Dual description of nonextensive ensembles

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Consider a quantum mechanical system with an unbounded hamiltonian. For such a system the entropic index $q$ of nonextensive thermodynamics has an upperbound $q_c \geq 1$ beyond which the formalism becomes meaningless. The expression $1/(q_c - 1)$ is the dimension of the state space (i.e. the manifold of density matrices) in the context of non-commutative geometry. For $q = q_c$ an ultraviolet cutoff $E \leq E_{ub}$ is needed to guarantee the existence of the equilibrium density matrix. Duality between $q > 1$ and $q < 1$-statistics via a $q \rightarrow 1/q$ transformation is established. It leads to an overall picture in which the meaning of both $q > 1$-statistics and $q < 1$-statistics is clarified. The hydrogen atom is considered as an example.

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The aim of this paper is to contribute to the physical understanding of nonextensive thermodynamics. It is obvious from the many applications (see e.g. [4]) that the formalism is physically relevant. Nevertheless the overall picture is still unclear. The open question treated below is whether physical systems should be described by an entropic index $q$ which is less than 1 or larger than 1. The $q > 1$-situation is easier to handle. On the other hand there are arguments in favor of $q < 1$. Both views are reconciled by the $q \rightarrow 1/q$-duality which was proposed in [3]. By working out this duality it becomes feasible to attach a physical meaning to both $q < 1$ and $q > 1$ formalisms.

In [3] the opinion is expressed that each hamiltonian has an intrinsic $q$-value, and that systems with short range interactions all belong to the universality class of $q = 1$-systems. Such an intrinsic value, denoted $q_c$, is proposed here. At first sight it does not seem to agree with the statement about the universality class of systems with short range interactions. However, at the end of the paper we will see that a hamiltonian with long range potential, like that of the hydrogen atom, does indeed determine a $q_c$-value different from 1.

A side effect of the present work is a link with noncommutative geometry as formulated in [3]. This mathematical theory generalizes concepts of differential geometry to quantum mechanics and could be essential in reconciling quantum mechanics with theories of gravity. An introductory text is [4]. An essential result of this theory is that in a non-commutative context the geometry of the manifold of states is fully determined by an operator which in the case of relativistic quantum mechanics is the Dirac operator. This correspondence is used here to interpret the expression $1/(q_c - 1)$ as a geometric dimension. At this moment it is not clear whether this correspondence will lead to new insights. It is however not excluded that non-extensivity plays an important role in the quantum mechanics of the microcosmos, as is also suggested by previous links between non-extensive thermodynamics and quantum groups [5], [6], resp. $q$-deformations AS97.

The Tsallis entropy is given by

$$S_q(\rho) = k_B \frac{1 - \text{Tr} \rho^q}{q - 1}$$

It depends on the entropic parameter $q \neq 1$ (we assume throughout the paper that $q > 0$) and on the density matrix $\rho$ ($\rho \geq 0$ and $\text{Tr} \rho = 1$). In the limit $q \rightarrow 1$ the usual Shannon entropy is recovered. Minimization of the free energy

$$F_q = U^H_q - TS_q$$

determines the equilibrium density matrix at temperature $T$. For the energy $U^H_q$ several proposals have been made, the latest of which is [3].

$$U^H_q(\rho) = \frac{\text{Tr} \rho^q H}{\text{Tr} \rho^q}$$

The hamiltonian $H$ has a discrete spectrum bounded from below. The inverse temperature will be denoted $\beta = 1/k_B T$ as usual.

Different situations occur whether $q > 1$ or $q < 1$. Let us first assume that $q > 1$. Because of the duality, which will be discussed later on, the equilibrium density matrix in the $q > 1$-case is denoted $\sigma$ instead of $\rho$. For the same reason the hamiltonian is denoted $K$ instead of $H$. The equilibrium density matrix is of the form

$$\sigma = \frac{1}{\zeta} \left[ 1 - \beta(1-q) \frac{K - U^K_q(\sigma)1}{\text{Tr} \sigma^q} \right]^{1/(1-q)}$$

with

$$\zeta = \text{Tr} \left[ 1 - \beta(1-q) \frac{K - U^K_q(\sigma)1}{\text{Tr} \sigma^q} \right]^{1/(1-q)}$$

Note that Eq. (4) is of the implicit type. One can prove that it has a unique solution, provided that the operator

$$1 - \beta(1-q) \frac{K - U^K_q(\sigma)1}{\text{Tr} \sigma^q}$$

is...
$K^{1/(1-q)}$ is trace class (see 3). Let us consider the latter condition in more detail. Let $(\psi_n)_n$ be a basis in which $K$ is diagonal, with eigenvalues $\epsilon_n$: $K\psi_n = \epsilon_n \psi_n$. Assume that the eigenvalues are isolated, with finite multiplicity, and ordered increasingly. Let $q_c$ be the lower bound of $q \geq 1$ for which the sequence $n^{1-q_c}\epsilon_n$ is bounded. Then obviously the eigenvalues of $K$ diverge as
\[
\epsilon_n \sim n^{q_c-1}
\]
(6)
Note that the dimension of the non-commutative state space equals $1/(q_c - 1)$. See e.g. 3, section 5.6. Let us consider some examples. If $K$ were bounded (which is assumed not to be the case) then $q_c$ would be 1. For the harmonic oscillator $q_c$ equals 2, which corresponds with a geometric dimension equal to 1. For a quantum particle in a $d$-dimensional box with reflecting walls $q_c = 1 + 2/d$. Hence the dimension of the manifold is $d/2$, which is only half of what is expected. The explanation is that the laplacean is a second order operator. The correct dimension is obtained when the Dirac operator is used as follows. If $q_c$ were 1 then the trace in (4) diverges generically. Finite values can be obtained by introducing a cutoff in energy, i.e. by fixing a large number $N$, and restricting the system to the finite Hilbert space spanned by the eigenvectors $\psi_n, n = 0, 1, \cdots, N - 1$. Note that the cutoff in energy $E \leq E_{ub}$ is related to $N$ by
\[
E_{ub} \sim N^{q_c - 1}
\]
(7)
In the limit of large $N$ the trace of (3) can be estimated in terms of the Dixmier trace $\text{Tr}_\omega$, which is defined by
\[
\text{Tr}_\omega A = \lim_{N \to \infty} \frac{1}{\ln N} \sum_{n=0}^{N-1} \langle \psi_n | A | \psi_n \rangle \quad \text{for all } A
\]
(8)
The expectation value of any observable $A$ is then given by
\[
\langle A \rangle = \lim_{N \to \infty} \text{Tr}_N \sigma_N A = \frac{\text{Tr}_\omega a1 + K^{1/(1-q_c)}A}{\text{Tr}_\omega a1 + K^{1/(1-q_c)}}
\]
(9)
with $a$ an arbitrary constant such that $a1 + K > 0$. Remarkable is that $\langle A \rangle$ does not depend on $\beta$. Its value is determined by the high energy tail of the spectrum of $K$. In the context of noncommutative geometry 3, is called the integral of $A$.

The $q$-averages are given by
\[
\langle A \rangle_q = \text{Tr} \rho_N A = \frac{\text{Tr} \rho_N^q A}{\text{Tr} \rho_N^q}
\]
(10)
These are the physical expectation values. They depend on temperature and cutoff via a rescaled inverse temperature
\[
\beta^* = \beta (\ln N)^{q_c-1}
\]
(11)
A straightforward calculation shows that
\[
\langle A \rangle_q \approx \frac{\text{Tr} (f(\beta^*) + K_N)/(1-q_c)A}{\text{Tr} (f(\beta^*) + K_N)/(1-q_c)}
\]
(12)
with $f$ the inverse of the function $g$ given by
\[
g(a) = \left( \frac{\text{Tr} (a + K)/(1-q_c)}{\text{Tr}_\omega (a + K)/(1-q_c)} \right)^{q_c-1}
\]
(13)
Let us now consider the case $0 < q < 1$. The equilibrium density matrix is the solution of the implicit equation
\[
\rho = \frac{1}{\zeta} \left[ 1 - \beta(1-q) \frac{H - U^H_q(\rho)}{\text{Tr} \rho^q} \right]^{1/(1-q)}
\]
(14)
with $[A]_+ = A$ on the subspace on which $A$ is positive, and $= 0$ on the subspace on which $A$ is negative, and with
\[
\zeta = \text{Tr} \left[ 1 - \beta(1-q) \frac{H - U^H_q(\rho)}{\text{Tr} \rho^q} \right]^{1/(1-q)}
\]
(15)
The proof that under certain conditions these equations determine a unique equilibrium density matrix is complicated by the presence of the high energy cutoff — see 3 for a full discussion: part of the problem is discussed below.

In 2 it was argued that a system in thermal contact with a finite heat bath is described by Tsallis thermodynamics with entropic index 0 < $q < 1$. In this context the appearance of an energy cutoff is very natural since the total energy of system plus heat bath is finite. This bound on the total energy belongs probably to the essence of nonextensive systems.

A $q \sim 1/q$-duality has been studied in 2. It is based on the observation that the relation $\rho = \sigma^q/\text{Tr} \sigma^q$ can be inverted to $\sigma = \rho^q/\text{Tr} \rho^q$ with $q' = 1/q$. This duality is worked out below by introduction of the effective Hamiltonian $H_{eff}$ of 1. Write the energy functional (3) in a $1$-homogeneous form
\[
U_q^H(\rho) = (\text{Tr} \rho) \frac{\text{Tr} \rho^q H}{\text{Tr} \rho^q}
\]
(16)
Then the effective Hamiltonian $H_{eff}$ is defined by variation of the energy functional
\[
H_{eff}(\rho) = \frac{\delta}{\delta \rho} U_q^H(\rho)
\]
(17)
(the variation is restricted to the subspace on which \( \rho \) is strictly positive). It is the generator of the time evolution (see [11]). For an equilibrium state \( [\rho, H] = 0 \) holds, in which case it is easy to obtain (putting \( \text{Tr} \rho = 1 \))

\[
H_{\text{eff}}(\rho) = U_q^H(\rho)1 + \frac{q}{\text{Tr} \rho} \rho^{q-1} (H - U_q^H(\rho)1) \tag{18}
\]

Note also that

\[
\text{Tr} \sigma H = \text{Tr} \rho H_{\text{eff}}(\rho) = U_q^H(\rho) \tag{19}
\]

because of the 1-homogeneity of (16). A short calculation now gives

\[
1 - \beta (1 - q) \frac{H - U_q^H(\rho)1}{\text{Tr} \rho^\alpha} = \left[1 - \beta (1 - \frac{1}{q}) \lambda \frac{H_{\text{eff}}(\rho) - U_q^H(\rho)1}{\text{Tr} \sigma^{1/q}}\right]^{-1} \tag{20}
\]

with \( \lambda = \text{Tr} \sigma^{1/q} / \text{Tr} \rho^\alpha \). The lhs of (20) is proportional to \( \rho^{1-q} \) on the subspace on which it is strictly positive. Hence from \( \sigma \sim \rho^\alpha \) follows

\[
\sigma = \frac{1}{\xi} \left[1 - \beta (1 - \frac{1}{q}) \lambda \frac{H_{\text{eff}}(\rho) - U_q^H(\rho)1}{\text{Tr} \sigma^{1/q}}\right]^{1/(1-1/q)} \tag{21}
\]

with \( \xi \) the normalization factor. It turns out that

\[
\xi = \zeta^q \text{Tr} \rho^\alpha \tag{22}
\]

There is no cutoff in (21) because \( H_{\text{eff}}(\rho) \) is zero on the subspace where the cutoff is active. (21) shows that \( \sigma \) is the equilibrium density matrix corresponding to the entropic index \( 1/q \) for a system with hamiltonian \( K = \lambda H_{\text{eff}}(\rho) \). One concludes that a nice duality between \( q < 1 \) and \( q > 1 \)-statistics is obtained if not only \( q \) is mapped onto \( 1/q \) and \( \rho \) is mapped onto \( \sigma \), but also \( H \) is mapped onto \( K = \lambda H_{\text{eff}}(\rho) \).

From this duality the following statements can be deduced.

- \( q > 1 \)-statistics is another way of looking at \( q < 1 \)-statistics. The population of energy levels as described by the \( q < 1 \)-density matrix \( \rho \) drops faster than exponentially with increasing energy, as it is expected in a non-extensive system in thermal contact with a finite heat bath. The density matrix \( \sigma \) of \( q > 1 \)-statistics is a renormalized density matrix in which the population of high energy levels has been increased in an artificial way.

- Not every system described with \( q > 1 \)-statistics can be obtained in this way. Indeed, due to the cutoff in (14) the effective hamiltonian \( H_{\text{eff}} \) is in most cases defined on a finite dimensional Hilbert space. Hence a cutoff should be applied to the \( q > 1 \)-hamiltonian \( K \) before considering it as an effective hamiltonian. Further complications are that the effective hamiltonian depends on temperature, and that it is not the result of a simple ultraviolet cutoff applied to a fixed hamiltonian.

- Two types of hamiltonians are involved. The hamiltonian \( H \) in the \( q < 1 \)-description is the operator which determines the energy of the system. The operator \( K \) of the \( q > 1 \)-description corresponds with the effective hamiltonian \( H_{\text{eff}} \) of the \( q < 1 \)-case and hence is also the generator of the dynamics. This observation is in agreement with the use of \( K \) in the context of noncommutative geometry to formulate Tomita-Takesaki-theory (see [4], section 5.7). The connection with linear respons theory and the KMS condition will be discussed elsewhere [12].

Let us now consider which kind of system at \( q < 1 \) corresponds by duality with a system with entropic index \( q \) satisfying \( 1 < q < q_c \). For most hamiltonians the equilibrium density matrix of the \( 0 < q < 1 \)-case will contain only a finite number of eigenvalues different from zero. This is a consequence of the high-energy cutoff in (14). However, there is one exception, when the hamiltonian \( H \) is bounded and has an accumulation of eigenvalues at the upper limit \( \epsilon_\infty \) of its spectrum. This is e.g. the case with the discrete part of the spectrum of the hydrogen atom. This is precisely the kind of hamiltonian for which \( q < 1 \)-statistics is physically meaningful because the usual Gibbs statistics cannot be applied - see [3]. Let \( \beta_\infty \) be the solution of the equation

\[
\text{Tr} \rho^\alpha = \beta (1 - q)(\epsilon_\infty - U_q^H(\rho)) \tag{23}
\]

If \( \beta > \beta_\infty \) then the energy cutoff is active and only a finite number of eigenvalues of the equilibrium density matrix differ from zero. At high temperatures, i.e. \( \beta < \beta_\infty \), the operator in (14) has a diverging trace and \( q \)-statistics is meaningless, as it is the case for \( q = 1 \). The inverse temperature \( \beta_\infty \) depends on \( q \). It tends to \( \infty \) when \( q \to 1 \) and when \( q \to 1/q_\infty \), with the critical entropic index \( q_\infty \) equal to the upperbound of \( q \)'s for which \( n^{q-1}(\epsilon_\infty - \epsilon_n) \) is bounded, i.e.

\[
\epsilon_\infty - \epsilon_n \sim \frac{1}{n^{1/q_\infty - 1}} \tag{24}
\]

One concludes that the thermodynamic equilibrium of \( q < 1 \)-statistics exists for \( q \) in the interval \((1/q_\infty, 1)\) and for low enough temperatures so that \( \beta > \beta_\infty \). For completeness, note that for a bounded hamiltonian in an infinite dimensional Hilbert space the free energy has no minimum. Indeed, the energy \( U_q(\rho) \) is bounded above, while the entropy \( S_q(\rho) \) can be made arbitrary large. Hence the free energy \( F_q(\rho) \) can be made arbitrary small. The density matrix given by (14) is only a relative minimum of the free energy. However it is the unique maximum of
the entropy $S_q(\rho)$ for a given value of the energy $\mathcal{U}_q(\rho)$ — see [9].

Consider the example of the discrete part of the spectrum of the hydrogen atom. It has $q_c = 5/3$ (indeed the spectrum consists of eigenvalues $-\alpha/n^2$, $n = 1, 2, \cdots$; the $n$-th level is $n^2$-times degenerate; due to the degeneracy, the eigenvalues $\epsilon_n$ tend to $\epsilon_\infty = 0$ as $-\alpha/n^{2/3}$; neglect the spin of the electron). The corresponding dimension equals $3/2$ (again, one would expect the dimension to be equal to 3; the extra factor $1/2$ disappears if the square root of minus the hamiltonian is the operator determining the geometry). See the figure for a plot of $\alpha \beta_-$ as a function of $q$ in the domain of existence $(3/5, 1)$.

![Figure 1. $\alpha \beta_-$ as a function of $q$.](image)

In [13] an anomaly is reported at $q_c = 9/7$ instead of $q_c = 5/3$. This value was taken from [14], which is a paper on stellar polytropes. Study of the latter paper makes clear that it concerns the same anomaly as the one studied here, namely the upper limit for which $q$-statistics is meaningful. However, it is not evident that $q_c$ should have the same value in a classical model of gravitation as in a quantum mechanical model of Coulomb attraction. Further differences between [13] and the present paper can be explained by the use of a different expression for the energy functional (3).

One concludes that a statistical description of the hydrogen atom is possible in the interval $q_c^{-1} < q < 1$. The temperature varies between zero for the ground state and the maximal value $T_- \equiv 1/k_B \beta_-$ which depends itself on $q$. If the heath bath is very large then $q$ is close to one and the abundance of energy destabilizes the system (i.e. $T_-$ tends to zero). If $q$ tends to $q_c$ then the Tsallis entropy diverges and again $T_-$ tends to zero.

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