



Thermodynamic consistency of the q -deformed Fermi–Dirac distribution in nonextensive thermostatistics

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ABSTRACT

The q -deformed statistics for fermions arising within the nonextensive thermostatistical formalism has been applied to the study of various quantum many-body systems recently. The aim of the present note is to point out some subtle difficulties presented by this approach in connection with the problem of thermodynamic consistency. Different possible ways to apply the q -deformed quantum distributions in a thermodynamically consistent way are considered.

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The q -deformed quantum distributions [1–10] inspired on the nonextensive thermostatistical formalism [11–13] have been the focus of considerable attention in recent years (see [14–19] and references therein). An interesting recent development along these lines was the formulation by Pereira, Silva, and Alcaniz (PSA) of a q -deformed equation of state for relativistic nuclear matter within Walecka's phenomenological relativistic approach [16]. The PSA equation of state may be relevant for the study of nuclear matter in neutron stars. Strictly speaking, however, the PSA equation of state as derived in [16] is not thermodynamically consistent. Here we will consider possible solutions to this difficulty. As we are going to demonstrate, the PSA approach can be implemented in a thermodynamically consistent way either by adopting a q -nonlinear form for thermodynamical quantities like the total energy E or the total number of particles N that in the standard thermostatistical formalism are linear functions of the (mean) occupation numbers or, alternatively, by recourse to a different choice of the entropy functional. This last procedure can, in turn, be implemented in two different ways. One possible re-definition of the entropy, accounting for the relevant equations of constraint, yields the same quantum distribution functions as solutions of the entropic variational principle as the one employed by PSA, and it preserves thermodynamic consistency.

Consider the q -deformed Fermi–Dirac distribution used by PSA which has the form

$$\begin{aligned} \bar{n}_i &= \frac{1}{1 + [1 + (\tilde{q} - 1)(\alpha + \beta\epsilon_i)]^{\frac{1}{\tilde{q}-1}}} \\ &= \frac{1}{1 + [1 + (\tilde{q} - 1)\beta(\epsilon_i - \mu)]^{\frac{1}{\tilde{q}-1}}}, \end{aligned} \quad (1)$$

where ϵ_i are the single particle energies, $\beta = 1/kT$ (T being the absolute temperature and k denoting Boltzmann's constant), $\mu = -\frac{\alpha}{\beta}$ is the chemical potential, and

$$\tilde{q} = \begin{cases} q & \text{if } \alpha + \beta\epsilon_i > 0, \\ 2 - q & \text{if } \alpha + \beta\epsilon_i \leq 0. \end{cases} \quad (2)$$

The physical and mathematical motivations for the prescription (2) are the same as those behind the celebrated Tsallis' cut-off condition, viz., to avoid unphysical negative values of the argument of the power function appearing in the distribution (1). It must be emphasized that Tsallis' cut-off condition, even if leading to thermodynamically consistent maximum entropy distributions, is not uniquely determined by the entropic variational principle itself. Other prescriptions are in principle possible. The one given by Eq. (2) has been analysed in detail in [20] and leads to a q -deformed Fermi distribution that has already been found useful for the description of various important physical systems [15,16,18,19].

As shown in [20], the Fermi mean occupation numbers (1) can be obtained from a maximum entropy principle based on the entropic measure

$$S_q^{(F)} = \sum_i C_q(\bar{n}_i), \quad (3)$$

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where the function $C_q(x)$ is defined by

$$C_q(x) = \begin{cases} \frac{x-x^q}{q-1} + \frac{(1-x)-(1-x)^q}{q-1} & \text{if } x \leq \frac{1}{2}, \\ \frac{x-x^{2-q}}{1-q} + \frac{(1-x)-(1-x)^{2-q}}{1-q} & \text{if } x > \frac{1}{2}, \end{cases} \quad (4)$$

and it is assumed that $q \geq 1$. The optimization of the entropic measure (3) under appropriate constraints corresponding to the total number of particles N and the total energy E leads to the variational problem

$$\delta \left\{ \frac{1}{k} S_q^{(F)}[\bar{n}] + \alpha \left(N - \sum_i \bar{n}_i^q \right) + \beta \left(E - \sum_i \epsilon_i \bar{n}_i^q \right) \right\} = 0, \quad (5)$$

where α and β denote the Lagrange multipliers associated, respectively, with the aforementioned two constraints. The solution of Eq. (5) is given by the q -deformed Fermi distribution (1). In the limit case $q \rightarrow 1$, the entropic functional (3) reduces to the well-known Fermi functional

$$S = - \sum_i [\bar{n}_i \ln \bar{n}_i + (1 - \bar{n}_i) \ln(1 - \bar{n}_i)], \quad (6)$$

and the q -distribution (1) reduces to the standard Fermi distribution.

Now, the most fundamental requirement of a thermostatistical formalism is thermodynamical consistency. That is, the formalism must comply with the standard thermodynamical relationships among thermodynamical variables such as entropy, energy, temperature, etc. For instance, one requires the well-known relationship

$$\left(\frac{\partial S}{\partial E} \right)_{V,N} = \frac{1}{T}, \quad (7)$$

between the entropy, the energy, and the temperature of a thermodynamical system at equilibrium to be satisfied. It can be shown (see [20,21] and references therein for details) that any thermostatistical formalism constructed on the basis of the constrained externalization of an entropic functional (that is, following Jayne's maximum entropy prescription) complies with the thermodynamical relationships (which, in the context of Jayne's' maxent formulation are usually referred to as Jayne's' relationships). To obtain a thermodynamically consistent formulation one has to make the appropriate identifications between relevant constraints and extensive thermodynamical quantities, on the one hand, and between the corresponding Lagrange multipliers and appropriate intensive thermodynamical quantities, on the other one. In the case of the formalism based upon the entropic variational principle (5) the appropriate identifications are

$$\begin{aligned} \sum_i \bar{n}_i^q &\rightarrow N, \\ \sum_i \bar{n}_i^q \epsilon_i &\rightarrow E, \end{aligned} \quad (8)$$

and

$$\begin{aligned} \beta &\rightarrow 1/kT, \\ -\alpha/\beta &\rightarrow \mu. \end{aligned} \quad (9)$$

The functional (3), of course, is to be identified with the entropy of the system. It is plain from (8) that, in order to compute physical quantities in a thermodynamically consistent way, one must not use directly the particle distribution given by Eq. (1) (as is done in [16], see Eqs. (17)–(20) in [16]) but, instead, use the effective particle distribution

$$\bar{n}_i^q = (1 + [1 + (\tilde{q} - 1)\beta(\epsilon_i - \mu)]^{\frac{1}{\tilde{q}-1}})^{-q}, \quad (10)$$

with \tilde{q} defined as in (2). For instance, if the energy of an ideal Fermi gas is to comply with the basic thermodynamical relationship (7), it has to be computed (according to (8)) as

$$E = \sum_i \epsilon_i (1 + [1 + (\tilde{q} - 1)\beta(\epsilon_i - \mu)]^{\frac{1}{\tilde{q}-1}})^{-q}. \quad (11)$$

It must be stressed that making the identification (8) does not imply any severe conceptual difficulty, since the \bar{n}_i are not probabilities and, consequently, are not normalized to unity (see [22] for a similar situation arising in connection with the q -generalization of the classical Boltzmann distribution). In fact, it is possible to reformulate the variational principle (5) in terms of linear constraints, by recourse to an appropriate re-definition of the entropic functional. Indeed, if one introduces the new entropy,

$$\tilde{S}_q^{(F)} = \sum_i C_q(\bar{n}_i^{1/q}), \quad (12)$$

with the function C_q still defined as in (4), then the variational principle

$$\delta \left\{ \frac{1}{k} \tilde{S}_q^{(F)}[\bar{n}] + \alpha \left(N - \sum_i \bar{n}_i \right) + \beta \left(E - \sum_i \epsilon_i \bar{n}_i \right) \right\} = 0, \quad (13)$$

is equivalent to the variational principle (5). The solution to this variational problem is given by the mean occupation numbers

$$\bar{n}_i = (1 + [1 + (\tilde{q} - 1)\beta(\epsilon_i - \mu)]^{\frac{1}{\tilde{q}-1}})^{-q}, \quad (14)$$

which are given by the same expression as the one given in (10). The thermodynamical quantities N and E are now expressed in terms of the mean occupation numbers (14) using the standard linear forms.

There is another possible modification of the maxent variational problem that can be implemented in order to recover thermodynamical consistency. One can redefine the entropy functional to be

$$S_q^* = S_q + \alpha_1 \sum_i (\bar{n}_i - \bar{n}_i^q) + \beta_1 \sum_i \epsilon_i (\bar{n}_i - \bar{n}_i^q). \quad (15)$$

In this case the variation of the entropy functional with the standard constraints $N = \sum_i \bar{n}_i$ and $E = \sum_i \epsilon_i \bar{n}_i$ is given by

$$\delta \left\{ S_q^* + \left(N - \alpha \sum_i \bar{n}_i \right) + \left(E - \beta \sum_i \epsilon_i \bar{n}_i \right) \right\} = 0, \quad (16)$$

where α_1 and β_1 are constants as q to be determined. Now if the following choices, $\alpha_1 = \alpha$ and $\beta_1 = \beta$ are made, the solution to the variational problem given in Eq. (16) is formally given by Eq. (1) where α and β are now determined by the standard equations of constraint since both variational equations, (5) and (16), are equivalent.

However, in order for this to be a useful result, it is essential that thermodynamic consistency is also preserved. In order to verify this it is necessary to evaluate $(\frac{\partial S_q^*}{\partial E})_{V,N}$. This can be done in the following manner,

$$\begin{aligned} \left(\frac{\partial S_q^*}{\partial E} \right)_{V,N} &= \left(\frac{\partial S_q^*}{\partial \bar{n}_i^*} \right)_{V,N} / \left(\frac{\partial E}{\partial \bar{n}_i^*} \right)_{V,N} \\ &= \frac{q \bar{n}_i^{q-1}}{\epsilon_i} \left[\beta \epsilon_i + \beta \epsilon_i \left(\frac{1}{q \bar{n}_i^{q-1}} - 1 \right) \right] \\ &= \beta \end{aligned} \quad (17)$$

as required.

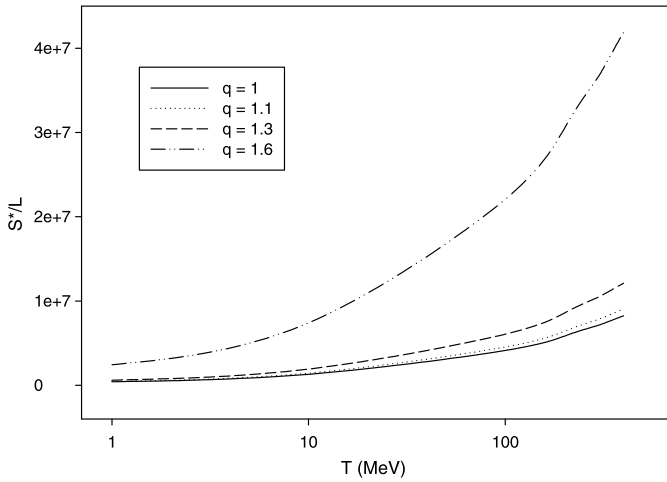


Fig. 1. S^*/L for $m = 1$ MeV and $\delta = 10^9$ MeV.

Thermodynamic consistency is therefore preserved when the following identifications are made

$$\begin{aligned} \sum_i \bar{n}_i &\rightarrow N, \\ \sum_i \bar{n}_i \epsilon_i &\rightarrow E, \end{aligned} \tag{18}$$

and

$$\begin{aligned} \beta &\rightarrow 1/kT, \\ -\alpha/\beta &\rightarrow \mu. \end{aligned} \tag{19}$$

It should also be noted that in the limit $q \rightarrow 1$, the last two terms in (15) cancel and it again reduces to (6). Requiring $S_q^* \rightarrow 0$ in the limit $T \rightarrow 0$ places the restriction $q < 2$.

To illustrate the behavior of this redefined entropy functional, consider the toy model of a one-dimensional Fermi gas. In this case the entropy density (entropy per unit length) can be calculated from

$$\frac{S^*}{L} = \int_0^\delta [C_q(\bar{n}) + (\epsilon - \mu)\beta(\bar{n} - \bar{n}^q)]g(\epsilon) d\epsilon \tag{20}$$

where δ is a high energy cutoff introduced for numerical purposes, and $g(\epsilon)d\epsilon = \frac{\sqrt{2m}}{\pi\hbar} \frac{1}{\sqrt{\epsilon}} d\epsilon$ is the one-dimensional density of states per unit length. For $m = 1$ MeV and $\delta = 10^9$ MeV, Fig. 1 shows S^*/L for various values of q . The entropy density increases at a given temperature for increasing values of q but remains a strictly convex function. Thus, this redefinition introduces no additional structure into the entropy density.

Similar results can be obtained for quantum systems given in terms of Bose–Einstein distributions. It is also interesting to note that analogous results can easily be obtained for a q -deformed classical entropy functional. Indeed, for the entropic measure

$$S_q^{(Classical)} = \sum_i C_q^{(Classical)}(\bar{\rho}_i), \tag{21}$$

where the function $C_q^{(Classical)}(x)$ is defined by

$$C_q^{(Classical)}(x) = \begin{cases} \frac{x-x^q}{q-1} & \text{if } x \leq 1, \\ \frac{x-x^{2-q}}{1-q} & \text{if } x > 1, \end{cases} \tag{22}$$

the variational principle

$$\delta \left\{ \frac{1}{k} S_q^{(Classical)}[\bar{\rho}] + \alpha \left(N - \sum_i \bar{\rho}_i^q \right) + \beta \left(E - \sum_i \epsilon_i \bar{\rho}_i^q \right) \right\} = 0, \tag{23}$$

yields a q -deformed generalization of the classical Maxwell–Boltzmann distribution,

$$\bar{\rho}_i = [1 + (\tilde{q} - 1)(\epsilon_i - \mu)\beta]^{-\frac{1}{\tilde{q}}}, \tag{24}$$

where \tilde{q} is again given by (2). The distribution (24) has the same form as the well-known Tsallis distribution, except for the fact that Tsallis’ cut-off condition is now replaced by the prescription (2). Notice, however, that the $\bar{\rho}_i$ in (24) are occupation numbers and not probabilities and, consequently, are not normalized to 1. In order for the distribution (24) to be normalizable at all, the single particle energy values ϵ_i must be bounded from below. Clearly, this distribution can also be obtained using standard linear constraints by redefining the entropy functional as in (15).

Alternatively, as in (12), one can also choose

$$\tilde{S}_q^{(Classical)} = \sum_i C_q^{(Classical)}(\bar{\rho}_i^{1/q}). \tag{25}$$

In this case the variation

$$\delta \left\{ \frac{1}{k} \tilde{S}_q^{(Classical)}[\bar{\rho}] + \alpha \left(N - \sum_i \bar{\rho}_i \right) + \beta \left(E - \sum_i \epsilon_i \bar{\rho}_i \right) \right\} = 0, \tag{26}$$

yields the distribution

$$\bar{\rho}_i = [1 + (\tilde{q} - 1)(\epsilon_i - \mu)\beta]^{-\frac{q}{\tilde{q}}}, \tag{27}$$

which is analogous to (14).

In the present work we have considered the q -deformed quantum entropy functional given in terms of Fermi–Dirac distribution functions. Modifying the entropy functional admits the possibility of using standard linear constraints such that thermodynamic consistency is preserved. Techniques similar to those developed by Hasegawa [23] can then be used to obtain exact as well as good approximate numerical solutions for q -generalized quantum systems.

Summing up, our main conclusions are the following.

- First, a straightforward application of the variational principle (5) is not consistent, from the thermodynamical point of view, with the use of the standard identifications $N \rightarrow \sum_i \bar{n}_i$ and $E \rightarrow \sum_i \epsilon_i \bar{n}_i$ for the total number of particles and the total energy, respectively (a similar problem occurs with other thermodynamical quantities that in the standard thermostistical formalism are expressed as linear functions of the mean occupation numbers).
- Thermodynamic consistency can be recovered by using the identifications $N \rightarrow \sum_i \bar{n}_i^q$ and $E \rightarrow \sum_i \epsilon_i \bar{n}_i^q$. This approach does not lead to serious conceptual problems, because the mean occupation numbers are not probabilities and are not normalized to one.
- Alternatively, thermodynamic consistency can be recovered by appropriately redefining the entropy functional. In the present work we have considered two alternative ways of implementing this last procedure.

Thermodynamical consistency is certainly a strong and fundamental constraint in the development of extended or generalized thermostistical formalisms of physical significance. However, in the case of the q -deformed Fermi–Dirac statistics, this requirement alone does not determine unequivocally a unique nonextensive

generalization of the standard statistics for fermions. As we have pointed out, there are several ways to implement a thermostatical formalisms for the q -deformed Fermi–Dirac distribution in a thermodynamically consistent way. Only when more experimental data is available, and more applications to concrete quantum many-body systems are investigated, will one definitively be able to ascertain which choices of the concomitant entropy functional and constraints should be used and under which circumstances. Any further developments along this lines will be very welcome.

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