} dy (\alpha + \lambda - T \ln_\kappa(y)).$$

This equals $T$ times $\langle\langle I \rangle\rangle_p$ provided that $\alpha$ is chosen equal to $-\lambda - TF_\kappa(0)$.

Note that the formalism developed in [26] deviates from the one presented here because energy constraints other than the standard (18) are considered. Such constraints are considered in the final part of this paper.

### 6.3 Kaniadakis’ entropy functional

Another example of $\kappa$-deformed logarithm has been introduced by Kaniadakis [5 27], namely

$$\ln_\kappa(x) = \frac{1}{2\kappa} \left( x^\kappa - x^{-\kappa} \right),$$

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with $\kappa$ a parameter with value between -1 and 1. The corresponding deformed exponential function is

$$\exp_\kappa(x) = \left(\kappa x + \sqrt{1 + \kappa^2 x^2}\right)^{1/\kappa}.$$  \hspace{1cm} (48)

With these definitions the entropy functional (19) becomes

$$\langle\langle I \rangle\rangle_p = \frac{1}{2\kappa(1 - \kappa)} \left(\sum_k p_k^{1-\kappa} - 1\right) + \frac{1}{2\kappa(1 + \kappa)} \left(1 - \sum_k p_k^{1+\kappa}\right). \hspace{1cm} (49)$$

The corresponding equilibrium distribution is

$$p_k = \left(\kappa[G(T) - H_k/T] + \sqrt{1 + \kappa^2[G(T) - H_k/T]^2}\right)^{1/\kappa}. \hspace{1cm} (50)$$

This distribution differs from the one studied in [5] because here normalization is not a prefactor.

7 Probability-dependent variables

In this final part of the paper the class of temperature dependent probabilities (9) is enlarged. One cannot expect that all open systems, weakly coupled with their environment, are described by equilibrium distributions of the form (9). Indeed, consider e.g. an open system consisting of a finite part of a 2-dimensional Ising lattice with nearest-neighbor interaction constant $J > 0$, in absence of an external field. Independent of how small $J$ is there is always a critical temperature $T_c$ (proportional to $J$) where the Ising lattice becomes unstable. This will be reflected by an instability of the entropy $S(U, B)$ of the open system. The idea is now to capture the essence of such instabilities by elements coming from mean-field theory.

Temperature-dependent variables are replaced by probability-dependent variables, which is a new notion that is introduced here. By definition, a probability-dependent variable is a function $f_k(x)$ depending on the microstate $k$ and on the probability $x$, which varies between 0 and 1. Its average or expectation is defined by

$$\langle\langle f \rangle\rangle_p = \sum_k \int_0^{p_k} dx \, f_k(x). \hspace{1cm} (51)$$
Note that this expression has the essential characteristics of a statistical average. It is linear, positive on positive functions, and normalized to one.

The most obvious example of a probability-dependent variable is information content, also called entropy functional. Indeed, Shannon’s measure of information $I(p)$ can be written as

$$I(p) = - \sum_k p_k \ln(p_k) = - \sum_k \int_0^{p_k} dx \left( \ln(x) + 1 \right) = \langle\langle I \rangle\rangle_p,$$

with the functions $I_k(x)$ defined by

$$I_k(x) = - \ln(x) - 1, \text{ independent of } k. \quad (53)$$

In fact, this is the reason why (19) was written in the form $\langle\langle I \rangle\rangle_p$, with the probability-dependent variable $I$ given by

$$I_k(x) = - \ln(x) - F_\kappa(0), \text{ independent of } k. \quad (54)$$

Notice that also energy may be a probability-dependent variable. Indeed, consider the following well-known mean-field Hamiltonian

$$H = -J\langle\sigma\rangle_p - h\sigma. \quad (55)$$

In this expression $J > 0$ and $h$ are model parameters, $\sigma$ is a spin variable taking on the value $\pm 1$ with probability $p_\pm$. The average value of the Hamiltonian $H$ can be written as

$$\langle H \rangle_p = -J\langle\sigma\rangle_p^2 - h\langle\sigma\rangle_p = \langle\langle \phi \rangle\rangle_p.$$

with potentials $\phi_\pm(x)$ given by

$$\phi_\pm(x) = -4Jx + J \mp h. \quad (57)$$

This shows that the energy of the mean-field model (55) is a probability-dependent variable.
A straightforward generalization of (57) is to consider potentials of the form

\[ \phi_k(x) = -J_k q x^{q-1} - h_k, \]  

(58)

where \( q \) is a fixed number, and \( J_k > 0 \) and \( h_k \) are model parameters. The corresponding average energy equals

\[ \langle \langle \phi \rangle \rangle_p = - \sum_k J_k p_k^q - \sum_k h_k p_k. \]  

(59)

Note that the non-linear constraint (35) coincides with this expression, with \( J_k < 0 \) and \( h_k = 0 \). Hence the critique of [20], that (35) lacks normalization, does not apply. Indeed, in the present context the average \( \langle \langle \phi \rangle \rangle_p \) is normalized to 1.

### 8 Generalized mean-field theory

The class of temperature-dependent pdfs (9) can now be enlarged by allowing all distributions of the form

\[ p_k = \exp_{\kappa} (G(T) - \psi_k(p_k)/T), \]  

(60)

where \( \psi_k(x) \) is a probability-dependent potential. The question, discussed below, is whether there exists a generalized mean-field model with probability-dependent potentials \( \phi_k(x) \), for which the equilibrium distributions are given by (60). The relation between the potentials \( \phi_k(x) \) and \( \psi_k(x) \) is allowed to be non-trivial.

Let entropy \( S \) be defined as before by \( S = \langle \langle I \rangle \rangle_p \). It is immediately clear that internal energy \( U \), defined by \( U = \langle \langle \psi \rangle \rangle_p \), still satisfies (17). However, the stability requirement that energy \( U \) is an increasing function of \( T \) is not always fulfilled. One can show, e.g., that it holds when the high temperature condition

\[ T \geq -\psi_k'(p_k) \exp_{\kappa}^G(G(T) - \psi_k(p_k)/T) \]  

(61)

is satisfied for all \( k \). It is not a surprise that in these mean-field models a thermodynamic instability can occur at low temperatures.
The variational principle is straightforward. Consider the problem of maximizing \( \langle \langle I \rangle \rangle_r \) under the constraint that \( \langle \langle \psi \rangle \rangle_r = U \). This leads to the Lagrange problem of minimizing

\[
\beta \langle \langle \psi \rangle \rangle_r - \langle \langle I \rangle \rangle_r - \alpha \sum_k r_k. \tag{62}
\]

Variation w.r.t. \( r_k \) leads to the equation

\[
\beta \psi_k(r_k) - I_k(r_k) = \alpha. \tag{63}
\]

This equation coincides with (60), when \( r = p, \beta = 1/T, \) and \( \alpha(T) - F_κ(0) = G(T) \).

However, the above variational calculation is not what one does traditionally with the mean-field model (55). Rather, one first studies the Hamiltonian \( H = -Jm\sigma - h\sigma \), where \( m \) is a constant which is taken equal to \( \langle \sigma \rangle_p \) only after finishing the calculation of thermodynamic equilibrium. In order to generalize this procedure, consider the problem of optimizing \( \langle \langle I \rangle \rangle_r \) under the constraint

\[
\sum_k r_k E_k = U, \tag{64}
\]

with constant energy levels \( E_k \). At the end they are taken equal to \( \psi_k(p_k) \). The corresponding Lagrange problem leads to the equation

\[
\beta E_k - I_k(r_k) = \alpha. \tag{65}
\]

It is clear that \( p_k \) given by (60) is the solution of this problem. However, (65) is not the equation corresponding with the problem of maximizing \( \langle \langle I \rangle \rangle_r \) given the constraint \( \langle \langle \psi \rangle \rangle_r = U \), but rather that corresponding with a constraint of the form \( \langle \langle \phi \rangle \rangle_r = U^* \), where the \( \phi \)-potentials satisfy

\[
\psi_k(y) = \frac{1}{y} \int_0^y \phi_k(x)dx. \tag{66}
\]

In the specific case of the mean-field Hamiltonian (55), in combination with Shannon’s measure of information, (65) reduces to the well known mean-field equation

\[
m = \tanh \left( \beta (Jm + h) \right) \quad \text{with} \quad m = r_+ - r_. \tag{67}
\]
The expression
\[ \beta \sum_k r_k E_k - \langle\langle I \rangle\rangle_r \] (68)
should be convex, with minimum at \( r = p \). The appropriate tool to investigate this point is relative information content, also called relative entropy or Kullback-Leibler distance. Its generalized definition is (see [14])
\[ I(r||p) = I(r) - I(p) + \sum_k (r_k - p_k) I_k(p_k). \] (69)
Using (54) this becomes
\[ I(r||p) = \sum_k \int_{p_k}^{r_k} p_k \, dx \left( \ln \kappa(x) - \ln \kappa(p_k) \right). \] (70)
A short calculation gives
\[ \beta \sum_k r_k E_k - \langle\langle I \rangle\rangle_r = \beta \sum_k p_k E_k - \langle\langle I \rangle\rangle_p + I(r||p). \] (71)
Because \( I(r||p) \) is a convex function, which is minimal if and only if \( r = p \), this shows that, if a pdf \( p \) exists, solving (60), then it minimizes (68). This does not mean that the pdf \( p \) is the only solution of (60). Indeed, we know that in the mean-field model (55) there can exist three solutions. But the corresponding energy levels \( E_k \) are different, so that each time (68) is minimal at \( r = p \).

Let us shortly return to the Tsallis formalism. Expression (32) gives the temperature dependence of the pdf as found in the context of Tsallis’ thermostatistics. It is straightforward to write these in the form (60). Indeed, let \( \psi_k(x) \) be given by
\[ \psi_k(x) = H_k q x^{q-1} \] (72)
(note that this is (58) with some change of notation) and let \( \ln \kappa(x) \) be given by (28). Then (60) reduces to (32), with \( G(T) \) given by
\[ G(T) = \frac{q}{q-1} (Z(T)^{1-q} - 1), \] (73)
and \( \beta^* = 1/T \). This means that Tsallis’ non-extensive thermostatistics is a special case of the present generalized mean-field theory.
9 Discussion

This paper proposes a generalized thermostatistics obtained by replacing exponential and logarithmic functions in the Boltzmann-Gibbs distribution, respectively Shannon’s entropy functional, by $\kappa$-deformed functions. The latter are rather arbitrary functions satisfying a minimal number of requirements. In the resulting formalism thermodynamic stability is automatically satisfied.

New in the present approach is the emphasis on the temperature dependence of equilibrium probability distributions. Such temperature dependence may be obtained by calculation of an open system in the standard formalism, or may, in principle, originate from an experiment. Next, a thermodynamic formalism is sought for in which these are the equilibrium distributions. This way of working eliminates the need for postulating specific entropy functions or energy constraints, as is the typical way of doing in non-extensive thermostatistics.

The thermodynamic relation between entropy $S$ and internal energy $U$ can be derived from the underlying microscopic statistical theory under the assumption that the interaction of the system with its environment is negligible. Goal of this paper is to show that this thermodynamic relation is also valid for systems weakly interacting with their environment. This has been shown for at least one example, namely a single spin interacting with its environment. However, one cannot expect this result to be generic because the system together with its environment may exhibit a phase transition. In such a case one expects that the system might be destabilized by its environment.

In order to be able to cope with the latter possibility a mean-field approach has been elaborated in the second part of the paper. The concept of probability-dependent variables has been introduced. The result is a rigorously defined mean-field theory. Its stability properties have been analyzed using a generalized notion of relative entropy. Although equilibrium states are not necessarily unique they still satisfy a variational principle. But the effective energy levels involved in this variational principle depend on the choice of equilibrium state.

A secondary goal of the present paper is to improve understanding of Tsallis’ formalism of non-extensive thermostatistics. With a specific choice of deformed logarithmic function the entropy functional becomes that of Tsallis. The resulting equilibrium distribution coincides with Tsallis’ distribution. If temperature dependence of the distributions is taken into account then the
Tsallis formalism describes mean-field models of the present approach. As a consequence, all applications of the Tsallis formalism are also applications of the present generalized thermostatistics. The same statement holds for the recently introduced formalism of superstatistics. Also the entropy functional proposed by Kaniadakis has been considered. The present formalism leads to an equilibrium distribution which differs from the one proposed by Kaniadakis because here normalization is not a prefactor but enters inside the deformed exponential function.

For simplicity only discrete probabilities have been considered. Generalization to continuous distributions is straightforward. The average of a function \( f \) over phase space \( \Gamma \) is given by

\[
\langle f \rangle_\rho = \int_{\Gamma} d\gamma \rho(\gamma)f(\gamma).
\]  

The analogue of (9) for the equilibrium density \( \rho(\gamma) \) is

\[
\rho(\gamma) = \exp_\kappa (G(\beta) - \beta H(\gamma)).
\]  

The probability-dependent generalization of (74) is

\[
\langle \langle f \rangle \rangle_\rho = \int_{\Gamma} d\gamma \int_0^{\rho(\gamma)} dx f(\gamma, x).
\]  

Also quantum statistical mechanics has not been considered. The ansatz for the equilibrium density matrix \( \rho \), given a Hamiltonian operator \( H \), is now

\[
\rho = \exp_\kappa (G(\beta) - \beta H).
\]  

It is not obvious how to introduce probability-dependent variables in this case. However, for functions of the density matrix, like information content \( I \), one can define

\[
\langle \langle I \rangle \rangle_\rho = \int_0^1 dx \operatorname{Tr} \rho I(x\rho).
\]  

It is then straightforward to reformulate the first part of the paper in a quantum context.

Open systems are most often described using stochastic differential equations. A recent effort in this direction is found in [28]. The connection with the present formalism has not yet been studied.
Acknowledgments

I thank S. Abe, G. Kaniadakis, and T. Wada, for helpful comments on a previous version of this paper. I thank an anonymous referee for numerous helpful comments.

Appendix A: Ising model

This appendix explains how the deformed logarithm is constructed in case of the one-dimensional Ising model.

For convenience, let $J^* = J/\Delta$. Introduce a function $\lambda(x)$, defined for $x$ between 0 and $1/2$, by the relation

$$
\lambda(p_-(T)) = \beta \Delta. \tag{79}
$$

The inverse function $\lambda^{-1}(z)$ is given by

$$
\lambda^{-1}(z) = \frac{1}{2} \left( \frac{\sinh(z/2)}{\sqrt{e^{-2J^*z} + \sinh^2(z/2)}} \right). \tag{80}
$$

If $J = 0$ then an explicit expression for $\lambda(x)$ is feasible. One finds in this case $\lambda(x) = \ln(1 - x) - \ln(x)$.

For $0 < x \leq 1/2$ the deformed logarithm must be of the form

$$
\ln_\kappa(x) = -\ln(2 \cosh(\lambda(x)/2)) - u(\lambda(x)) - \frac{\lambda(x)}{2}, \tag{81}
$$

with $u(z)$ still to be determined. The definition for $1/2 \leq x < 1$ is then given by

$$
\ln_\kappa(x) = \ln_\kappa(1 - x) + \lambda(1 - x). \tag{82}
$$

The derivative of (81) reads

$$
\frac{d}{dx} \ln_\kappa(x) = -\lambda'(x) \left[ \frac{1}{2} \left( 1 + \tanh \left( \frac{\lambda(x)}{2} \right) \right) \right] + u'(\lambda(x)). \tag{83}
$$
Because $\lambda(x)$ is decreasing and the deformed logarithm must be an increasing function one obtains the condition that

$$2u'(z) + \tanh(z/2) > -1.$$  \hspace{1cm} (84)

Because $\ln_\kappa(x)$ must also increase for $1/2 \leq x < 1$ one has further that

$$2u'(z) + \tanh(z/2) < 1.$$  \hspace{1cm} (85)

The condition that $\ln_\kappa(1) = 0$ can be analyzed easily. The result is that $u(z)$ must vanish in the limit of large $z$. The condition that $\ln_\kappa(x)$ is concave in $x = 1/2$ requires that $u'(0) \geq 0$.

The condition of concavity of $\ln_\kappa(x)$ is more difficult because $\lambda(x)$ is necessarily convex for $x$ close to zero, while $\lambda''(1/2) = -16J^*$. This wrong curvature of $\lambda(x)$ close to $x = 1/2$ should be compensated by the curvature of $u(z)$ for $z$ close to zero.

The above analysis suggests to choose $u$ as follows

$$u(z) = \frac{1}{2} J^*(1 + z)e^{-z}.$$  \hspace{1cm} (86)

The factor $J^*$ has been included to ensure that the deformed logarithm coincides with the natural logarithm in case $J^* = 0$. The above conditions on $u(z)$ are satisfied provided $J^*$ is less than $J^*_{\text{max}} \simeq 3.83$.

It is rather hard to check concavity of the deformed logarithm in an analytic manner. However, by numerical evaluation one can convince oneself that the function is concave as long as $J^*$ is not too large.

**Appendix B: Thermodynamic stability**

In this appendix is shown that the probability distributions considered in the present paper are automatically stable under thermodynamic perturbations. It is a tradition (see [17]) to require also that pressure is a decreasing function of volume. However, here the notion of volume dependence is absent.

Consider the problem of maximizing entropy $\langle\langle I\rangle\rangle_r$ under the constraints that average energy $\langle H \rangle$ and average magnetization $\langle M \rangle$ have given values $U$, respectively $B$:

$$\langle H \rangle = \sum_k r_k H_k = U$$
\[ \langle M \rangle = \sum_k r_k M_k = B. \]  

Introduce Lagrange multipliers \( \alpha, \beta, \) and \( \gamma, \) and minimize the expression

\[ \beta \sum_k r_k H_k + \gamma \sum_k r_k M_k - \langle \langle I \rangle \rangle_r - \alpha \sum_k r_k. \]  

Variation w.r.t. \( r_k \) gives the condition

\[ 0 = \beta H_k + \gamma M_k + \ln(\kappa(r_k)) + F(0) - \alpha. \]  

Hence the probability distribution maximizing \( \langle \langle I \rangle \rangle_r \) must be of the form

\[ \ln(\kappa(r_k)) = -F(0) + \alpha - \beta H_k - \gamma M_k. \]  

The parameter \( \alpha \) must be such that \( \sum_k r_k = 1 \) and will be considered as a function of \( \beta \) and \( \gamma. \) The value of \( \langle \langle I \rangle \rangle_r \) at equilibrium is denoted \( S(\beta, \gamma). \)

Introduce escort probabilities \( P_k(\beta, \gamma) \) by

\[ P_k(\beta, \gamma) = \frac{1}{Z(\beta, \gamma)} \exp(\kappa(-F(0) + \alpha - \beta H_k - \gamma M_k)). \]  

where

\[ Z(\beta, \gamma) = \sum_k \exp(\kappa(-F(0) + \alpha - \beta H_k - \gamma M_k)). \]  

Then, using (91), one obtains

\[ \frac{\partial U}{\partial \beta} = Z(\beta, \gamma) \sum_k P_k H_k \left[ \frac{\partial \alpha}{\partial \beta} - H_k \right] \]

\[ \frac{\partial U}{\partial \gamma} = Z(\beta, \gamma) \sum_k P_k H_k \left[ \frac{\partial \alpha}{\partial \gamma} - M_k \right] \]

\[ \frac{\partial B}{\partial \beta} = Z(\beta, \gamma) \sum_k P_k M_k \left[ \frac{\partial \alpha}{\partial \beta} - H_k \right] \]

\[ \frac{\partial B}{\partial \gamma} = Z(\beta, \gamma) \sum_k P_k M_k \left[ \frac{\partial \alpha}{\partial \gamma} - M_k \right]. \]  

(93)
Now, from $\sum_k r_k = 1$ follows

$$
\frac{\partial \alpha}{\partial \beta} = \langle H \rangle_*, \quad \frac{\partial \alpha}{\partial \gamma} = \langle M \rangle_*, \quad (94)
$$

where we introduced the notation that $\langle X \rangle_* = \sum_k P_k X_k$.

This leads to the result that

$$
\frac{\partial U}{\partial \beta} = -Z(\beta, \gamma) \left[ \langle H^2 \rangle_* - \langle H \rangle_*^2 \right], \\
\frac{\partial U}{\partial \gamma} = \frac{\partial B}{\partial \beta} = -Z(\beta, \gamma) \left[ \langle HM \rangle_* - \langle H \rangle_* \langle M \rangle_* \right], \\
\frac{\partial B}{\partial \gamma} = -Z(\beta, \gamma) \left[ \langle M^2 \rangle_* - \langle M \rangle_*^2 \right]. \quad (95)
$$

A short calculation using (90) and (19) gives

$$
\frac{\partial S}{\partial \beta} = \beta \frac{\partial U}{\partial \beta} + \gamma \frac{\partial B}{\partial \beta}, \\
\frac{\partial S}{\partial \gamma} = \beta \frac{\partial U}{\partial \gamma} + \gamma \frac{\partial B}{\partial \gamma}. \quad (96)
$$

Introduce the notation

$$
D(\beta, \gamma) = \frac{\partial U}{\partial \beta} \frac{\partial B}{\partial \gamma} - \frac{\partial U}{\partial \gamma} \frac{\partial B}{\partial \beta}. \quad (97)
$$

Then one has, using (96),

$$
\frac{\partial S}{\partial U} = \frac{1}{D(\beta, \gamma)} \left[ \frac{\partial S}{\partial \beta} \frac{\partial B}{\partial \gamma} - \frac{\partial S}{\partial \gamma} \frac{\partial B}{\partial \beta} \right] = \beta \quad (98)
$$

and similarly

$$
\frac{\partial S}{\partial B} = \gamma. \quad (99)
$$
Let us now put everything together. The matrix of second derivatives of $S$ as a function of $U$ and $B$ equals

\[
\begin{pmatrix}
\frac{\partial^2 S}{\partial U^2} & \frac{\partial^2 S}{\partial U \partial B} \\
\frac{\partial^2 S}{\partial B \partial U} & \frac{\partial^2 S}{\partial B^2}
\end{pmatrix} = \frac{1}{D(\beta, \gamma)} \begin{pmatrix}
\frac{\partial B}{\partial \beta} & -\frac{\partial U}{\partial \beta} \\
-\frac{\partial B}{\partial \gamma} & \frac{\partial B}{\partial \gamma}
\end{pmatrix}
\]

\[= -\frac{Z(\beta, \gamma)}{D(\beta, \gamma)} \begin{pmatrix}
\langle M^2 \rangle_* - \langle M \rangle_*^2 & -\langle HM \rangle_* + \langle H \rangle_* \langle M \rangle_* \\
-\langle HM \rangle_* + \langle H \rangle_* \langle M \rangle_* & \langle H^2 \rangle_* - \langle H \rangle_*^2
\end{pmatrix}, \tag{100}
\]

From Schwartz’s inequality follows that

\[| - \langle HM \rangle_* + \langle H \rangle_* \langle M \rangle_* |^2 \leq \left[ \langle M^2 \rangle_* - \langle M \rangle_*^2 \right] \left[ \langle H^2 \rangle_* - \langle H \rangle_*^2 \right]. \tag{101}\]

This inequality suffices to show that the matrix in the r.h.s. of (100) has positive eigenvalues and that $D(\beta, \gamma) \geq 0$. Hence, entropy is a concave function of $U$ and $B$. This shows thermodynamic stability of the probability distribution $r$.

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