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# $q$ -thermostatistics and the analytical treatment of the ideal Fermi gas

S. Martínez\*, F. Pennini, A. Plastino, M. Portesi

*Instituto de Física La Plata, Universidad Nacional de La Plata and CONICET, C.C. 727, 1900 La Plata, Argentina*

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## Abstract

We discuss relevant aspects of the exact  $q$ -thermostatistical treatment for an ideal Fermi system. The grand-canonical exact generalized partition function is given for arbitrary values of the non-extensivity index  $q$ , and the ensuing statistics is derived. Special attention is paid to the mean occupation numbers of single-particle levels. Limiting instances of interest are discussed in some detail, namely, the thermodynamic limit, considering in particular both the high- and low-temperature regimes, and the approximate results pertaining to the case  $q \sim 1$  (the conventional Fermi–Dirac statistics corresponds to  $q = 1$ ). We compare our findings with previous Tsallis’ literature. © 2003 Elsevier B.V. All rights reserved.

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## 1. Introduction

Nonextensive thermostatistics<sup>1</sup> [1–5] constitutes a new paradigm for statistical mechanics. It is based on Tsallis’ nonextensive information measure [6]

$$S_q = k_B \frac{1 - \sum p_n^q}{q - 1}, \quad (1)$$

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\* Corresponding author.

*E-mail addresses:* [martinez@fisica.unlp.edu.ar](mailto:martinez@fisica.unlp.edu.ar) (S. Martínez), [pennini@fisica.unlp.edu.ar](mailto:pennini@fisica.unlp.edu.ar) (F. Pennini), [plastino@fisica.unlp.edu.ar](mailto:plastino@fisica.unlp.edu.ar) (A. Plastino), [portesi@fisica.unlp.edu.ar](mailto:portesi@fisica.unlp.edu.ar) (M. Portesi).

<sup>1</sup> A periodically updated bibliography on nonextensive thermostatistics can be found in the URL <http://tsallis.cat.cbpf.br/biblio.htm>.

where  $\{p_n\}$  is a set of normalized probabilities and  $k_B$  stands for Boltzmann constant ( $k_B = 1$  hereafter). The real parameter  $q$  is called the index of nonextensivity, the conventional Boltzmann–Gibbs statistics being recovered in the limit  $q \rightarrow 1$ .

The new theory comes in several flavors, though. Within the literature on Tsallis’ thermostatics, three possible choices are considered for the evaluation of expectation values in a nonextensive scenario. As a set of (nonextensive) expectation values are always regarded as constraints in the associated  $q$ -MaxEnt approach [7], three different generalized probability distributions ensue. Let  $p_n$  ( $n = 1, \dots, W$ ) stand for the microscopic probability that a system is in the  $n$ th microstate, and consider the (classical) physical quantity  $O$  that in the microstate  $n$  adopts the value  $o_n$ . The first choice [6] for the expectation value of  $O$ , used by Tsallis in his seminal paper, was the conventional one:  $\sum_{n=1}^W p_n o_n$ . The second choice [8],  $\sum_{n=1}^W p_n^q o_n$ , was regarded as the canonical definition until quite recently and is the only one that is guaranteed to yield, always, an analytical solution to the associated MaxEnt variational problem [9]; notice, however, that the average value of the identity operator is not equal to one. Elaborate studies of the so-called  $q$ -Fermi gas problem, which will constitute the focus of our attention here, have been performed using this “Curado–Tsallis flavor” [10–14]. Nowadays most authors consider that the third choice [5,15], usually denoted as the Tsallis–Mendes–Plastino (TMP) one,

$$\langle O \rangle_q \equiv \frac{\sum_{n=1}^W p_n^q o_n}{\sum_{n'=1}^W p_{n'}^q} \tag{2}$$

is the most appropriate definition.

We employ the latter choice in order to accommodate the available a priori information and thus obtain the pertinent probability distribution via Jaynes’ MaxEnt approach [16,17], extremizing the  $q$ -entropy  $S_q$  subject to normalization ( $\sum_{n=1}^W p_n = 1$ ) and prior knowledge of a set of  $M$  nonextensive expectation values  $\{\langle O_j \rangle_q, j = 1, \dots, M\}$ . As usual the constrained extremization is accomplished by introducing  $M + 1$  Lagrange multipliers; in practice two (equivalent) procedures can be followed to do this. First, the variational procedure followed by Tsallis et al. in Ref. [15] gives the Tsallis’ probability distribution in the form

$$p_n = \frac{f_n^{1/(1-q)}}{\bar{Z}_q}, \tag{3}$$

where [15]

$$f_n = 1 - \frac{(1-q) \sum_{j=1}^M \lambda_j^{(TMP)} (o_{j,n} - \langle O_j \rangle_q)}{\sum_{n'=1}^W p_{n'}^q} \tag{4}$$

is the so-called configurational characteristic, and  $\bar{Z}_q = \sum_n f_n^{1/(1-q)}$  represents a “pseudo” partition function (in the limit  $q \rightarrow 1$  it goes to  $Z_1 e^{\sum_{j=1}^M \lambda_j \langle O_j \rangle}$  instead of  $Z_1$ ).  $f_n$  should be positive (otherwise  $f_n \equiv 0$ ) in order to guarantee that probability  $p_n$  be real for arbitrary  $q$  (Tsallis’ cutoff condition [7,18]); as a consequence, the sum in  $\bar{Z}_q$  is restricted to those states for which  $f_n$  is positive.

Notice that the expression obtained for  $p_n$  following the TMP recipe is *explicitly self-referential*. This fact often leads to numerical difficulties in concrete applications

(see, for instance, Ref. [19]); more important, it obscures the underlying physics because the concomitant Lagrange multipliers lose their traditional physical meaning [20]. Martínez et al. [21] devised a way to circumvent these problems by recourse to the introduction of new, putatively *optimal* Lagrange multipliers (OLM) for the Tsallis' variational problem. The idea is to extremize the  $q$ -entropy with centered mean values (a legitimate alternative procedure) which entails recasting the constraints in the fashion

$$\sum_{n=1}^W p_n^q (o_{j_n} - \langle O_j \rangle_q) = 0, \quad j = 1, \dots, M. \quad (5)$$

The ensuing microscopic probabilities are formally given by Eq. (3), where now

$$f_n = 1 - (1 - q) \sum_{j=1}^M \lambda_j (o_{j_n} - \langle O_j \rangle_q). \quad (6)$$

In this way, the configurational characteristic obtained with the OLM recipe *does not depend explicitly on the set of probabilities*  $\{p_n\}$ .

It is obvious that the solution of a constrained extremizing problem via the celebrated Lagrange method depends exclusively on the functional form one is dealing with as well as on the constraints, the Lagrange multipliers being just auxiliary quantities to be eliminated at the end of the process. As a consequence, TMP and OLM results should coincide. However their *manipulation* is, in the latter instance, considerably simpler (notice that the OLM variational procedure [21–26] solves *directly* for the optimized Lagrange multipliers). Comparing then the TMP and OLM approaches for a given problem, one realizes that the resultant probabilities (as well as the pseudo partition functions) are identical if

$$\lambda_j = \frac{\lambda_j^{(TMP)}}{\sum_{n=1}^W p_n^q} = \bar{Z}_q^{q-1} \lambda_j^{(TMP)}, \quad j = 1, \dots, M, \quad (7)$$

where use has been made of the relation  $\sum_n p_n^q = \bar{Z}_q^{1-q}$  [15,21] which is valid under the assumption of the knowledge available a priori.

For the sake of completeness, let us write down [25] the set of equations that constitute the basic information-theory relations in Jaynes' version of statistical mechanics [16,17]:

$$\frac{\partial}{\partial \langle O_j \rangle_q} (\ln \bar{Z}_q) = \lambda_j, \quad (8)$$

$$\frac{\partial}{\partial \lambda_j} (\ln Z_q) = -\langle O_j \rangle_q \quad (9)$$

for  $j = 1, \dots, M$ . Here the partition function  $Z_q$  is defined by [21]  $\ln Z_q \equiv \ln \bar{Z}_q - \sum_{j=1}^M \lambda_j \langle O_j \rangle_q$ . While the above OLM equations involve ordinary logarithms, the analogous TMP relations [15] employ the so-called  $q$ -logarithms,  $\ln_q x \equiv (1 - x^{1-q})/(q-1)$ ; thus in the latter case, the basic Jaynes' relations are not recovered and the physical sense becomes somewhat obscured.

### 1.1. Our goal

Motivated by the success of the OLM procedure, and in view of some recent and quite interesting applications of the quantum distributions (see, for instance, Ref. [27] for anomalous behaviors in thermodynamic quantities for ideal Fermi gases below two dimensions), we wish to address here with such a technique the noninteracting Fermi–Dirac (FD) gas. The Tsallis generalized treatment of such a system was originally advanced in Ref. [10] using the Curado–Tsallis flavor. Büyükkılıç et al. further investigated [11] the generalized distribution functions employing an approximation to deal with nonextensive quantum statistics called the factorization approach (FA). This approach, which turns out to give approximate results in the region  $q \sim 1$ , is valid for a dilute gas (i) ignoring the correlations between particles and (ii) regarding the states of different particles as statistically independent. Most succeeding works on the nonextensive treatment of quantum systems are based on these approximate generalized distribution functions. The nonextensive fermion distribution was further analyzed in Ref. [13] in the context, again, of the second choice, but without recourse to that sort of approximations. It was seen there that the FA faces some difficulties. Other interesting studies on the subject have been presented by Ubriaco [12] and, quite recently, by Aragão-Rêgo et al. [28], employing the third-choice expectation values along the TMP lines. The latter work focuses attention upon the thermodynamic limit and provides elegant analytical results.

The Fermi gas problem is rather cumbersome to treat using the TMP algorithm. We will show here that the OLM approach allows for an exact treatment of Fermi distributions in a nonextensive scenario, in a simpler way. This, in turn, will make it possible to re-discuss the nature of the approximation scheme of Büyükkılıç et al. The paper is organized as follows: in Section 2 we sketch the quantum version of the OLM technique. Section 3 is devoted specifically to the grand-canonical description of quantum gases in a nonextensive framework. Our main results concerning Fermi systems are developed in Section 4, where a careful study of the mean occupancy of discrete single-particle (s.p.) levels is given. Next we present approximate results for values of  $q$  close to unity, and compare them with previous works on the subject. The thermodynamic limit is addressed in Section 6, by appealing to integral transform methods that are summarized in the appendix. Finally, some conclusions are drawn.

## 2. The OLM procedure in quantum language

Since we are going to address the ideal Fermi gas, we have to adapt our nonextensive OLM–Tsallis statistical language to a quantal environment. Our main tool will be the equilibrium density operator  $\hat{\rho}$ , that can be obtained by recourse to the Lagrange multipliers’ method. Within the nonextensive framework one has to extremize the information measure [1,2,6]

$$S_q[\hat{\rho}] = \frac{1 - \text{Tr}(\hat{\rho}^q)}{q - 1} \quad (10)$$

subject to the normalization requirement and the assumed a priori knowledge of the generalized expectation values of, say  $M$ , relevant observables, namely

$$\langle \hat{O}_j \rangle_q = \frac{Tr(\hat{\rho}^q \hat{O}_j)}{Tr(\hat{\rho}^q)}, \quad j = 1, \dots, M. \tag{11}$$

In the quantum version of the OLM instance the constraints are recast in the manner

$$Tr(\hat{\rho}) = 1, \tag{12}$$

$$Tr[\hat{\rho}^q(\hat{O}_j - \langle \hat{O}_j \rangle_q)] = 0, \quad j = 1, \dots, M, \tag{13}$$

where the  $q$ -expectation values  $\{\langle \hat{O}_1 \rangle_q, \dots, \langle \hat{O}_M \rangle_q\}$  constitute the external a priori information. Performing the constrained extremization of Tsallis entropy one obtains [21]

$$\hat{\rho} = \frac{\hat{f}_q^{1/(1-q)}}{\bar{Z}_q}, \tag{14}$$

where the quantal configurational characteristic has the form

$$\hat{f}_q = \hat{\mathbb{1}} - (1 - q) \sum_{j=1}^M \lambda_j \delta_q \hat{O}_j \tag{15}$$

if the quantity in the right-hand side (r.h.s.) is positive definite, otherwise  $\hat{f}_q = 0$  (cutoff condition [15,18]). Here  $\{\lambda_1, \dots, \lambda_M\}$  stands for the set of optimal Lagrange multipliers, and we have defined for brevity the generalized deviation as  $\delta_q \hat{O} \equiv \hat{O} - \langle \hat{O} \rangle_q$ . The normalizing factor in Eq. (14) corresponds to the OLM generalized partition function which is given, in analogy with the classical situation, by [21–26]

$$\bar{Z}_q = Tr(\hat{f}_q^{1/(1-q)}) = Tr \left[ e_q \left( - \sum_{j=1}^M \lambda_j \delta_q \hat{O}_j \right) \right], \tag{16}$$

where the trace evaluation is to be performed with due caution in order to account for Tsallis' cutoff, and

$$e_q(x) \equiv [1 + (1 - q)x]^{1/(1-q)} \tag{17}$$

is a generalization of the exponential function, which is recovered when  $q \rightarrow 1$ . Let us remark that the density operator à la OLM is not self-referential.

It is to be pointed out that within the TMP framework one obtains from the normalization condition on the equilibrium density operator  $\hat{\rho}$  the following relation that the OLM approach inherits [15,21–26], namely,

$$Tr[\hat{f}_q^{1/(1-q)}] = Tr[\hat{f}_q^{q/(1-q)}]. \tag{18}$$

Making use of this relation, one can obtain the value of the extremized  $q$ -entropy as

$$S_q = \ln_q(\bar{Z}_q). \tag{19}$$

For the sake of completeness, we can write down the generalized mean value of a quantum operator  $\hat{O}$  in terms of the quantal configurational characteristic as

$$\langle \hat{O} \rangle_q = \frac{\text{Tr}[\hat{f}_q^{q/(1-q)} \hat{O}]}{\text{Tr}[\hat{f}_q^{q/(1-q)}]} . \tag{20}$$

We recapitulate in the appendix how to employ a quite useful method for calculating the generalized partition function and expectation values of relevant operators, by recourse to suitable integral representations. The procedure, which is based on the definition of the Euler gamma function, has been used in the literature by many authors [22,23,26,28–32] as it enables to express  $q$ -generalized quantities in terms of the conventional ( $q = 1$ ) ones, thus providing an alternative analytic approach.

### 3. Quantum gas in a generalized grand canonical ensemble

It is our aim here that of developing formally the statistical description of quantum systems, particularly fermions, in a generalized framework. For this purpose, we will make use of the OLM–Tsallis version of nonextensive statistics. The Hamiltonian of the system is assumed to be of the form

$$\hat{H} = \sum_k \varepsilon_k \hat{n}_k$$

while the number operator exhibits the appearance  $\hat{N} = \sum_k \hat{n}_k$ , where  $\varepsilon_k$  and  $\hat{n}_k$  denote, respectively, the energy and occupation number operator of the  $k$ th s.p. level for a discrete-energy spectrum, with  $\varepsilon_1 < \varepsilon_2 < \dots$ .

Following a grand-canonical-ensemble description, the configurational characteristic is given by

$$\hat{f}_q = \hat{\mathbb{1}} - (1 - q)\beta(\hat{H} - U_q) - (1 - q)\alpha(\hat{N} - N_q) , \tag{21}$$

where the Lagrange multipliers  $\beta$  and  $\alpha \equiv -\beta\mu$  are related to the temperature and chemical potential  $\mu$  of the system, respectively, and we have designated the generalized mean values of  $\hat{H}$  and  $\hat{N}$  by  $U_q$  and  $N_q$ , respectively. The OLM-generalized grand partition function for this ideal quantum gas is obtained by inserting the last expression into Eq. (16).

In order to simplify the notation we now define  $\varepsilon_k^* \equiv \varepsilon_k - \mu$  and the Legendre transform (“free energy”)  $\hat{H}^* \equiv \hat{H} - \mu\hat{N} = \sum_k \varepsilon_k^* \hat{n}_k$ . The quantities whose mean value is assumedly known, i.e., the internal energy and the particle number, are then combined in the fashion

$$\langle \hat{H}^* \rangle_q = U_q - \mu N_q \equiv U_q^* . \tag{22}$$

This notation allows one to treat the grand-canonical ensemble as if it were the canonical one, but with grand-canonical traces. In terms of the new (“star”) quantities, the configurational characteristic reads

$$\hat{f}_q = \hat{\mathbb{1}} - (1 - q)\beta(\hat{H}^* - U_q^*) \equiv \frac{\beta}{\beta_q} \hat{g}_q , \tag{23}$$

where

$$\beta_q = \frac{\beta}{1 + (1 - q)\beta U_q^*} \tag{24}$$

and

$$\hat{g}_q = \hat{\mathbb{1}} - (1 - q)\beta_q \hat{H}^* \tag{25}$$

are auxiliary quantities. (It will be seen below that  $\beta_q$  corresponds to the inverse temperature, while  $\hat{g}_q$  to the configurational characteristic, in a Curado–Tsallis treatment [10–14].)

Our partition function can therefore be written as

$$\bar{Z}_q = \left(\frac{\beta}{\beta_q}\right)^{1/(1-q)} Tr(\hat{g}_q^{1/(1-q)}) = e_q(\beta U_q^*) Tr[e_q(-\beta_q \hat{H}^*)], \tag{26}$$

where the last expression resembles the form of this function in conventional, orthodox  $q=1$  statistics. Once again, evaluation of the trace involves the cutoff restriction which now reads:  $(\beta/\beta_q)\hat{g}_q$  should be positive definite. From Eqs. (20) and (23), the scalar quantity  $U_q^*$  becomes

$$U_q^* = \frac{Tr(\hat{g}_q^{q/(1-q)} \hat{H}^*)}{Tr(\hat{g}_q^{q/(1-q)})}. \tag{27}$$

Similar expressions hold for  $U_q$  and  $N_q$  separately, employing the corresponding operator inside the pertinent (upper) trace. A comparison of these generalized mean values with the concomitant Curado–Tsallis results [10–14] allows for the identification of the auxiliary quantity  $\beta_q$  with the inverse temperature defined in the unnormalized context.

The generalized heat capacity is defined as

$$C_{Vq} \equiv \left. \frac{\partial U_q}{\partial T} \right|_{N_q, V} = -\beta^2 \left. \frac{\partial U_q}{\partial \beta} \right|_{N_q, V}, \tag{28}$$

that, after a little algebra can be expressed as

$$C_{Vq} = \frac{1}{1 - q} \times \frac{q\beta_q[\langle \hat{g}_q^{-1} \delta_q \hat{H} \rangle_q - \langle \hat{g}_q^{-1} \delta_q \hat{H} \delta_q \hat{N} \rangle_q \langle \hat{g}_q^{-1} \delta_q \hat{N} \rangle_q / \langle \hat{g}_q^{-1} (\delta_q \hat{N})^2 \rangle_q]}{1 - q\beta_q[\langle \hat{g}_q^{-1} \delta_q \hat{H} \rangle_q - \langle \hat{g}_q^{-1} \delta_q \hat{H} \delta_q \hat{N} \rangle_q \langle \hat{g}_q^{-1} \delta_q \hat{N} \rangle_q / \langle \hat{g}_q^{-1} (\delta_q \hat{N})^2 \rangle_q]}. \tag{29}$$

#### 4. Ideal Fermi gas results

In this section, we present our fundamental results related to the nonextensive description of fermion systems, emphasizing the consequences of dealing with a discrete s.p. energy spectrum. We start by reminding that in the conventional statistical treatment of an ideal FD gas, the grand partition function reads [33,34]

$$Z_1 = Tr(e^{-\beta \hat{H}^*}) = \sum_{N=0}^{\infty} \sum'_{\{n_k\}} e^{-\beta \sum_k \varepsilon_k^* n_k}, \tag{30}$$

where the  $n_k$ 's take just two values (0 or 1) and the primed summation means that they add up to  $N$ . This fermionic partition function can be expanded as

$$Z_1 = 1 + \sum_{N=1}^{\infty} \sum_{k_1 < \dots < k_N=1}^{\infty} e^{-\beta \sum_{i=1}^N \varepsilon_{k_i}^*} \tag{31}$$

in a form that, on the one hand, emphasizes the contribution of each possible value of  $N$  and, on the other, illustrates the manner of performing the trace operation. Note that, if the number of s.p. levels is finite, say  $K$ , both infinite sums in Eq. (31) nicely terminate when one reaches  $k_i = K$  and  $N = K$ . This way of performing the pertinent sums, which is not the typical textbook procedure to deal with thermodynamic quantities in the case of Fermi systems, is of a general quantal (*fermionic*) character, no matter what the summands' content is. One could have, for instance

$$\text{Tr}[\varphi(-\beta \hat{H}^*)] = 1 + \sum_{N=1}^{\infty} \sum_{k_1 < \dots < k_N=1}^{\infty} \varphi\left(-\beta \sum_{i=1}^N \varepsilon_{k_i}^*\right), \tag{32}$$

involving an arbitrary analytical function  $\varphi$ . If  $\varphi$  is a generalized  $q$ -exponential we obtain Eq. (33) below. Indeed, in the framework of the  $q$ -thermostatistics one deals with the same sort of expansion, with a crucial difference: *one faces, instead of the trace of ordinary exponentials, the trace of  $q$ -exponentials*. Without recourse to the integral transform methods discussed in the appendix, one can easily *circumvent the main problem of the generalized Tsallis' treatment*: the fact that  $q$ -exponentials do not follow the distributive law with respect to sums over states, an important result of the present endeavor.

Using the above considerations one thus recasts the Tsallis trace in Eq. (26) in the fashion

$$\bar{Z}_q = \left(\frac{\beta}{\beta_q}\right)^{1/(1-q)} \left[ 1 + \sum_{N \geq 1} \sum_{k_1 < \dots < k_N} \left( 1 - (1-q)\beta_q \sum_{i=1}^N \varepsilon_{k_i}^* \right)^{1/(1-q)} \right], \tag{33}$$

where, however, one has to take proper account of the cutoff requirement. Let us analyze this important point with some detail.

The cutoff condition can be stated in the following manner:

$$q < 1: \quad \sum_{i=1}^N \varepsilon_{k_i}^* < \frac{1}{(1-q)\beta} + U_q^*, \tag{34}$$

$$q > 1: \quad \sum_{i=1}^N \varepsilon_{k_i}^* > \frac{1}{(1-q)\beta} + U_q^* \tag{35}$$

for every possible (ordered) configuration  $(k_1, \dots, k_N)$ , and for all  $N = 1, \dots, K$ . In other words, those configurations not fulfilling the above inequalities *do not* contribute to the trace, i.e., the concomitant configurational characteristic is set to zero. Notice that the right side of both inequalities is nothing but  $[(1-q)\beta_q]^{-1}$  and, in principle, could have positive or negative sign. Nevertheless, it can be easily seen that the requirement of positive probabilities (cutoff condition) is straightforwardly fulfilled by negative-



definite “displaced” hamiltonians (whose spectrum is  $\varepsilon_k - \mu$ ) in the case  $q < 1$  with  $U_q^* > -[(1 - q)\beta]^{-1}$ , and by positive-definite ones for  $q > 1$  with  $U_q^* < [(q - 1)\beta]^{-1}$ . In these two cases, one can be sure that *all* configurations contribute with nonzero probability; but any other situation should be handled with some care. It is interesting to notice that the same sort of conditions are found in Ref. [32] in the context of integral transform methods for the unnormalized (second flavor), canonical-ensemble problem. However, let us stress that in the present situation the analytic calculations can be fully implemented, with no other hardship than properly accounting for Tsallis cutoff as already mentioned, in summing over states in  $\bar{Z}_q$  (and other thermodynamic quantities).

Let us now introduce, for the sake of brevity, the auxiliary scalar quantity

$$g_q(k_1, \dots, k_N) = 1 - (1 - q)\beta_q \sum_{i=1}^N \varepsilon_{k_i}^* \tag{36}$$

which corresponds to the eigenvalue of the operator  $\hat{g}_q$  for the state with  $N$  occupied levels:  $n_{k_1} = \dots = n_{k_N} = 1$ , otherwise  $n_k = 0$ . In terms of these new scalars, the partition function reads

$$\bar{Z}_q = \left( \frac{\beta}{\beta_q} \right)^{1/(1-q)} \left[ 1 + \sum_{N \geq 1} \sum_{k_1 < \dots < k_N} g_q(k_1, \dots, k_N)^{1/(1-q)} \right]. \tag{37}$$

Moreover, one can obtain  $U_q^*$  from Eq. (27), evaluating the traces as exemplified with reference to  $\bar{Z}_q$ . Thus,

$$U_q^* = \frac{\sum_{N \geq 1} \sum_{k_1 < \dots < k_N} \left( \sum_{i=1}^N \varepsilon_{k_i}^* \right) g_q(k_1, \dots, k_N)^{q/(1-q)}}{1 + \sum_{N \geq 1} \sum_{k_1 < \dots < k_N} g_q(k_1, \dots, k_N)^{q/(1-q)}}. \tag{38}$$

Again,  $U_q$  and  $N_q$  will also be given by similar expressions, replacing  $\varepsilon_{k_i}^*$  by either  $\varepsilon_{k_i}$  or  $-\mu$ , respectively. One easily ascertains that  $U_q^*$  becomes  $U_1^* = U_1 - \mu N$  in the extensive limit, and  $U_1^* = -\partial \ln Z_1 / \partial \beta$ . Let us comment that in the case one wishes to determine, for instance, the dependence of the  $q$ -energy with temperature, one should *consistently* work out the above expressions in order to solve for the desired thermodynamic quantity.

We tackle finally the evaluation of the  $q$ -mean value of the occupation number operator,  $\langle \hat{n}_l \rangle_q$ . To such an effect we, again, evaluate the traces in the form indicated above and obtain an *exact expression* for the generalized fermion occupation numbers,

$$\langle \hat{n}_l \rangle_q = \frac{\sum_{N \geq 1} \sum_{k_1 < \dots < k_N} \left( \sum_{i=1}^N \delta_{lk_i} \right) g_q(k_1, \dots, k_N)^{q/(1-q)}}{1 + \sum_{N \geq 1} \sum_{k_1 < \dots < k_N} g_q(k_1, \dots, k_N)^{q/(1-q)}}. \tag{39}$$

This expression can be further worked out employing a property of the auxiliary quantities  $g_q(k_1, \dots, k_N)$ , which are not altered under a permutation of indices. Thus, we obtain

$$\langle \hat{n}_l \rangle_q = \frac{g_q(l)^{q/(1-q)} + \sum_{N \geq 2} \sum_{k_1 < \dots < k_{N-1} (k_i \neq l)} g_q(k_1, \dots, k_{N-1}, l)^{q/(1-q)}}{1 + \sum_{N \geq 1} \sum_{k_1 < \dots < k_N} g_q(k_1, \dots, k_N)^{q/(1-q)}}. \tag{40}$$

Notice that  $\langle \hat{n}_l \rangle_q$  depends on the generalized internal energy  $U_q^*$  through  $\beta_q$ .

### 5. Approximate results for $q \sim 1$ : comparison with previous work

Since the exact results discussed above exhibit a rather formidable appearance, and in order to gain a better grasp of the nonextensive thermostatistics of the Fermi gas, it is useful to consider the situation  $q \rightarrow 1$ . It is obligatory in this context to cite the pioneering work of Büyükkılıç et al. [11], in which quantum gases are tackled in approximate fashion. They evaluate the partition function by recourse to the so-called factorization approach, whose essential feature is that of ignoring interparticle correlations for the case of a dilute quantum gas. In other words, this is equivalent to treat the  $q$ -exponentials (17) as if they were ordinary exponentials, what is approximately true when  $q \sim 1$ . The ensuing average occupation numbers have been widely employed in the literature (see footnote 1). It is to be stressed that these FA results were developed for the unnormalized second Tsallis flavor mentioned in the introduction, namely, the Curado–Tsallis formulation (recently, some of us have brought this approximation up to date using the OLM recipes and applied the ensuing results to the black-body problem [26]).

Since we are here in possession of exact results for the Fermi gas, we can indeed perform a check on the accuracy of the FA. If we treat the  $q$ -exponentials as if they were ordinary exponentials we have

$$g_q(k_1, \dots, k_N)^{1/(1-q)} \approx \prod_{i=1}^N g_q(k_i)^{1/(1-q)} .$$

Strictly speaking, we are making use of an approximation for the  $q$ -exponential of a sum of entities in the form

$$e_q \left( \sum_{i=1}^N x_i \right) \approx \prod_{i=1}^N e_q(x_i)$$

which is valid for  $q$  sufficiently close to 1 such that the following inequality holds:  $|(1 - q)[(\sum x_i)^2 - \sum x_i^2]| \ll 1$ . In our case,  $x_i = -\beta_q \varepsilon_{k_i}^*$ .

Therefore we obtain, from Eq. (39), the following FA-inspired approximate expression:

$$\langle \hat{n}_l \rangle_q \approx \frac{\sum_{N \geq 1} \sum_{k_1 < \dots < k_N} \left( \sum_{i'=1}^N \delta_{lk_{i'}} \right) \prod_{i=1}^N [1 - (1 - q)\beta_q \varepsilon_{k_i}^*]^{q/(1-q)}}{1 + \sum_{N \geq 1} \sum_{k_1 < \dots < k_N} \prod_{i=1}^N [1 - (1 - q)\beta_q \varepsilon_{k_i}^*]^{q/(1-q)}} \quad (41)$$

that can be cast as

$$\langle \hat{n}_l \rangle_q \approx \frac{[1 - (1 - q)\beta_q \varepsilon_l^*]^{q/(1-q)} \prod_{k, k \neq l} \{1 + [1 - (1 - q)\beta_q \varepsilon_k^*]^{q/(1-q)}\}}{\prod_k \{1 + [1 - (1 - q)\beta_q \varepsilon_k^*]^{q/(1-q)}\}} \quad (42)$$

leading straightforwardly to

$$\langle \hat{n}_l \rangle_q \approx \frac{1}{1 + [1 - (1 - q)\beta_q \varepsilon_l^*]^{-q/(1-q)}} \quad (43)$$

which is the FA result of Ref. [11], except that the power  $1/(1 - q)$  in the result under an unnormalized context is changed to  $q/(1 - q)$  under OLM strictures. It is clear then that the FA approximation is reasonably consistent in the  $q \rightarrow 1$  limit.

By using Eq. (43) one arrives to (formally) simple expressions for both the number of particles and the internal energy,

$$N_q \approx \sum_k \frac{1}{[1 - (1 - q)\beta_q \varepsilon_k^*]^{-q/(1-q)} + 1}, \tag{44}$$

$$U_q \approx \sum_k \frac{\varepsilon_k}{[1 - (1 - q)\beta_q \varepsilon_k^*]^{-q/(1-q)} + 1}, \tag{45}$$

similar to the ones obtained using the FA. We dare say that the present treatment is simpler than the one found in Ref. [10]. The simple appearance we are emphasizing here is deceptive, though. In order to perform any practical calculation one has to solve a coupled system due to the presence of  $\beta_q$ . This problem, in turn, can be overcome by noticing that  $\beta_q$  satisfies the approximate relation

$$\frac{\beta}{\beta_q} \approx 1 + (1 - q)\beta \sum_k \frac{\varepsilon_k^*}{[1 - (1 - q)\beta_q \varepsilon_k^*]^{-q/(1-q)} + 1} \tag{46}$$

which allows one to obtain  $\beta_q$  in terms of  $\beta$  and, as a consequence, to decouple Eqs. (44) and (45).

In this context, which we recall is valid for  $q \sim 1$ , we will now discuss the thermodynamic limit inspired in calculations performed by Ubriaco [12]. We consider a system of massive spinless particles in a volume  $V$  at temperature  $T$ . Going over to the thermodynamic limit in Eqs. (44) and (45) we find that

$$N_q \approx \frac{V}{\lambda_T^3} \left( \frac{\beta}{\beta_q} \right)^{3/2} f_{3/2}^*(z, q) \tag{47}$$

and

$$U_q \approx \frac{3}{2} T \frac{V}{\lambda_T^3} \left( \frac{\beta}{\beta_q} \right)^{5/2} f_{5/2}^*(z, q), \tag{48}$$

where  $\lambda_T = h/\sqrt{2\pi mT}$  is the usual thermal wavelength and  $z$  is the fugacity. We have introduced the following Fermi-like integral:

$$f_n^*(z, q) \equiv \frac{1}{\Gamma(n)} \int_0^\infty dx \frac{x^{n-1}}{[1 + (q - 1)x - (q - 1)(\beta_q/\beta) \ln z]^{q/(q-1)} + 1}. \tag{49}$$

Using the definition of Eq. (17), the first term in the denominator can be re-expressed as  $[e_q(-x + (\beta_q/\beta) \ln z)]^{-q}$  so that

$$f_n^*(z, q) = \frac{1}{\Gamma(n)} \int_0^\infty dx \frac{x^{n-1}}{[e_q(-x + (\beta_q/\beta) \ln z)]^{-q} + 1} \tag{50}$$

and in this form it is easy to see that it gives the expected result  $z^{-1} e^x$  when  $q = 1$ .

The ratio  $\beta/\beta_q$  can be obtained from the thermodynamic limit of Eq. (46) as

$$\frac{\beta}{\beta_q} \approx 1 + (1 - q) \frac{V}{\lambda_T^3} \left[ \frac{3}{2} \left( \frac{\beta}{\beta_q} \right)^{5/2} f_{5/2}^*(z, q) - \ln z \left( \frac{\beta}{\beta_q} \right)^{3/2} f_{3/2}^*(z, q) \right]. \quad (51)$$

Making use of the approximate results in Eqs. (47) and (48) we can express it in the fashion

$$\frac{\beta}{\beta_q} \approx \frac{1 + (q - 1)N_q \ln z}{1 + (q - 1)N_q \frac{3}{2}(f_{5/2}^*(z, q)/f_{3/2}^*(z, q))}. \quad (52)$$

Then, we can write down the generalized energy per particle  $u_q \equiv U_q/N_q$  in a useful form as

$$u_q \approx \frac{3}{2} T \frac{f_{5/2}^*(z, q)}{f_{3/2}^*(z, q)} \frac{1 + (q - 1)N_q \ln z}{1 + (q - 1)N_q \frac{3}{2}(f_{5/2}^*(z, q)/f_{3/2}^*(z, q))} \quad (53)$$

that resembles the conventional result.

Let us discuss the behavior of the generalized specific heat per particle within the present context. We have computed it, following the usual procedure, by taking the temperature derivative of  $u_q$  while keeping constant values for (i) the volume and (ii)  $N_q$ . The resulting expression for  $C_{V,q}/N_q$  is somewhat involved and will not be given here in order to save space. It can be written in terms of  $q - 1$ ,  $N_q$ ,  $\ln z$  and the Fermi-like integrals  $f_n^*(z, q)$  with  $n = \frac{1}{2}$ ,  $\frac{3}{2}$  and  $\frac{5}{2}$ . It is of interest to compare this generalized result against its conventional  $q=1$  counterpart,  $C_V/N$ , to which it tends for  $q \rightarrow 1$ . Let us effect this comparison by assuming that the value of the nonextensivity parameter  $q$  is very close to unity. Thus, we are allowed to use Taylor expansions for all the involved generalized quantities and keep just first-order terms (in  $q - 1$ ). Defining

$$C_{V,q}/N_q \equiv C_V/N[1 + (q - 1)\mathcal{C}^{(1)} + \mathcal{O}((q - 1)^2)], \quad (54)$$

one is to look for the (relative) first-order correction  $\mathcal{C}^{(1)}$  as a (rather complicated) function of  $z$  and  $N$ .

In order to see the effects of nonextensivity on the specific heat for an ideal Fermi gas, we consider the two extreme regimes of very low and very high temperatures. Our main conclusions are that: (i)  $C_{V,q}(T=0)=0$  for arbitrary  $q$ ; (ii) when  $T \gtrsim 0$  (in which case  $\ln z$  is of the order of  $\mu_F/T \gg 1$ , where  $\mu_F$  stands for the Fermi energy),  $\mathcal{C}^{(1)}$  represents a *positive* contribution that behaves as  $N \ln z$  plus smaller terms, so that  $C_{V,q}/N_q \lesssim C_V/N$  for  $q \lesssim 1$ ; and (iii) when  $T \rightarrow \infty$  (in which case  $z$  is approximately  $\lambda_T^3 N/V \ll 1$ ),  $\mathcal{C}^{(1)}$  represents a *negative* contribution that also behaves mainly as  $N \ln z$ , so that  $C_{V,q}/N_q \gtrsim C_V/N$  for  $q \lesssim 1$  (in the case  $q \gtrsim 1$ , the same finding is reported by Ubriaco [12]).

Finally, let us pinpoint the differences between the present results and the calculations of Ref. [12]. These differences manifest themselves in the presence of powers of  $(\beta/\beta_q)$  in Eqs. (47)–(49) and are ultimately due to the definition one chooses for the generalized mean values. As discussed in the previous sections, instead of using unnormalized mean values we work here within a *normalized* Tsallis framework, in its OLM

version. Moreover, we compute, for consistency's sake, the  $q$ -generalized expectation value for the number operator instead of dealing simply with  $\langle \hat{N} \rangle_1$ .

## 6. The thermodynamic limit

Let us discuss the thermodynamic limit in a more general context, and present our results for the internal energy and specific heat of an ideal fermion gas in the thermodynamic limit for any  $q > 1$ -value (in the  $0 < q < 1$  case we encounter a serious convergence problem on account of the cutoff condition. It is only easily tractable in the  $q \rightarrow 1$  case). Following usual practice, in the limit of large volume (coordinate space) we can convert summations over discrete s.p. levels into integrations in phase space. If the energy spectrum of a particle in the gas is of the form  $\varepsilon(\mathbf{p}) = A|\mathbf{p}|^s$  with degeneracy  $g$ , we can write these integrals in terms of the continuous s.p. energy. In doing so we need the density of states, given by

$$D(\varepsilon) d\varepsilon = g \frac{L^d}{h^d} \frac{2\pi^{d/2}}{\Gamma(d/2)} \frac{1}{As} \left(\frac{\varepsilon}{A}\right)^{d/s-1} d\varepsilon \equiv a\varepsilon^{b-1} d\varepsilon, \quad (55)$$

where we have assumed that the gas is contained in a hypercube of volume  $L^d$  in a  $d$ -dimensional space. In the case of massive spinless particles in 3D, one has  $a = 2\pi V(2m)^{3/2}/h^3$  and  $b = 3/2$ ; while for electrons in the ultra-relativistic limit one has  $a = 8\pi V/(hc)^3$  and  $b = 3$ . The conventional ( $q = 1$ ) grand partition function for an ideal fermion gas whose density of states is of the form (55), is given by [33,34]

$$\ln Z_1(\{\beta, \alpha\}, V \rightarrow \infty) = a \Gamma(b) \frac{f_{b+1}(e^{-\alpha})}{\beta^b} \quad (56)$$

with  $\beta > 0$  and  $b > 0$ . The function  $f_n$  stands for the usual FD integral, which in terms of the fugacity  $z = e^{-\alpha}$  reads

$$f_n(z) = \frac{1}{\Gamma(n)} \int_0^\infty dx \frac{x^{n-1}}{z^{-1}e^x + 1} = \sum_{l=1}^\infty (-1)^{l-1} \frac{z^l}{l^n}.$$

One can now write down the generalized grand partition function  $\bar{Z}_q$  making use of an integral representation (see appendix). We consider here the real representation (Hilhorst transform) of Eq. (A.3). To this end, the function  $Z_1$  is evaluated for the transformed Lagrange multipliers  $\beta' = t(q-1)\beta$  and  $\alpha' = t(q-1)\alpha$ . Thus, in the thermodynamic limit we find, for any index  $q$  greater than one (and provided that the grand-canonical configurational characteristic is positive definite), the following exact expression:

$$\bar{Z}_q = \frac{1}{\Gamma(1/(q-1))} \int_0^\infty dt t^{1/(q-1)-1} \times \exp\left(-t[1 - (q-1)I_q] + a \Gamma(b) \frac{f_{b+1}(e^{-t(q-1)\alpha})}{[t(q-1)\beta]^b}\right), \quad (57)$$

where  $I_q$  stands for  $\beta U_q + \alpha N_q = \beta U_q^*$ , from which one gets  $1 - (q-1)I_q = \beta/\beta_q$ .

6.1. Classical limit

Let us consider now the case of sufficiently small values of  $z$ , which corresponds to the classical limit. In such a case, the FD integrals that appear in the different thermodynamic quantities of interest can be expanded in the fugacity, up to second order, as  $f_n(z) \simeq z - z^2/2^n$ . The ensuing OLM generalized partition function becomes then

$$\begin{aligned} \bar{Z}_q = & e_q(I_q) + a \frac{\Gamma(b)\Gamma(1/(q-1)-b)}{\Gamma(1/(q-1))} e_q(I_q - \alpha) \left( \frac{1 - (q-1)(I_q - \alpha)}{(q-1)\beta} \right)^b \\ & - \frac{a}{2} \frac{\Gamma(b)\Gamma(1/(q-1)-b)}{\Gamma(1/(q-1))} e_q(I_q - 2\alpha) \left( \frac{1 - (q-1)(I_q - 2\alpha)}{2(q-1)\beta} \right)^b \\ & + a^2 \frac{\Gamma(b)^2 \Gamma(1/(q-1) - 2b)}{\Gamma(1/(q-1))} e_q(I_q - 2\alpha) \left( \frac{1 - (q-1)(I_q - 2\alpha)}{(q-1)\beta} \right)^{2b} \\ & + \dots \end{aligned} \tag{58}$$

In the process we must take care of some restrictions on the parameters that arise from the use of the definition of the gamma function Eq. (A.1). They are: (i)  $q > 1$ , (ii)  $1 - (q-1)I_q > 0$ , and (iii)  $1/(q-1) - 2b > 0$ . As a consequence, the present findings are valid within the region  $1 < q < \min\{1 + 1/(2b), 1 + 1/I_q\}$ . We can also obtain  $U_q$  and  $N_q$  in this case, in the form prescribed in Eq. (A.4). Keeping only terms up to first order in the fugacity, we are able to express the ratio between the generalized mean energy and particle number in the fashion

$$u_q \equiv \frac{U_q}{N_q} \simeq bT \frac{1 - (q-1)[\beta U_q + \alpha(N_q - 1)]}{1 - (q-1)b} \tag{59}$$

from which we can obtain

$$u_q \simeq bT \frac{1 - (q-1)\alpha(N_q - 1)}{1 + (q-1)b(N_q - 1)}, \tag{60}$$

where one can easily recognize the appropriate result for the classical energy per particle when  $q=1$ . In the present situation, we also find  $I_q = (b+\alpha)N_q/[1+(q-1)b(N_q-1)]$ . The implicit relation between  $\langle \hat{N} \rangle_q$  and its corresponding Lagrange multiplier can be cast in the following way:

$$\begin{aligned} N_q & \left( \frac{1 - (q-1)\alpha(N_q - 1)}{1 - (q-1)(\alpha N_q + b)} \right)^{1/(q-1)+1} \left( \frac{1 + (q-1)b(N_q - 1)}{1 - (q-1)\alpha(N_q - 1)} \right)^b \\ & = a\Gamma(b) \frac{\Gamma(1/(q-1)-b)}{\Gamma(1/(q-1))} e_q(b) \left( \frac{1/(q-1)-b}{\beta} \right)^b \end{aligned} \tag{61}$$

from which one could, in principle, solve for  $\alpha$  as a function of  $N_q$ . Introducing this result into the expression given above for  $u_q$ , one finally would obtain the generalized mean energy per particle as a function of temperature (and of  $N_q$ ). Therefore, in this limit we are able to overcome the eventual possible complications introduced, within

the OLM formalism, by the presence of the term  $I_q = \sum_{j=1}^M \lambda_j \langle \hat{O}_j \rangle_q$  in the expressions for the generalized partition function and other thermodynamic quantities.

### 6.2. Low temperature limit

Let us face now the particular situation in which the fugacity is extremely large:

$$z \gg 1 \quad \text{i.e., } \alpha \rightarrow -\infty$$

which corresponds to the low temperature limit with finite chemical potential. Notice that, in this case, the transformed variable  $e^{-I(q-1)\alpha}$  becomes very large as well. We can make use of Sommerfeld’s lemma [33,35]

$$f_n(z) = \frac{(\ln z)^n}{\Gamma(n+1)} \left[ 1 + \frac{\pi^2}{6} n(n-1) \frac{1}{(\ln z)^2} + \mathcal{O}\left(\frac{1}{(\ln z)^4}\right) \right] \tag{62}$$

which gives an asymptotic expansion of the FD integrals for  $z \gg 1$ . As can be seen, the dominant term in the expansion is of order  $(-\alpha)^n$ . We can evaluate the integral in Eq. (57) up to this order, getting an expression valid for all  $q > 1$  in the low temperature limit:

$$\bar{Z}_q \simeq e_q \left( I_q - \frac{a}{b(b+1)} \left( \frac{-\alpha}{\beta} \right)^b (-\alpha) \right). \tag{63}$$

Additional quantities evaluated up to the same order are

$$U_q \simeq \frac{a}{b+1} \mu^{b+1} \quad \text{and} \quad N_q \simeq \frac{a}{b} \mu^b \tag{64}$$

independently of the value of  $q$ , in agreement with previous results obtained using the OLM formalism [21]. Using the above relations we can derive the Fermi potential as  $\mu_F = (N_q b/a)^{1/b}$ ; and we can also identify the Fermi temperature as  $T_F \equiv \mu_F = (N_q b/a)^{1/b}$ . Besides, it is easy to obtain  $I_q^{(0)}$  and then simplify the expression for  $\bar{Z}_q$ , leading to

$$\bar{Z}_q \simeq e_q(2I_q^{(0)}) = e_q \left( -\frac{2a}{b(b+1)} \beta \mu^{b+1} \right). \tag{65}$$

It is worth pointing out that the mean energy per particle in the OLM–Tsallis framework *does not depend explicitly on the value of  $q$* . Indeed, in the limit under consideration we have  $U_q^{(0)}/N_q = \mu_F b/(b+1)$ .

Performing calculations up to the next order of approximation we arrive, after a little algebra, at the following results which are valid for any  $q > 1$ :

$$N_q \simeq \frac{a}{b} \mu^b \left[ 1 + \frac{\pi^2}{6} (b-1)b \left( \frac{T}{\mu} \right)^2 \frac{\mathcal{F}^2}{1-(q-1)} + \dots \right], \tag{66}$$

where the quantity  $\mathcal{F} \equiv 1 - (q-1)\beta\{U_q - \mu[N_q - a\mu^b/b(b+1)]\} = 1 - (q-1)(I_q - I_q^{(0)})$  is very close to unity. Actually, the second term in  $\mathcal{F}$  vanishes if one keeps just terms corresponding to the lowest order approximation, which eliminates the term  $I_q$

introduced by the OLM procedure (see Eqs. (13), (15), and (21)). For the chemical potential we find

$$\mu^{(2)} = \mu_F \left[ 1 - \frac{\pi^2}{6} (b-1) \left( \frac{T}{T_F} \right)^2 \frac{\mathcal{J}^2}{1-(q-1)} \right] \quad (67)$$

whereas the generalized mean energy becomes

$$U_q^{(2)} = \frac{a}{b+1} \mu_F^{b+1} \left[ 1 + \frac{\pi^2}{6} (b+1) \left( \frac{T}{T_F} \right)^2 \frac{\mathcal{J}^2}{1-(q-1)} \right]. \quad (68)$$

From this expression we derive the generalized specific heat at constant volume

$$C_{V,q}^{(2)} = N_q \frac{\pi^2}{3} b \frac{T}{T_F} \frac{1}{1-(q-1)}, \quad (69)$$

where we have assumed  $\mathcal{J}^2 = 1$ . Notice the linear behavior of the specific heat with temperature and that the only difference with the conventional results (see, e.g., Ref. [33]) is a factor  $1/(2-q)$  which tends to unity in the limit  $q \rightarrow 1^+$ .

## 7. Conclusions

In this communication, we have presented an exact statistical treatment for the ideal Fermi system in the generalized, nonextensive thermostatistics framework of the third Tsallis-flavor, the TMP one. Our main innovation is that of employing the OLM approach to nonextensivity [21–26], which allows one to obtain analytical results unavailable if one uses other algorithms that revolve around the concept of Tsallis' entropy.

Additionally, we have (i) solved in exact fashion the Fermi–TMP equations, (ii) introduced a method for evaluating traces that bypasses the use of the gamma representation, (iii) devised a rather simple treatment of  $q \approx 1$  instances, and (iv) studied interesting limiting situations. More specifically, the exact generalized partition function in the grand-canonical ensemble has been given, and we derived the ensuing statistics for arbitrary positive values of the nonextensivity index  $q$ . Several limit instances of interest were discussed here in some detail:

1. the thermodynamic limit,
2. the case  $q \sim 1$  ( $q = 1$  corresponds to the conventional FD statistics),
3. the low-temperature regime, where we obtained results that are independent of the specific  $q$ -values.

In writing down the generalized expectation value for the occupation number operator we were able to explicitly display the *correlation* among the occupations of different levels, which is a typical nonextensive effect. Indeed, the distinct mean occupation numbers are seen to disentangle from each other as one approaches the conventional  $q = 1$  statistics. Finally, we discussed the limits of validity of the FA of Büyükkılıç et al. [11].



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**Appendix. Integral representations**

In this appendix, we summarize a practical method for calculating the generalized partition function (16) and expectation values (20) of relevant observables, by recourse to integral representations based on the definition of the Euler gamma function. We start with the identity

$$\int_0^\infty dt t^{v-1} e^{-t\eta} = \eta^{-v} \Gamma(v) \tag{A.1}$$

for  $\Re(\eta) > 0$  and  $\Re(v) > 0$  (see for instance Ref. [36, p. 342]). One can then write

$$\hat{f}_q^{1/(1-q)} = \frac{1}{\Gamma(1/(q-1))} \int_0^\infty dt t^{1/(q-1)-1} e^{-t\hat{f}_q} \tag{A.2}$$

with the restrictions that (i)  $\hat{f}_q$  be positive (which is indeed always complied with because of Tsallis’ cutoff condition [18]), and (ii)  $q > 1$ . The usefulness of the transformation becomes evident, as the power-law form is converted into an exponential factor.

Evaluating the trace of the above expression—see final comments below—and introducing the OLM quantal configurational characteristic, one arrives at an integral representation (Hilhorst transform [29]) for the OLM generalized partition function (16) of index  $q > 1$ , in the form

$$\bar{Z}_q = \frac{1}{\Gamma(1/(q-1))} \int_0^\infty dt t^{1/(q-1)-1} e^{-t[1+(1-q)\sum_k \lambda_k \langle \hat{O}_k \rangle_q]} Z_1(\{\lambda'_i\}). \tag{A.3}$$

Here the integrand contains the corresponding *conventional partition function*  $Z_1$  evaluated for the set of *transformed Lagrange multipliers*  $\{\lambda'_i(t) = t(q-1)\lambda_i, i = 1, \dots, M\}$ . Notice that this transformation preserves the sign of the Lagrange parameters (this fact is used in the text). The generalized expectation values (11) can be expressed, for  $q > 1$ , in terms of integrals involving  $Z_1$  and its derivative with respect to the associated Lagrange multiplier. Indeed, one realizes that

$$\langle \hat{O}_j \rangle_q = - \frac{\int_0^\infty dt t^{1/(q-1)} e^{-t[1+(1-q)\sum_k \lambda_k \langle \hat{O}_k \rangle_q]} \partial Z_1(\{\lambda'_i\}) / \partial \lambda'_j}{\int_0^\infty dt t^{1/(q-1)} e^{-t[1+(1-q)\sum_k \lambda_k \langle \hat{O}_k \rangle_q]} Z_1(\{\lambda'_i\})}. \tag{A.4}$$

Let us mention that one can obtain alternative integral representations for  $\bar{Z}_q$  and  $\langle \hat{O}_j \rangle_q$  in the range  $0 < q < 1$  by recourse, for instance, to the following complex

representation of the Euler gamma function:

$$\int_{-\infty}^{\infty} dt (\zeta + it)^{-\nu} e^{(\zeta+it)\eta} = 2\pi\eta^{\nu-1} / \Gamma(\nu) \tag{A.5}$$

for  $\eta > 0$ ,  $\Re(\nu) > 0$  and  $\Re(\zeta) > 0$  [36, p. 343]. In this case (that may be called the Prato–Lenzi transform [30,31]) the partition function can be written as

$$\begin{aligned} \bar{Z}_q &= \frac{1}{2\pi} \Gamma\left(\frac{q-2}{q-1}\right) \int_{-\infty}^{\infty} dt (1+it)^{1/(q-1)-1} \\ &\times e^{(1+it)[1+(1-q)\sum_k \lambda_k \langle \hat{O}_k \rangle_q]} Z_1(\{\tilde{\lambda}_i\}), \end{aligned} \tag{A.6}$$

where  $\tilde{\lambda}_i(t) \equiv (1+it)(1-q)\lambda_i$  for each  $i=1, \dots, M$ , and the region of validity is  $q < 1$  or  $q > 2$ . The associated mean values take the form

$$\langle \hat{O}_j \rangle_q = - \frac{\int_{-\infty}^{\infty} dt (1+it)^{1/(q-1)} e^{(1+it)[1+(1-q)\sum_k \lambda_k \langle \hat{O}_k \rangle_q]} \partial Z_1(\{\tilde{\lambda}_i\}) / \partial \tilde{\lambda}_j}{\int_{-\infty}^{\infty} dt (1+it)^{1/(q-1)} e^{(1+it)[1+(1-q)\sum_k \lambda_k \langle \hat{O}_k \rangle_q]} Z_1(\{\tilde{\lambda}_i\})} \tag{A.7}$$

for  $j = 1, \dots, M$  and  $q < 1$ .

Some additional remarks are necessary. A quite detailed analysis concerning integral representations for the  $q$ -thermostatistics can be found in the recent preprint [32] by Solis and Esguerra, who pay special attention to practical details of the representations discussed above. One has to make sure that *all* states are contributing to the evaluation of the trace—in the sense that there is no cutoff—in order to get  $Z_1$  on the r.h.s. of Eqs. (A.3) or (A.6). Solis and Esguerra point out that this fact has not been taken into account in the majority of Tsallis-related works (see, for instance, Ref. [28]). In our particular case, the condition to be imposed in order to ensure that the Hilhorst-type representation can be safely used can be stated in the following terms:  $\hat{f}_q$  as given by Eq. (21) should be positive definite for all states, i.e., the lowest energy eigenvalue (or the greatest lower bound of the Hamiltonian) should be greater than or equal to  $\mu(\hat{N} - N_q) + U_q - 1/[\beta(q-1)]$ . (Notice that the simpler requirement given in Ref. [32], namely that  $\hat{H}$  be greater than  $-1/[\beta(q-1)]$ , originates in the fact that a canonical-ensemble description is performed and also that unnormalized, Curado–Tsallis mean values are employed.)

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