Eur. Phys. J. B **10**, 353–359 (1999)

THE EUROPEAN PHYSICAL JOURNAL B
EDP Sciences

Perturbation expansion, Bogoliubov inequality and integral representations in nonextensive Tsallis statistics

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Received 19 November 1998

Abstract. By using integral representations the perturbation expansion and the Bogoliubov inequality in nonextensive Tsallis statistics are investigated in a unified way. This procedure extends the analysis performed recently by Lenzi *et al.* [Phys. Rev. Lett. **80**, 218 (1998)] to the quantum (discrete spectra) case, for $q < 1$. An example is presented in order to illustrate the method.

PACS. 05.70.Ce Thermodynamic functions and equations of state – 05.20.-y Classical statistical mechanics – 05.30.Ch Quantum ensemble theory

1 Introduction

Despite the great success of the usual statistical mechanics (Boltzmann-Gibbs (BG) statistics) there are situations where its applications do not lead to reasonable conclusions. A good example, among others, where the usual statistical mechanics fails is related to the study of systems with long-range (gravitational) interactions [1–5]. On the other hand, it was recently proposed a generalization of the statistical mechanics [6] (Tsallis statistics) based on the entropy(Tsallis entropy) which is labeled by a parameter $q \in \mathcal{R}$, where q specifies the different nonextensive statistics (the BG statistics is recovered in the limit $q \to 1$).

Motivated by the above characteristics, the Tsallis statistics has been largely employed in the study of nonextensive phenomena. For example: Lévy-type anomalous superdiffusion [7], Euler turbulence [8], self-gravitating systems [8–12], cosmic background radiation [13], linear response theory [14] and electron-phonon interaction [15], peculiar velocities in galaxies [16] and ferrofluid-like systems [17]. Furthermore, it was stressed by Lavenda *et al.* [18] that any new entropy must have the correct concavity property, and this is the case of Tsallis entropy [6]. However, the calculations employing the Tsallis statistics are usually difficult. In order to circumvent this difficulty, some approximate methods were developed, such as semiclassical approximation [19], perturbation expansion [20] and variational method [20,21]. In particular, the last two methods presented in [20] deserve a more complete analysis because the quantum case for $q < 1$ has not been analyzed yet. These difficulties have also led to the use of integral representations. They sensibly simplify the calculational task since they permit to connect the generalized partition function with the usual one. Moreover, the relevance of these integral representations is reinforced by the fact that the Green functions [22] and the path integral prescription [23] in Tsallis statistics are nicely formulated in terms of integral representations. For example, the first analytical solution of a quantum many-body problem was obtained by using integral representation [24].

In this work, we employ the integral representation in order to complete the analysis of the perturbation and variational methods presented in reference [20], *i.e.*, we develop the perturbation expansion and prove the generalized Bogoliubov inequality for the quantum (discrete spectra) case, for $0 < q < 1$. These developments are presented in a unified way and, in addition, we will show that the inequality preserves its original form also for $q < 1$.

This work is organized in five sections. In Section 2, a brief introduction to the Tsallis statistics and integral representations is given. The perturbation expansion is developed in Section 3. By using the results of Section 3, the Bogoliubov inequality is demonstrated in Section 4. Finally, in Section 5, the conclusions are given.

2 Integral representations in Tsallis statistics

The nonextensive Tsallis statistics is based on the Tsallis entropy [6], and q-expectation value for an observable A [6,25]. They are defined respectively by

$$S_q = k\,\mathrm{Tr}\frac{\hat{\rho}-\hat{\rho}^q}{q-1}, \tag{1}$$

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and

$$\langle \hat{A} \rangle_q = \mathrm{Tr}\hat{\rho}^q \hat{A}, \tag{2}$$

where $\hat{\rho}$ is the density matrix, $q \in \mathbf{R}$ characterizes the degree of nonextensivity and k is a positive constant. Without loss of generality, we can take $k = 1$ in the present discussion in order to simplify the notation. Another possible choice for the q-expectation value is given by

$$\langle\langle \hat{A} \rangle\rangle_q = \frac{\mathrm{Tr}\hat{\rho}^q \hat{A}}{\mathrm{Tr}\hat{\rho}^q} \tag{3}$$

and it was analyzed in details recently [26]. We will give further comments on this subject in Section 4 and in the conclusions.

The canonical distribution is obtained from the entropy (1) by using the maximum entropy principle [6,25,27], with the constraints given by (2) (with $\hat{A} = \hat{H}$, where $\hat{H}$ is the Hamiltonian of the system) and the normalization of the density matrix $\hat{\rho}$, $\mathrm{Tr}\hat{\rho} = 1$. Thus, the canonical distribution becomes

$$\hat{\rho} = [1 - (1-q)\beta\hat{H}]^{1/(1-q)}/Z_q, \tag{4}$$

where

$$Z_q = \mathrm{Tr}\left[1 - (1-q)\beta\hat{H}\right]^{1/(1-q)} \tag{5}$$

is the generalized partition function, and β is the inverse of temperature T. In the energy basis, the probabilities in the canonical distribution are

$$p(E_n) = \langle n|\hat{\rho}|n\rangle = \left[1 - (1-q)\,\beta E_n\right]^{1/(1-q)}/Z_q, \tag{6}$$

where $\{E_n\}$ and $\{|n\rangle\}$ are the eigenvalues and the eigenvectors of the Hamiltonian $\hat{H}$, respectively. Then, equation (5) can be written as

$$Z_q = \sum_n \left[1 - (1-q)\beta E_n\right]^{1/(1-q)}. \tag{7}$$

Furthermore, in order to obtain a consistent probabilistic interpretation of $p(E_n)$, the term $[1 - (1-q)\,\beta E_n]^{1/(1-q)}$ is replaced by zero when $1 - (1-q)\,\beta E_n \le 0$. As example, in the classical case this cut-off condition leads to a restriction in the integration limits in the phase space, and the integration region is given by the condition $1 - (1-q)\,\beta H \ge 0$ (see for instance [20]).

It should be reminded that, in the usual thermodynamics, there are several relations among the thermodynamic quantities which also incorporate the multiple equivalent representations by using the Legendre transformations, such as the Helmholtz potential (or Helmholtz free energy or just called "free energy") representation. On the other hand, in thermostatistical theory, these thermodynamic quantities are connected with the partition function. These Legendre transforms are also incorporated in the Tsallis statistics; for instance, the free energy satisfies [25]

$$F_q = U_q - TS_q = -\frac{1}{\beta}\frac{Z_q^{1-q} - 1}{1-q}, \tag{8}$$

where $U_q = \sum_n [p(E_n)]^q E_n$ is the generalized internal energy. Note that the previous expressions are reduced to the usual ones in the limit case $q \to 1$. Furthermore, the above expressions will be useful to discuss the nonextensive variational method in the next section.

In general, the calculations employing the Tsallis statistics are more difficult than those within standard statistics since the former contains the latter as a limit case. Consistently, it is natural to investigate the possibility of obtaining the Tsallis thermodynamic functions from the usual ones. At the present date these investigations are based on the integral representations. Moreover, according to what we have mentioned in the introduction, the integral representations are useful to obtain analytical solutions of quantum many-body problems and to formulate Tsallis statistics in terms of a path integral and Green functions. In the present work, we employ the integral representation in order to demonstrate the Bogoliubov inequality in the nonextensive quantum Tsallis statistics for $0 < q < 1$, as well as for developing the perturbation expansion in this parameter region. In the case $q > 1$ we can also work in a similar fashion.

We describe now the basic mathematical tools which we will use in the next section. First, let us consider the Euler definition of the Gamma function

$$\int_0^\infty \mathrm{d}x\, x^{\alpha-1}\exp(-x) = \Gamma(\alpha), \tag{9}$$

with $\mathrm{Re}\,\alpha > 0$. We use the variable v defined by equality $x = [1 - (1-q)\beta E_n]v$ instead of x, hence the identity (9) becomes

$$[1 - (1-q)\beta E_n]^{-\alpha} = \int_0^\infty \mathrm{d}v\, K_>(v;\alpha)\exp(-\tilde{\beta}E_n), \tag{10}$$

where

$$K_>(v;\alpha) = \frac{v^{\alpha-1}\exp(-v)}{\Gamma(\alpha)}, \tag{11}$$

and

$$\tilde{\beta} = (q-1)v\beta. \tag{12}$$

It is worthwhile to note that, for arbitrary positive temperature ($\beta > 0$) and $E_n \ge 0$, the above integral representation can only be applied for $q > 1$.

In terms of this integral representation and using operator notation, the statistical weight and partition function can be written as

$$[1 - (1-q)\beta\hat{H}]^{-1/(q-1)} = \int_0^\infty \mathrm{d}v\, K_>\left(v;\frac{1}{q-1}\right)\exp(-\tilde{\beta}\hat{H}), \tag{13}$$

and

$$Z_q(\beta) = \int_0^\infty \mathrm{d}v\, K_>\left(v;\frac{1}{q-1}\right)Z_1(\tilde{\beta}), \tag{14}$$

where Z_1 is the usual partition function. The present integral representation was first proposed by Hilhorst [28]. Certainly, this representation of $Z_q(\beta)$ is valid for $q > 1$, too.

For $q < 1$, we know that there are two kinds of integral representations: the first one was proposed by Prato [29] and cannot be applied for $q = (n-2)/(n-1)$, where n is an integer. The second one does not have this restriction [30]. In the present work we use the second integral representation which is based on the following identity [31]

$$\frac{\exp(ab)b^{1-z}}{2\pi}\int_{-\infty}^{\infty} \mathrm{d}v \frac{\exp(ivb)}{(a+iv)^z} = \frac{1}{\Gamma(z)} \text{ for } b > 0, \qquad = 0 \text{ for } b < 0, \tag{15}$$

with $a > 0, \mathrm{Re}\, z > 0$, and $-\pi/2 < \arg(a+iv) < \pi/2$. If we choose $a = 1$, $b = 1-(1-q)\beta\hat{H}$ and $z = \alpha+1$ in the above expression, the desired integral representation is obtained, *i.e.*,

$$[1-(1-q)\beta\hat{H}]^\alpha = \int_{-\infty}^{\infty} \mathrm{d}v K_<(v;\alpha)\exp(-\bar{\beta}\hat{H}), \tag{16}$$

where

$$K_<(v;\alpha) = \frac{\Gamma(\alpha+1)}{2\pi}\frac{\exp(1+iv)}{(1+iv)^{\alpha+1}}, \tag{17}$$

and

$$\bar{\beta} = (1-q)(1+iv)\beta. \tag{18}$$

Therefore, the partition function Z_q can be expressed in terms of the usual one, namely

$$Z_q(\beta) = \int_{-\infty}^{\infty} \mathrm{d}v K_<\left(v;\frac{1}{1-q}\right) Z_1(\bar{\beta}). \tag{19}$$

Note that the present integral representation incorporates naturally the cut-off introduced for $q < 1$ in order to obtain a consistent probabilistic interpretation. In other words, the integral (15) makes all the terms equal to zero when $b = [1-(1-q)\beta E_n] < 0$. Consequently, the summation over $[1-(1-q)\beta E_n]^\alpha$ by index n can be applied without any problem for arbitrary value of E_n and any value of α. This feature constitutes an ingredient which sensibly simplifies the calculations.

3 Nonextensive perturbation expansion

In order to develop the perturbation method in the generalized statistical mechanics we consider the following Hamiltonian

$$H = H_0 + \lambda H_I, \tag{20}$$

where H_0 typically is the Hamiltonian of a soluble model, λH_I is considered as a perturbation of H_0 (H_0 and H_I do not necessarily commute), and λ is the parameter which regulates the intensity of the perturbation. The perturbation expansion of the free energy in terms of λ is given by

$$F_q(\lambda) = F_q^{(0)} + \lambda F_q^{(1)} + \frac{\lambda^2}{2}F_q^{(2)} + \ldots \tag{21}$$

The term $F_q^{(0)}$ is the free energy for the case without perturbation, *i.e.*,

$$F_q^{(0)} = F_q(0). \tag{22}$$

If we take the first derivative of $F_q(\lambda)$ at $\lambda = 0$, we obtain the first-order correction to the free energy

$$F_q^{(1)} = \frac{\partial F_q(0)}{\partial\lambda} = -\frac{1}{\beta Z_q^q}\frac{\partial Z_q}{\partial\lambda}\bigg|_{\lambda=0}. \tag{23}$$

The next term in the expansion of the free energy (21) is

$$F_q^{(2)} = \frac{\partial^2 F_q(0)}{\partial\lambda^2} = \left[\frac{q}{\beta Z_q^{q+1}}\left(\frac{\partial Z_q}{\partial\lambda}\right)^2 - \frac{1}{\beta Z_q^q}\frac{\partial^2 Z_q}{\partial\lambda^2}\right]\bigg|_{\lambda=0}. \tag{24}$$

Of course, we can see from these expressions that the calculation of the nth term of the expansion reduces to the evaluation of $\partial^n Z_q/\partial\lambda^n$. Let us now proceed to calculate $\partial^n Z_q/\partial\lambda^n$ for the case $q < 1$. By using the integral representation (16) with $\alpha = 1/(1-q)$ we can write

$$\frac{\partial Z_q}{\partial\lambda} = \frac{\partial}{\partial\lambda}\int_{-\infty}^{\infty}\mathrm{d}v K_<\left(v;\frac{1}{1-q}\right)\mathrm{Tr}\exp(-\bar{\beta}\hat{H}). \tag{25}$$

Employing the following identity [32]

$$\frac{\partial\exp(\hat{A})}{\partial\alpha} = \int_0^1 \mathrm{d}\gamma\exp(\gamma\hat{A})\frac{\partial\hat{A}}{\partial\alpha}\exp[(1-\gamma)\hat{A}] \tag{26}$$

for $\hat{A} = -\bar{\beta}\hat{H}$ and $\alpha = \lambda$, we find that

$$\frac{\partial Z_q}{\partial\lambda} = -\beta\ \mathrm{Tr}\ \left\{\hat{H}_I\int_{-\infty}^{\infty}\mathrm{d}v K_<\left(v;\frac{q}{1-q}\right)\exp(-\bar{\beta}\hat{H})\right\} = -\beta Z_q^q\langle\hat{H}_I\rangle_q. \tag{27}$$

To obtain the last equation we have used that the orders of the derivative, integral and trace can be commuted between them, and also the definition of the q-mean value (2). Since the above calculation was performed for arbitrary λ, the first-order correction for F_q becomes

$$F_q^{(1)} = \langle\hat{H}_I\rangle_q^{(0)}, \tag{28}$$

where the superscript (0) indicates that the q-mean value is calculated for $\lambda = 0$.

Next, we calculate the second derivative of Z_q. To do that, we derive (27) with respect to λ

$$\frac{\partial^2 Z_q}{\partial\lambda^2} = -\beta\frac{\partial}{\partial\lambda}\mathrm{Tr}\left\{\hat{H}_I\int_{-\infty}^{\infty}\mathrm{d}v\ K_<\left(v;\frac{q}{1-q}\right)\exp(-\bar{\beta}\hat{H})\right\}. \tag{29}$$

Again, commuting the orders of the derivative with respect to the integral and to the trace, and using the identity (26), equation (29) becomes

$$\frac{\partial^2 Z_q}{\partial \lambda^2} = q\beta^2 \int_{-\infty}^{\infty} \mathrm{d}v K_< \left(v; \frac{2q-1}{1-q}\right) \times \mathrm{Tr}\left\{\hat{H}_I \int_0^1 \mathrm{d}\gamma \exp(-\gamma\bar{\beta}\hat{H})\hat{H}_I \exp[-(1-\gamma)\bar{\beta}\hat{H}]\right\}. \quad (30)$$

In this expression, let us introduce the completeness relation in the energy basis between $\exp(-\gamma\bar{\beta}\hat{H})$ and $\hat{H}_I$ to calculate the trace by using the same basis. In this way, after the integration in γ and exchanging the order between integral and the sum over energy states, equation (30) can be written as

$$\frac{\partial^2 Z_q}{\partial \lambda^2} = -\beta \sum_n \sum_{m\neq n} |\langle m|\hat{H}_I|n\rangle|^2 \int_{-\infty}^{\infty} \mathrm{d}v K_< \left(v; \frac{q}{1-q}\right) \frac{\exp(-\bar{\beta}E_m) - \exp(-\bar{\beta}E_n)}{E_m - E_n} + q\beta^2 \sum_n |\langle n|\hat{H}_I|n\rangle|^2 \int_{-\infty}^{\infty} \mathrm{d}v K_< \left(v; \frac{2q-1}{1-q}\right) \exp(-\bar{\beta}E_n). \quad (31)$$

To simplify this expression we use again the equation (16), and obtain

$$\frac{\partial^2 Z_q}{\partial \lambda^2} = q\beta^2 \sum_n |\langle n|\hat{H}_I|n\rangle|^2 \left[1-(1-q)\beta E_n\right]^{(2q-1)/(1-q)} + \beta \sum_n \sum_{m\neq n} \frac{|\langle m|\hat{H}_I|n\rangle|^2}{E_n - E_m} \left([1-(1-q)\beta E_m]^{q/(1-q)} - [1-(1-q)\beta E_n]^{q/(1-q)}\right). \quad (32)$$

Identifying in this expression the probabilities (6) we obtain

$$\frac{\partial^2 Z_q}{\partial \lambda^2} = q\beta^2 Z_q^{2q-1} \sum_n |\langle n|\hat{H}_I|n\rangle|^2 \left[p(E_n)\right]^{2q-1} + \beta Z_q^q \sum_n \sum_{m\neq n} \frac{|\langle m|\hat{H}_I|n\rangle|^2}{E_n - E_m} \{[p(E_m)]^q - [p(E_n)]^q\}. \quad (33)$$

The previous procedure can also be applied to evaluate the higher order derivatives of Z_q. However, as in the case of the second derivative, it is important to remark that the integral representation (16) is restricted to a certain range of values of the entropic parameter q. Indeed, the integrals in equation (31) are well defined only for $q/(1-q) > 0$. In general, this restriction is given by $q > 1 - 1/(n-1)$ in order to calculate $\partial^n Z_q/\partial\lambda^n$. It must be emphasized that this limitation is not a specific consequence of the integral representation. Indeed, this restriction also occurs in the classical case, where the integral representation was not employed [20].

Substituting the derivatives (27, 33) with $\lambda = 0$ into (24) we obtain the second-order correction to the free energy,

$$F_q^{(2)} = \frac{\partial^2 F_q(0)}{\partial \lambda^2} = -\beta q \left(Z_q^{(0)}\right)^{q-1} \times \sum_n p(E_n^{(0)}) \left\{\left[[p(E_n^{(0)})]^{q-1} \langle n|H_I|n\rangle - \langle H_I\rangle_q^{(0)}\right]^2\right\} - \sum_n \sum_{m\neq n} \left|\langle n\,|H_I|\,m\rangle^{(0)}\right|^2 \frac{\left[p\left(E_m^{(0)}\right)\right]^q - \left[p\left(E_n^{(0)}\right)\right]^q}{E_n^{(0)} - E_m^{(0)}}. \quad (34)$$

When H_0 and H_I commute (in the classical case, for instance) the expression (34) is simpler since the second term on the right-hand side is null because $\langle n\,|H_I|\,m\rangle$ vanishes. Notice that equations (28, 34) are correct for any λ, but in this case it is necessary to consider the dependence of $|\,n\rangle$ with λ and substitute $E_n^{(0)}$ by E_n. The other corrections for the free energy can be calculated following the same procedure that was employed in the first two corrections. Moreover, as discussed in the last paragraph, the interval for possible values of the parameter q becomes reduced with the increase of n in $F_q^{(n)}$. Summarizing, the free energy up to the corrections calculated above is given by

$$F_q(\lambda) = F_q(0) + \lambda\langle H_I\rangle_q^{(0)} - \frac{\lambda^2}{2}\beta q \left(Z_q^{(0)}\right)^{q-1} \times \sum_n p(E_n^{(0)}) \left\{\left[\left[p(E_n^{(0)})\right]^{q-1} \langle n|H_I|n\rangle - \langle H_I\rangle_q^{(0)}\right]^2\right\} - \frac{\lambda^2}{2} \sum_n \sum_{m\neq n} |\langle n\,|H_I|\,m\rangle|^2 \frac{[p(E_m^{(0)})]^q - [p(E_n^{(0)})]^q}{E_n^{(0)} - E_m^{(0)}} + \mathcal{O}\left(\lambda^3\right), \quad (35)$$

where $|\,n\rangle$ is evaluated with $\lambda = 0$. It should be mentioned that, in the case $q > 1$, the perturbation expansion can be established and analyzed by using the integral representation (10). Of course, it can also be analyzed without the use of any integral representation [20]; as expected the results are the same.

4 Generalized Bogoliubov inequality

To study the Bogoliubov inequality, we decompose the Hamiltonian into two parts,

$$\hat{H} = \hat{H}_0 + \hat{H}_I. \quad (36)$$

For concrete applications, $\hat{H}_0$ is chosen in such way that it is the Hamiltonian of a solvable model, although for the present arguments this is not necessary. In the following discussion it is more convenient to use a Hamiltonian that interpolates continuously between $\hat{H}_0$ and $\hat{H}$. This Hamiltonian is $\hat{H} = \hat{H}_0 + \lambda \hat{H}_I$ with $\lambda \in [0,1]$; therefore, the results of the previous section can be employed. These results, together with the general identity

$$F_q(\lambda) = F_q(0) + \lambda F_q'(0) + \frac{\lambda^2}{2} F_q^{''}(\lambda_0), \qquad (37)$$

for free energy are all that is needed to obtain the Bogoliubov inequality in the context of Tsallis statistics. The prime in (37) indicates the derivative with respect to λ, and λ_0 is chosen in order to satisfy the equality (37).

If $F_q^{''}(\lambda_0) \leq 0$, then the inequality

$$F_q \leq F_q(0) + \lambda F_q^{'}(0) \qquad (38)$$

follows. Substituting in this inequality the equations (22, 28), and choosing $\lambda = 1$ in order to recover the system described by the Hamiltonian (36), we obtain that

$$F_q \leq F_q^{(0)} + \langle H_I \rangle_q^{(0)}. \qquad (39)$$

This inequality is the desired result, *i.e.*, the Bogoliubov inequality in the Tsallis statistics. As we can see immediately, this inequality is a natural generalization of the usual one, $F \leq F^{(0)} + \langle H_I \rangle^{(0)}$. In other words, the Bogoliubov inequality is *form invariant with respect to the parameter q*.

The inequality (39) is different from the one proposed in [21].This is due to the fact that we have used different mathematical inequalities to derive our final results. The derivation of the generalized Bogoliubov inequality obtained in this section is based on Feynman's proof [33]. To complete the demonstration of (39), it is necessary to verify that $F_q^{''}(\lambda_0) \leq 0$. This condition occurs independently of λ_0. In fact, each term of (34) is negative because the first term clearly is always negative, valid for any λ, and for the second term, we have: $[p(E_n)]^q \leq [p(E_m)]^q$ for $E_n > E_m$ and $[p(E_n)]^q \geq [p(E_m)]^q$ for $E_n < E_m$.

Before performing any calculation it is important to make further remarks about the ground state energy of the exact and the approximate Hamiltonians in the present context with $q < 1$ and $T > 0$. For the positive exact ground state energy, $E_0 > 0$, there is an inaccessible temperature region given by the inequality, $1-(1-q)E_0/T_0 < 0$, *i.e.*, $T_0 < (1-q)E_0$. On the other hand, if we consider the approximate analysis, it is necessary to consider the ground state energy of the Hamiltonian H_0, $E_0^{(0)}$. In this case, the inaccessible temperature is dictated by the inequality $T_0^{(0)} < (1-q)E_0^{(0)}$. In order to overcome this forbidden temperature region in the approximate analysis, it is convenient to choose H_0 in such way that $E_0^{(0)} = 0$. Finally, by taking the limit $T \to T_0^{(0)} = (1-q)E_0^{(0)}$ with $T > T_0$, $F_q^{(0)}$ and $\langle H_I \rangle_q^{(0)}$ reduce respectively to $E_0^{(0)}$ and $\langle 0|H_I|0\rangle$ ($|0\rangle$ represents the ground state of H_0). Thus, the Bogoliubov inequality, equation (39), gives an upper bound for the exact ground state energy, *i.e.*, $E_0 \leq E_0^{(0)} + \langle 0|H_I|0\rangle$. In other words, the well known quantum variational principle is recovered in the limit of very low temperature, *independently* of the q value. Furthermore, by using the last variational principle, the exact inaccessible temperature region is given by the inequality $T_0 \leq (1-q)(E_0^{(0)} + \langle 0 \mid H_I \mid 0\rangle)$.

Another important remark is about the new version of the generalized statistical mechanics which based on the constraint (3) instead of the constraint (2). The formalism based on equation (2) was successful in the discussion of nonextensive systems, however, it contains some unfamiliar properties, for instance, $\langle 1 \rangle_q \neq 1$ and a dependence on the choice of origin of the energy spectrum. On the other hand, the new version does not present these undesirable properties. It is important to emphasize that the statistical mechanics based on equation (3) retains the main, with successful, aspects of the old formalism (Eq. (2)). This conclusion is based on the fact that the canonical distribution corresponding to the constraint (3) is given by

$$p'(E_n) = [1-(1-q)\beta(E_n - U_q')/g]^{1/(1-q)}/Z_q \qquad (40)$$

where $U_q' = \langle\langle \hat{H} \rangle\rangle_q$, $g = \sum_n p(E_n)^q$ and

$$Z_q' = \sum_n [1-(1-q)\beta(E_n - U_q')/g]^{1/(1-q)}. \qquad (41)$$

Moreover, if we define β' as

$$\beta' = \frac{\beta}{g + (1-q)\beta U_q'} \qquad (42)$$

Equations (40, 41) reduce to equations (5, 6) with β replaced by β'. Thus, the main aspects (including calculational ones) of the old formalism are preserved in the new one (a complete discussion of this question is developed in Ref. [26]). In particular, the calculations developed in this work are a good example of the aspect preserved in the new formalism. Indeed, this fact justify the utility of the analysis developed here to study the new version of the generalized statistical mechanics by employing perturbative and variational methods.

5 Application

To illustrate the above inequality we will now discuss a simple system, namely a one-dimensional harmonic oscillator. We will approximate this system by a particle in a square well potential. We can calculate the partition function of the unperturbed system and the q-expectation value for $H_I = H - H_0$ by using (2) and (5). In order to eliminate inaccessible positive temperatures in the present example, we choose H and H_0 in such way that $E_0 = E_0^{(0)} = 0$. Thus, the Hamiltonian of a one-dimensional harmonic oscillator is given by

$$H = \frac{p^2}{2m} + \frac{m}{2}\omega^2 x^2 - \frac{\hbar\omega}{2} \qquad (43)$$

and of the square well potential is

$$H_0 = \frac{p^2}{2m} + V_0 - \frac{\pi^2\hbar^2}{2mL^2}, \quad (44)$$

where

$$V_0 = \begin{cases} 0 & \text{for } |x| < L/2 \\ \infty & \text{for } |x| > L/2. \end{cases} \quad (45)$$

By taking the above considerations and by using (5, 27, 28) we find that

$$Z_q^{(0)} = \sum_{n=0}^{\infty} \left[1 - (1-q)\beta E_n^{(0)}\right]^{1/(1-q)}, \quad (46)$$

where $E_n^{(0)} = \pi\hbar^2((n-1)^2 - 1)/(2mL^2)$ and

$$\langle H - H_0\rangle_q^{(0)} = \sum_{n=0}^{\infty} \left(p_{q,n}^{(0)}\right)^q \langle\psi_n|H - H_0|\psi_n\rangle^{(0)} \quad (47)$$

with

$$\langle\psi_n|H - H_0|\psi_n\rangle^{(0)} = \frac{L^2 m\omega^2}{24}\left[1 - \frac{6}{n^2\pi^2}\right] + \frac{\pi^2\hbar^2}{2mL^2} - \frac{\hbar\omega}{2}\cdot \quad (48)$$

The free energy $F_q^{(0)}$ can be immediately obtained by substituting (46) into (8).

The optimum approximation for the free energy is evaluated by taking the minimization of $F_q^{(0)} + \langle H - H_0\rangle_q^{(0)}$ with respect to L, and then the result is substituted again into $F_q^{(0)} + \langle H - H_0\rangle_q^{(0)}$. Figure 1 shows the approximate and the exact results for the free energy for some typical values of q. Notice that these curves resemble the curves of classical free energy [20].

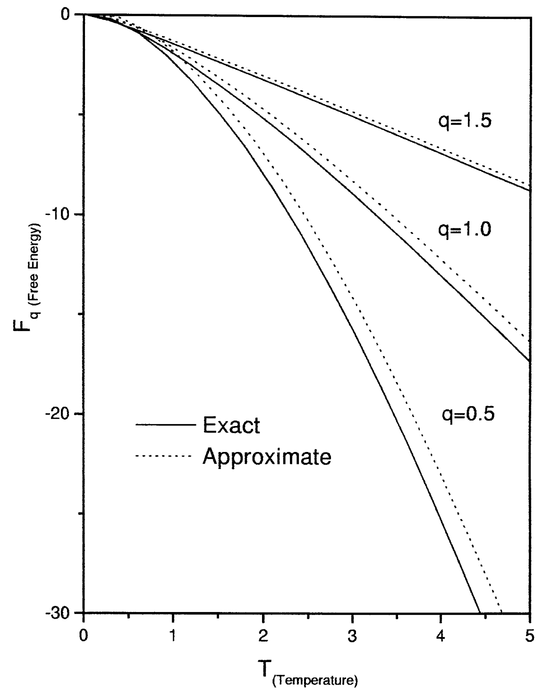

Fig. 1. Free energy *vs.* temperature for typical values of q. The exact and approximate free energy are represented by dashed and solid lines, respectively.

6 Conclusions

In this work we have developed, in a unified way, the generalized perturbation and variational methods in a nonextensive context by using integral representations. In this approach, we have obtained a generalization of the Bogoliubov inequality which turns out to be form-invariant for all $q > 0$. This form-invariance property was first presented in reference [20], but under more restricted conditions. When compared with the results presented in that reference, the analysis developed here was extended to the important case of discrete spectra in the range $0 < q < 1$.

In the classical context, the higher derivatives of Z_q in relation to λ lead to the decrease of the range of the possible q values [20]. This reduction is governed by the inequality $q > 1 - 1/(n-1)$, where n is the order of perturbation term, $F_q^{(n)}$. The application conditions of the integral representation for $q < 1$ lead consistently to the same decrease in the range of q values. Therefore, this restriction in the possible values of q is not a consequence of using the integral representation employed here, but it is a feature of the theory. In summary, the results obtained in this work unify the perturbation and variational methods in the classical (continuous spectra) and quantum (discrete spectra) contexts. Moreover, the present arguments reinforce the power of the integral representations which can be used to solve a series of problems in Tsallis statistics. Finally, we believe that the present approaches could be useful in the discussion of the anomalies currently associated with nonextensive systems by using the generalized statistical mechanics based on unnormalized (Eq. (2)) or normalized (Eq. (3)) constraints.

We also thank CNPq and PRONEX (Brazilian agencies) for partial financial support.

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