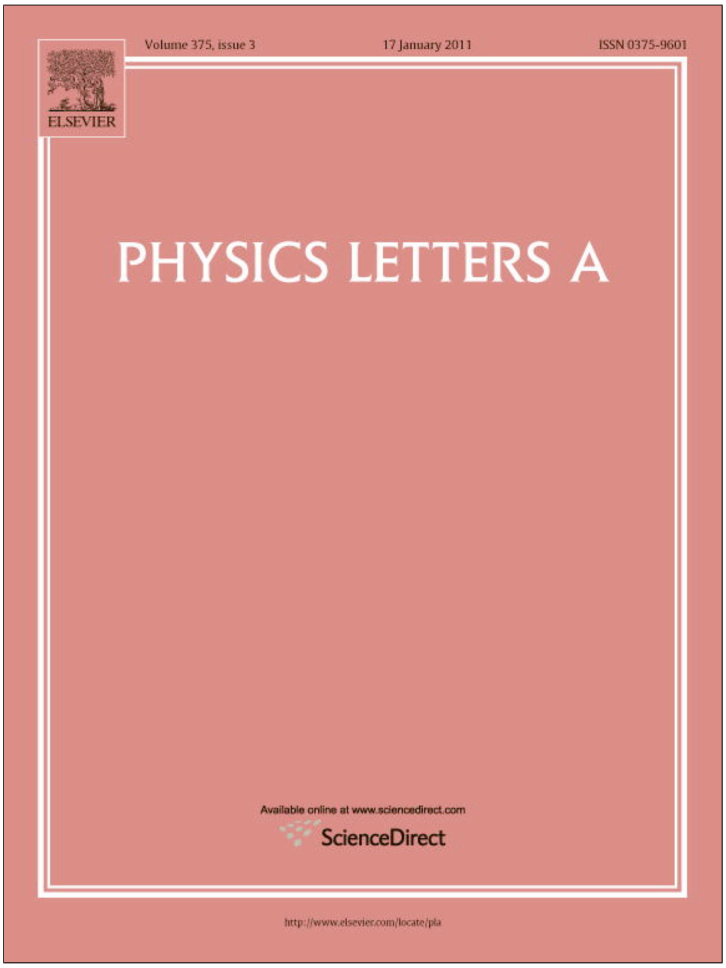
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# Nonextensive formalism and continuous Hamiltonian systems

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ABSTRACT

A recurring question in nonequilibrium statistical mechanics is what deviation from standard statistical mechanics gives rise to non-Boltzmann behavior and to nonlinear response, which amounts to identifying the emergence of "statistics from dynamics" in systems out of equilibrium. Among several possible analytical developments which have been proposed, the idea of nonextensive statistics introduced by Tsallis about 20 years ago was to develop a statistical mechanical theory for systems out of equilibrium where the Boltzmann distribution no longer holds, and to generalize the Boltzmann entropy by a more general function $S_q$ while maintaining the formalism of thermodynamics. From a phenomenological viewpoint, nonextensive *statistics* appeared to be of interest because maximization of the generalized entropy $S_q$ yields the $q$-exponential distribution which has been successfully used to describe distributions observed in a large class of phenomena, in particular power law distributions for $q > 1$. Here we re-examine the validity of the nonextensive *formalism* for continuous Hamiltonian systems. In particular we consider the $q$-*ideal gas*, a model system of quasi-particles where the effect of the interactions are included in the particle properties. On the basis of exact results for the $q$-*ideal gas*, we find that the theory is restricted to the range $q < 1$, which raises the question of its formal validity range for continuous Hamiltonian systems.



## 1. Introduction

Many phenomena in natural systems and in laboratory experiments are observed and measured under nonequilibrium conditions, and therefore do not obey the standard statistical mechanics description. In particular the distributions which characterize such systems are not Boltzmann-like and do not follow from linear response. Instead these distributions exhibit "fat tails" and power law decays and often they can be fitted by $q$-exponential functions which generalize the usual Boltzmann exponential distribution [1]. A recurring question is what deviation from standard statistical mechanics gives rise to this behavior, which amounts to the question of the emergence of "statistics from dynamics" as emphasized by E.G.D. Cohen [2]. There are several possible analytical developments from which $q$-exponential distributions can be obtained: superstatistics [3] by statistical average over the $\chi$-square distribution of an intensive variable, nonlinear response theory [4] by the solution of the generalized Fokker–Planck equation, and nonextensive statistics [5] by optimization of the generalized entropy.

It was precisely the original idea of nonextensive statistics introduced by Tsallis about 20 years ago [5] to develop a statistical mechanical theory for systems out of equilibrium where the Boltzmann distribution no longer holds, and to generalize the Boltzmann entropy by a more general function $S_q$ while maintaining the formalism of thermodynamics. From a practical viewpoint, the nonextensive statistics formulation appeared to be of interest because maximization of the generalized entropy under the usual constraints (normalized probabilities, fixed internal energy) yields the $q$-exponential distribution which has been successfully used to describe distributions observed in a large class of phenomena [6]. Indeed for a certain range of values of the index $q$, these $q$-exponential distributions exhibit a power law decay (when $q > 1$), a feature observed in a large class of experimental phenomena which cannot be straightforwardly interpreted in the context of classical theories. At the same time, a large literature concerning the internal self-consistency of the nonextensive formalism has developed addressing such questions as the stability of the entropy functional [7], the method of calculating averages [8–10] and the positivity of the specific heat [11,12].

Many explicit applications of the nonextensive formalism involve the assumption of independent particles: e.g., noninteracting particles that can occupy a set of discrete energy levels or, in the classical case, the ideal gas. These applications may appear paradoxical as the assumption of nonextensivity implies an interaction between components of the system (given classically by a potential term in the Hamiltonian). An alternative point of view, adopted here, is that there is no paradox because the underlying physical

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system does involve interactions (even long-ranged interactions): the independent particles are not the constituents of the physical system, but rather are understood to be quasi-particles in which the effect of the interactions are, to a first approximation, included in their properties (effective mass, statistics, etc.). This model system of quasi-particles is called the *q-ideal gas*. With this point of view, the adoption of the nonextensive formalism is another part of the effective one-body description required to account for aspects of the interactions that cannot be otherwise modeled. Accordingly we revisit the formalism for the $q$-ideal gas.

Even this simple case of the $q$-ideal gas has been subject to questions of internal consistency. In particular, that the nonextensive formalism has limited range of validity [8], gives negative specific heats [11] and even, recently, negative values for the second cumulant of the energy (a positive defined quantity!) [12]. Here we re-examine these issues using both the Tsallis entropy and, as suggested recently [7], the homogeneous entropy.

## 2. The homogeneous entropy

We start with the homogeneous entropy (or normalized Tsallis entropy) $S_q^H$ which was proven to be stable against small perturbations in the probability distribution function $\rho(\Gamma)$ while the Tsallis entropy $S_q$ is not [7]. For continuous systems the $H$-entropy is given by

$$S_q^H = k_B \frac{1-(K\int d\Gamma\,\rho^{1/q}(\Gamma))^q}{1-q}, \tag{1}$$

where $q$ is the index characterizing the entropy functional, $\Gamma$ denotes the phase space variable, and $K$ must be a quantity with the dimensions of $[\Gamma]^{\frac{1-q}{q}}$, i.e. $K=\hbar^{ND(\frac{1-q}{q})}$ with $N$, the number of degrees of freedom of the system with dimension $D$ and Hamiltonian $H$. In the limit $q\to 1$, the classical Boltzmann–Gibbs formulation is retrieved.[1]

Optimization of the $H$-entropy (1) with the normalization and energy constraints:

$$1=\int \rho(\Gamma)\,d\Gamma; \qquad U=\int \rho(\Gamma)H\,d\Gamma, \tag{2}$$

by the method of Lagrange multipliers leads to

$$\begin{aligned} 0 &= \frac{\delta}{\delta\rho(\Gamma)}\bigg(S_q^H-\alpha\Big(\int\rho(\Gamma)\,d\Gamma-1\Big) \\ &\quad -\beta\Big(\int\rho(\Gamma)H\,d\Gamma-U\Big)\bigg) \\ &= \frac{-q(K\int\rho^{1/q}(\Gamma)\,d\Gamma)^{q-1}K\frac{1}{q}\rho^{\frac{1}{q}-1}(\Gamma)}{1-q}-\alpha-\beta H, \end{aligned} \tag{3}$$

which is solved to give

$$\begin{aligned} \rho(\Gamma) &= \bigg(\frac{(q-1)\alpha}{(K\int\rho^{1/q}(\Gamma)\,d\Gamma)^{q-1}K} \\ &\quad + \frac{(q-1)\beta}{(K\int\rho^{1/q}(\Gamma)\,d\Gamma)^{q-1}K}H\bigg)_+^{\frac{q}{1-q}} \\ &= \mathcal{Z}_q^q(\alpha'+\beta' H)_+^{\frac{q}{1-q}}, \end{aligned} \tag{4}$$

where $\mathcal{Z}_q = K\int\rho^{1/q}(\Gamma)\,d\Gamma$, $\alpha'=(q-1)\alpha/K$, $\beta'=(q-1)\beta/K$, and where the notation $(x)_+$ means $x$ if $x>0$ and zero otherwise. $\rho(\Gamma)$ is the physical probability distribution, which must be real, positive and normalizable; so we must have

$$1=\mathcal{Z}_q^q\int(\alpha'+\beta' H)_+^{\frac{q}{1-q}}\,d\Gamma. \tag{5}$$

We will also consider the first moments of the Hamiltonian

$$\langle H^m\rangle = \int\rho(\Gamma)H^m\,d\Gamma = \mathcal{Z}_q^q\int(\alpha'+\beta' H)_+^{\frac{q}{1-q}}H^m\,d\Gamma; \tag{6}$$

in particular we are interested in

$$\begin{aligned} U=\langle H\rangle &= \frac{\int(\alpha'+\beta' H)^{\frac{q}{1-q}}H\,d\Gamma}{\int(\alpha'+\beta' H)^{\frac{q}{1-q}}\,d\Gamma}; \\ \langle H^2\rangle &= \frac{\int(\alpha'+\beta' H)^{\frac{q}{1-q}}H^2\,d\Gamma}{\int(\alpha'+\beta' H)^{\frac{q}{1-q}}\,d\Gamma}, \end{aligned} \tag{7}$$

where we used the normalization condition in (2). So the integrals to be considered have the form

$$I_m=\int(\alpha'+\beta' H)_+^{\frac{q}{1-q}}H^m\,d\Gamma, \tag{8}$$

and the result of the integration will depend on the sign of the Lagrange multipliers; therefore we must consider the following possible cases: (i) $\alpha'>0$ and $\beta'<0$, (ii) $\alpha'>0$ and $\beta'>0$, and (iii) $\alpha'<0$ and $\beta'>0$ (if both $\alpha',\beta'<0$, there is no solution to the normalization condition (5)).

## 3. The *q*-ideal gas

Besides the physical meaning of the $q$-ideal gas which was explained in the introductory section, it is legitimate to discuss its validity in the context of the nonextensive formalism because, if the formalism is to be used for continuous Hamiltonian systems, it should first pass the test of the $q$-ideal gas (as in classical statistical mechanics).

For the $q$-ideal gas, the Hamiltonian reduces to its kinetic part and the configuration integral in (8) is straightforward and yields a factor given by the space volume $V^N$. With a change of variable $X=\frac{\beta'}{\alpha'}\frac{p^2}{2m}$, (8) for $\alpha'>0$ and $\beta'<0$ (case (i)) becomes

$$\begin{aligned} I_m^{IG} &= V^N S_{DN}(2m)^{ND/2}\frac{1}{2}\alpha'^{\frac{q}{1-q}}\left(\frac{\alpha'}{|\beta'|}\right)^{\frac{ND}{2}+m} \\ &\quad\times\int_0^\infty(1-X)^{\frac{q}{1-q}}X^{\frac{ND}{2}+m-1}\,dX \\ &= V^N S_{DN}(2m)^{ND/2}\frac{1}{2}\alpha'^{\frac{q}{1-q}}\left(\frac{\alpha'}{|\beta'|}\right)^{\frac{ND}{2}+m} \\ &\quad\times B\left(\frac{1}{1-q},\frac{ND}{2}+m\right), \end{aligned} \tag{9}$$

where $B(k,l)$ is the Beta function provided $q<1$ (i.e. $\alpha<0$, and $\beta>0$), and excludes the possibility $q>1$ (with $\alpha>0$ and $\beta<0$). Then we have

$$\frac{I_m^{IG}}{I_0^{IG}}=\left(\frac{\alpha'}{|\beta'|}\right)^m\frac{B(\frac{1}{1-q},\frac{ND}{2}+m)}{B(\frac{1}{1-q},\frac{ND}{2})}, \tag{10}$$

which, with (7), gives

$$\frac{\alpha'}{|\beta'|}=U\left(1+\frac{2}{(1-q)ND}\right), \tag{11}$$

[1] For simplicity the Boltzmann factor $k_B$ in (1) will be omitted and reincluded explicitly when necessary.

$$\langle H^2\rangle - \langle H\rangle^2 = \left(\frac{\alpha'}{|\beta'|}\right)^2 \frac{B(\frac{1}{1-q}, \frac{ND}{2}+2)}{B(\frac{1}{1-q}, \frac{ND}{2})} - U^2$$
$$= \frac{4U^2}{ND(2+(1-q)(2+ND))}. \tag{12}$$

Note that $\langle H^2\rangle - \langle H\rangle^2$ is always positive since the $q$ index must be $q < 1$. It also follows from these results that the explicit expression of the distribution function for the $q$-ideal gas is given by

$$\rho^{IG}(\Gamma) = \left(\frac{\mathcal{Z}_q}{K}\right)^{\frac{q}{1-q}} \left(1-(1-q)\frac{\beta}{\mathcal{Z}_q^q}(H-U)\right)_+^{\frac{q}{1-q}}, \tag{13}$$

or, with the notation $\exp_q = (1+(1-q)x)_+^{\frac{1}{1-q}}$,

$$\rho^{IG}(\Gamma) = \frac{(\exp_q \frac{-\beta}{\mathcal{Z}_q^q}(H-U))^q}{\int \exp_q \frac{-\beta}{\mathcal{Z}_q^q}(H-U)\,d\Gamma}. \tag{14}$$

Noting that $\mathcal{Z}_{q=1} = 1$, it is clear that for $q = 1$, one retrieves the classical exponential distribution.

Proceeding along the same lines for case (ii): $\alpha', \beta' > 0$, i.e. $\alpha, \beta > 0$ with $q > 1$, or $\alpha, \beta < 0$ with $q < 1$, we obtain

$$\frac{I_m^{IG}}{I_0^{IG}} = \left(\frac{\alpha}{\beta}\right)^m \frac{B(\frac{ND}{2}+m, \frac{q}{q-1}-(\frac{ND}{2}+m))}{B(\frac{ND}{2}, \frac{q}{q-1}-\frac{ND}{2})}, \tag{15}$$

if and only if $1 < q < 1 + \frac{1}{\frac{ND}{2}+m-1}$. This gives

$$\frac{\alpha}{\beta} = U\left(\frac{2}{ND(q-1)} - 1\right),$$
$$\langle H^2\rangle - \langle H\rangle^2 = \frac{4U^2}{ND(2-(q-1)(2+ND))}, \tag{16}$$

which is valid (positive definite) when $1 < q < 1 + \frac{2}{ND+2}$. Notice that this range of the $q$ index is vanishingly small for $ND \gg 1$ and therefore physically negligible. In this case $\alpha, \beta > 0$, but the case $\alpha, \beta < 0$ (with $q < 1$) is excluded.

For $\alpha' < 0$ and $\beta' > 0$ (case (iii)), we have

$$I_m = V^N S_{DN}(2m)^{ND/2}\frac{1}{2}|\alpha'|^{\frac{q}{1-q}}\left(\frac{|\alpha'|}{\beta'}\right)^{\frac{ND}{2}+m}$$
$$\times \int_0^\infty (-1+X)^{\frac{q}{1-q}} X^{\frac{ND}{2}-1+m}\,dX, \tag{17}$$

which, whether $q < 1$ or $q > 1$, has no solution. So the cases $q > 1$ with $\alpha < 0$, and $\beta > 0$, and $q < 1$ with $\alpha > 0$, and $\beta < 0$ are excluded.

In summary, we have shown that, except for the physically negligible range $1 < q < 1 + \frac{2}{ND+2}$, the distribution function $\rho(\Gamma)$ for the $q$-ideal gas is normalizable only for $q < 1$ (with $\alpha < 0$, and $\beta > 0$), and that, contrary to some recent claim [12], the positivity of the energy mean squared fluctuations $\langle (H - \langle H\rangle)^2\rangle$ is always satisfied.

If, instead of the homogeneous entropy (1), we start from the Tsallis entropy [5] for continuous systems $S_q = \frac{K\int d\Gamma\,\rho_T^q(\Gamma)-1}{1-q}$, and use the same optimization procedure (2) (except that $U$ must then be computed with the escort average $U = \frac{\int \rho_T^q(\Gamma) H\,d\Gamma}{\int \rho_T^q(\Gamma)\,d\Gamma}$), we obtain the distribution function

$$\rho_T(\Gamma) = \left(\alpha'' - \alpha''(1-q)\frac{\beta}{\mathcal{Z}_T}(H-U)\right)_+^{\frac{1}{1-q}}, \tag{18}$$

where $\alpha'' = \frac{q}{1-q}\frac{K}{\alpha}$, and $\mathcal{Z}_T = K\int \rho^q(\Gamma)\,d\Gamma$. Therefrom performing the computation for the $q$-ideal gas (see Appendix A) leads to conclusions that are the same as above and are in essential agreement with some results by Abe [8,11]; in particular we find that the normalized distribution function exists only for $q < 1$ (besides the physically vanishingly small (for $N \gg 1$) range $1 < q < 1 + \frac{2}{ND+2}$) with the additional observation that $\rho_T(\Gamma)$ has a singular point at $q = 0$.

## 4. Thermodynamic quantities

We now evaluate the homogeneous entropy starting from (1) rewritten as

$$S_q^H = k_B\frac{1-\mathcal{Z}_q^q}{1-q}, \tag{19}$$

with

$$\mathcal{Z}_q^q = \frac{(K\int(\alpha'+\beta' H)_+^{\frac{1}{1-q}}\,d\Gamma)^q}{\int(\alpha'+\beta' H)_+^{\frac{q}{1-q}}\,d\Gamma} = K^q\frac{I^q}{I_0}. \tag{20}$$

For the $q$-ideal gas with $q < 1$ and $\beta > 0$, using (9), we find

$$\mathcal{Z}_q^q = K^q\left(V^N S_{DN}(2m)^{ND/2}\frac{1}{2}\right)^{q-1}\left(\frac{\alpha'}{|\beta'|}\right)^{\frac{ND}{2}(q-1)}$$
$$\times \frac{(B(\frac{2-q}{1-q}, \frac{ND}{2}))^q}{B(\frac{2-q}{1-q}, \frac{ND}{2})}, \tag{21}$$

where

$$\frac{(B(\frac{2-q}{1-q}, \frac{ND}{2}))^q}{B(\frac{2-q}{1-q}, \frac{ND}{2})} = \frac{B^{q-1}(\frac{1}{1-q}, \frac{ND}{2})}{(1+(1-q)\frac{ND}{2})^q}, \tag{22}$$

and

$$\frac{\alpha'}{|\beta'|} = U\left(1 + \frac{2}{(1-q)ND}\right). \tag{23}$$

Combining these results, we obtain

$$\mathcal{Z}_q^q = \frac{K^q R^H(V;q)}{U^{(1-q)\frac{ND}{2}}}, \tag{24}$$

with

$$R^H(V;q) = \left(V^N S_{DN}(2m)^{ND/2}\frac{1}{2}\frac{(1+(1-q)\frac{ND}{2})^{\frac{ND}{2}-\frac{q}{q-1}}}{((1-q)\frac{ND}{2})^{\frac{ND}{2}}}\right.$$
$$\left.\times B\left(\frac{1}{1-q}, \frac{ND}{2}\right)\right)^{q-1} \tag{25}$$

and

$$S_q^H = k_B\frac{1 - K^q R^H(V;q) U^{\frac{ND}{2}(q-1)}}{1-q}. \tag{26}$$

The thermodynamic temperature of the $q$-ideal gas then follows from this result. Since nonextensive statistics was developed on the basis of three axioms (the $q$-entropy, the normalization constraint and the free energy constraint) while maintaining the formalism of thermodynamics, the most logical implementation of this program is to retain the standard thermodynamic definition of temperature via the relation $1/T = dS/dU$.[2] From (26) we have

$$\frac{1}{T_q^H} = \frac{\partial S_q^H}{\partial U} = k_B K^q R^H(V;q)\frac{ND}{2}U^{\frac{ND}{2}(q-1)-1}. \tag{27}$$

In the limit $q \to 1$, $K = 1$ and $R^H(V; q \to 1) = 1$, so that for the classical ideal gas, where $U = \frac{ND}{2}k_B T$, we retrieve the expression $\frac{\partial S}{\partial U} = \frac{1}{T}$. The specific heat is then readily obtained

$$C_V^H = \left(\frac{\partial T_q^H}{\partial U}\right)^{-1} = k_B\frac{ND}{2}K^q R^H(V;q)\frac{U^{(q-1)\frac{ND}{2}}}{1+(1-q)\frac{ND}{2}}, \tag{28}$$

which is always positive for $q < 1$, and, for $q = 1$, gives the classical result $C_V = \frac{ND}{2}k_B$. Note that using (12), (24) and (27), (28) can also be written as

$$C_V^H = \frac{\langle H^2\rangle - \langle H\rangle^2}{k_B(T_q^H)^2}\mathcal{C}_q \tag{29}$$

with $\mathcal{C}_q = \mathcal{Z}_q^{-q}(1 + \frac{1-q}{1+(1-q)\frac{ND}{2}})$, which generalizes the expression of the specific heat given in terms of the energy fluctuations $C_V = \langle(\Delta E)^2\rangle/(k_B T^2)$.

When we perform the same computation with the Tsallis formulation (see Appendix A), we find the specific heat

$$C_V^q = k_B\frac{ND}{2}KR(V;q)\frac{U^{(1-q)\frac{ND}{2}}}{1-(1-q)\frac{ND}{2}}, \tag{30}$$

which, in the limit $q \to 1$, gives the classical expression for $C_V$, but where the denominator is *negative* for $q < 1$, except when $q = 1 - \epsilon$ with $\epsilon < \frac{2}{ND} \ll 1$. So, except in this narrow range, the Tsallis entropy formalism gives a negative specific heat for the $q$-ideal gas (see also [8] and [13]).

## 5. Concluding comments

We have shown that optimization of the $H$-entropy for continuous Hamiltonian systems combined with normalization and energy constraints gives an expression for the distribution function which is computed explicitly for the $q$-ideal gas and that, in the thermodynamic limit, the distribution function exists only in the $q \leqslant 1$ index range. Our results show that:

(i) in the range $q < 1$ the mean squared energy fluctuations are always positive, in contradition to recent claims that were a result of not taking into account the existence of intermediate integrals in the evaluation [12]; and that
(ii) in the usual Tsallis formulation the specific heat of the $q$-ideal gas is negative for $q < 1$.

We conclude that the use of the nonextensive formalism to "explain" observed $q$-exponential distributions on the basis of non-interacting quasi-particles is problematic when $q > 1$, the range where the $q$-exponential function exhibits power law decay. Furthermore, in the range $q < 1$ where the normalized distribution function exists, the Tsallis formalism is also questionable as it gives a negative specific heat for the $q$-ideal gas. Its applicability to Hamiltonian systems with continuous canonical variables has also been questioned recently by Abe from a different viewpoint [14].

As discussed in the Introduction, there are two aspects to the nonextensive approach to the study of nonequilibrium systems. (i) Nonextensive *statistics* has been applied successfully to analyze and to interpret observations in Hamiltonian systems which exhibit power law decay [6]; these interpretations are based on phenomenological analyses in accordance with $q$-exponential distributions. (ii) The nonextensive *formalism* was constructed on the basis of a few axioms and accordingly should develop with self-consistency. Our analysis gives strong indication that the range of validity of the latter is limited. While this does not preclude the pragmatic application of nonextensive *statistics* in phenomenological analyses of experimental results, it raises the question of the limits of validity of the *formalism* for continuous Hamiltonian systems.

[2] It has been proposed in the literature to modify this classical definition for various reasons (such as the introduction of a factor $c_q$ as a consequence of the use of the escort distribution [10,13]), but exploration of this possibility is outside the scope of the standard program.

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## Appendix A. The $q$-entropy

Starting with the Tsallis entropy $S_q = k_B\frac{K\int d\Gamma\,\rho_T^q(\Gamma)-1}{1-q}$, using the same optimization procedure (2) and noting that $U$ must now be computed with the escort average ($U = \frac{\int\rho_T^q(\Gamma)H\,d\Gamma}{\int\rho_T^q(\Gamma)\,d\Gamma}$), we obtain the distribution function

$$\rho_T(\Gamma) = \left(\alpha'' - \alpha''(1-q)\frac{\beta}{\mathcal{Z}_T}(H-U)\right)_+^{\frac{1}{1-q}}, \tag{31}$$

where $\alpha'' = \frac{q}{1-q}\frac{K}{\alpha}$, and $\mathcal{Z}_T = K\int\rho^q(\Gamma)\,d\Gamma$ (here $K$ has the dimensions $[\Gamma]^{q-1}$). For the computational convenience, we rewrite the distribution as

$$\rho_T(\Gamma) = \big(\Lambda - \Psi H(\Gamma)\big)^{\frac{1}{1-q}}\Theta\big(\Lambda - \Psi H(\Gamma)\big), \tag{32}$$

where the constants $\Lambda$ and $\Psi$

$$\Lambda = K\frac{q}{\alpha}\left(\frac{1}{1-q} + \frac{\beta U}{\mathcal{Z}_T}\right); \qquad \Psi = K\frac{q}{\alpha}\frac{\beta}{\mathcal{Z}_T};$$

$$\text{i.e. } \frac{\Lambda}{\Psi} = \frac{\mathcal{Z}_T}{\beta}\frac{\tilde{\Lambda}2}{1-q}, \tag{33}$$

are determined from the constraints

$$1 = \int\big(\Lambda - \Psi H(\Gamma)\big)^{\frac{1}{1-q}}\Theta\big(\Lambda - \Psi H(\Gamma)\big)\,d\Gamma, \tag{34}$$

$$U = \frac{\int(\Lambda - \Psi H(\Gamma))^{\frac{q}{1-q}}\Theta(\Lambda - \Psi H(\Gamma))H(\Gamma)\,d\Gamma}{\int(\Lambda - \Psi H(\Gamma))^{\frac{q}{1-q}}\Theta(\Lambda - \Psi H(\Gamma))\,d\Gamma}. \tag{35}$$

These integrals, and others of relevance, can be summarized in the form

$$I_m = \int\big(\Lambda - \Psi H(\Gamma)\big)^{\frac{q}{1-q}}\Theta\big(\Lambda - \Psi H(\Gamma)\big)\big(H(\Gamma)\big)^m\,d\Gamma. \tag{36}$$

For the $q$-ideal gas, $H(\Gamma) = \sum_{i=1}^N p_i^2/2m$ and the integral can be written with a change of variable as

$$I_m A = V^N S_{DN}(2m)^{ND/2}\frac{1}{2} \times \int_0^\infty(\Lambda - \Psi Y)^{\frac{q}{1-q}}\Theta(\Lambda - \Psi Y)Y^{\frac{ND}{2}-1+m}\,dY.$$

Considering the various possible combinations of signs of $\Lambda$ and $\Psi$, we find that the constraints requirements can be satisfied in two cases, giving:

$$q<1;\qquad \Lambda>0;\qquad \Psi>0,$$
$$\frac{\Lambda}{\Psi}=U\left(1+\frac{2}{(1-q)ND}\right);$$
$$\frac{I_m}{I_0}=\left(\frac{\Lambda}{\Psi}\right)^m\frac{B(\frac{1}{1-q},\frac{ND}{2}+m)}{B(\frac{1}{1-q},\frac{ND}{2})},\tag{37}$$

and

$$1<q<1+\frac{1}{\frac{ND}{2}+m-1};\qquad \Lambda>0>\Psi,$$
$$\frac{\Lambda}{|\Psi|}=U\left(\frac{2}{ND(q-1)}-1\right);$$
$$\frac{I_m}{I_0}=\left(\frac{\Lambda}{|\Psi|}\right)^m\frac{B(\frac{ND}{2}+m,-\frac{q}{1-q}-\frac{ND}{2}-m)}{B(\frac{ND}{2},-\frac{q}{1-q}-\frac{ND}{2})}.\tag{38}$$

We now consider the energy fluctuations

$$\langle H^2\rangle-\langle H\rangle^2=\frac{I_2}{I_0}-U^2.\tag{39}$$

In the first case, this gives

$$\langle H^2\rangle-\langle H\rangle^2=\left(\frac{\Lambda}{\Psi}\right)^2\frac{B(\frac{1}{1-q},\frac{ND}{2}+2)}{B(\frac{1}{1-q},\frac{ND}{2})}-U^2$$
$$=\frac{4U^2}{ND(2+(1-q)(2+ND))}\tag{40}$$

which is clearly positive for $q<1$. The second case gives

$$\langle H^2\rangle-\langle H\rangle^2=\left(\frac{\Lambda}{|\Psi|}\right)^2\frac{B(\frac{ND}{2}+2,\frac{1}{q-1}-\frac{ND}{2}-1)}{B(\frac{ND}{2},\frac{1}{q-1}-\frac{ND}{2}+1)}-U^2$$
$$=\frac{4U^2}{ND(2-(q-1)(2+ND))}\tag{41}$$

which is positive if $1<q<1+\frac{2}{ND+2}$.

When positivity is satisfied in (31), the distribution function can be written as

$$\rho_T(\Gamma)=e^{-\frac{1}{1-q}\log(\frac{1-q}{q}\frac{\alpha}{K})}\exp_q\left(-\frac{\beta(H-U)}{\mathcal{Z}_T}\right),\tag{42}$$

and the results for the $q$-ideal gas are summarized as follows:

(1) The solution to the variational problem does exist for $q<1$ and does not exist for all other values of $q$ (except in the physically narrow ($N\gg 1$) range $1<q<1+\frac{2}{ND}$) with the following ranges for $\alpha$ and $\beta$:

$$0<q<1:\quad \beta>0 \text{ and } \alpha>0,$$
$$\beta<0 \text{ and } \alpha<0:\quad \frac{|\beta|U}{\mathcal{Z}_T}>\frac{1}{1-q};$$
$$q<0:\quad \beta<0 \text{ and } \alpha>0:\quad \frac{|\beta|U}{\mathcal{Z}_T}>\frac{1}{1-q};$$
$$1<q<1+\Delta:\quad \beta>0 \text{ and } \alpha<0:\quad \frac{\beta U}{\mathcal{Z}_T}<\frac{ND}{2}+1.$$

For $q\to 1$ (with $\mathcal{Z}_T=1$ and $K=1$) the classical limit is retrieved, but for $q=0$, the distribution function $\rho_T(\Gamma)$ vanishes.

(2) The second moment only exists for $q<1$ and for $1<q<1+\frac{2}{ND+2}$, and is given by

$$\langle H^2\rangle-\langle H\rangle^2=\frac{4U^2}{ND(2+(1-q)(2+ND))}.\tag{43}$$

This expression is always positive, if $q$ is in the allowed ranges.

Inserting the explicit expression of the distribution function into the $q$-entropy, we have

$$S_q=k_B\frac{1-K\int{\rho_T}^q(\Gamma)\,d\Gamma}{q-1}$$
$$=k_B\frac{1-K\int(\Lambda-\Psi H(\Gamma))^{\frac{q}{1-q}}\Theta(\Lambda-\Psi H(\Gamma))\,d\Gamma}{q-1}.\tag{44}$$

The new quantity to be computed is the integral $\int{\rho_T}^q(\Gamma)\,d\Gamma$ which for the $q$-ideal gas, with $\Lambda,\Psi>0$,[3] reads

$$\int{\rho_T}^q(\Gamma)\,d\Gamma$$
$$=V^NS_{DN}(2m)^{ND/2}\frac{1}{2}\int_0^\infty(\Lambda-\Psi Y)^{\frac{q}{1-q}}\Theta(\Lambda-\Psi Y)Y^{\frac{ND}{2}-1}\,dY$$
$$=V^NS_{DN}(2m)^{ND/2}\frac{1}{2}\Lambda^{\frac{q}{1-q}}\left(\frac{\Lambda}{\Psi}\right)^{\frac{ND}{2}}B\left(\frac{1}{1-q},\frac{ND}{2}\right)$$
$$=V^{N(1-q)}S_{DN}^{1-q}(2m)^{ND(1-q)/2}2^{q-1}U^{\frac{ND}{2}(1-q)}$$
$$\times\left(1+\frac{2}{(1-q)ND}\right)^{\frac{ND}{2}(1-q)}\frac{B(\frac{1}{1-q},\frac{ND}{2})}{B^q(\frac{1}{1-q},\frac{ND}{2})}.\tag{45}$$

Thus,

$$S_q=k_B\frac{1-U^{\frac{ND}{2}(1-q)}R(V;q)}{q-1}\tag{46}$$

with

$$R(V;q)=V^{N(1-q)}S_{DN}^{1-q}(2m)^{ND(1-q)/2}2^{q-1}$$
$$\times\left(1+\frac{2}{(1-q)ND}\right)^{\frac{ND}{2}(1-q)}$$
$$\times B^{1-q}\left(\frac{1}{1-q},\frac{ND}{2}\right),\tag{47}$$

and the temperature of the $q$-ideal gas is given by

$$\frac{1}{T_q}=\frac{\partial S_q}{\partial U}=k_BK\frac{ND}{2}U^{\frac{ND}{2}(1-q)-1}R(V;q).\tag{48}$$

In the limit $q\to 1$

$$\frac{\partial S_{q\to 1}}{\partial U}=k_B\frac{ND}{2}\frac{1}{U}R(V;q\to 1)=k_B\frac{ND}{2}\frac{1}{U},\tag{49}$$

and with $U=\frac{ND}{2\beta}$ for the ideal gas, we retrieve the classical thermodynamic expression $\frac{1}{T}=\frac{\partial S}{\partial U}$.

According to the thermodynamic expression $C_V=\frac{\partial U}{\partial T}$, the specific heat of the $q$-ideal gas as obtained from the Tsallis entropy then reads

$$C_V^q=\frac{ND}{2}k_BKR(V;q)\frac{U^{(1-q)\frac{ND}{2}}}{1-(1-q)\frac{ND}{2}}.\tag{50}$$

Clearly, in the limit $q\to 1$, this gives the classical expression $C_V=\frac{ND}{2}k_B$. However in the normalization validity range, the denominator in $C_V^q$ is *negative* for $q<1$.

[3] We do not show the case $1<q<1+\frac{2}{ND+2}$ which reduces to the classical result ($q=1$) in the thermodynamic limit.

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