A Variational Perturbation Approximation Method in Tsallis Non-Extensive Statistical Physics

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Abstract

For the generalized statistical mechanics based on the Tsallis entropy, a variational perturbation approximation method with the principle of minimal sensitivity is developed by calculating the generalized free energy up to the third order in variational perturbation expansion. The approximation up to the first order amounts to a variational approach which covers the variational method developed in Phys. Rev. Lett. 80, 218 (1998) by Lenzi et al, and the approximations up to higher orders can systematically improve variational result. As an illustrated example, the generalized free energy for a classical harmonic oscillator (considered in the Lenzi’s joint work) are calculated up to the third order, and the resultant approximations up to the first, second, and third orders are numerically compared with the exact result.

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I. INTRODUCTION

Tsallis non-extensive statistical physics (TNESP) is one of theories for generalizing the Boltzmann-Gibbs statistical mechanics and thermodynamics. Its formalism is based on the Tsallis entropy with a parameter $q$, the index of non-extensiveness for a system. It takes the conventional statistical mechanics as its special case of $q \to 1$. A distinct feature of it is the power-law distributions ($q \neq 1$) instead of the exponential law in the conventional statistical mechanics. Since Tsallis’ pioneered work in 1988, the TNESP has greatly developed, and successfully been used for investigating many systems with a long-range interaction, long-time memory, or fractal structured space-time, in which the non-extensive effect exists.

For a new physical theory, to develop basic and analytic approximation tools for the TNESP should be a fundamental task for developing and employing it. To finish this task is particularly necessary for the TNESP because to perform calculation with the Tsallis statistics is usually difficult due to the presence of the power-law distributions. Since the TNESP with $q = 1$ is reduced to the conventional statistical mechanics, it will be natural to generalize variational method and perturbational theory, the two basic approximation methods in the conventional statistical mechanics, to the TNESP. In fact, some progress has been made in this direction. Early in 1993, employing concavity properties of Tsallis entropy, Plastino and Tsallis established a generalized Bogoliubov inequality and accordingly developed a scheme of variational approximation for the free energy in the generalized canonical ensemble. Later in 1998, Lenzi et al. generalized the perturbation method by deriving approximate expressions of the generalized free energy (GFE) up to the second order and obtained, through analyzing the approximate expression up to the second order, another generalized Bogoliubov inequality which affords a different variational method. Recently, Mendes et al. gave a comparative study on the aforementioned variational methods, and illustrated that the variational method in Ref. gives a better approximation for $q < 1$ and is easier to perform than the variational method in Ref., albeit the latter can lead to a better approximation than the former for the case of $1 < q < 2$.

Nevertheless, the usefulness of both variational and perturbation methods is limited. The variational approximate scheme in Ref. is valid only for the case of $q < 2$, and the variational approximate scheme in Ref. works only for the case of $q > 0$. As for the
perturbation method, the $n$th-order perturbation approximation can be used only when $q > (1 - \frac{1}{n})$. Moreover, as is well known in the conventional statistical mechanics, to control the approximate accuracy of variational methods is not straightforward, and the perturbation method is valid only for an exactly soluble system with a really small perturbation. Hence, for systematically improving variational method and extending the valid range of $q$, it is worthwhile developing new approximate approaches.

In the conventional statistical mechanics and some other branches of physics, a variational perturbation idea which collects merits and overcomes drawbacks of both the perturbation and the variational methods has developed and now becomes a powerful tool called variational perturbation theory (sometimes nominated other names.). The author or with his collaborators also developed some schemes for the variational perturbation theory (Refs. have briefly introduced references on the schemes for variational perturbation theory). In the present paper, we intend to generalize the variational perturbation theory to the TNESP. In the generalized canonical ensemble, we will consider an expansion for the GFE analogous to that in Ref. but with artificially introduced some auxiliary parameter $\mu$ and an expansion index $\epsilon$, and derive the expressions of the first four terms in the expansion series which will lead to approximations for the GFE up to the third order. From the truncated expressions of the GFE at the first, second and third orders (with taking $\epsilon = 1$), the auxiliary parameter $\mu$ will be determined according to a principle of minimal sensitivity (PMS) at the first, second and third orders, respectively. The value of $\mu$ determined at some order entering the truncated expression of the GFE at the same order produces the approximation for the GFE up to the same order. One will see that the adoption of the PMS is crucial to the variational perturbation approximation (VPA) method. It is the PMS that guarantees the meaningfulness, non-perturbational nature and effectiveness of the VPA results. To illustrate the method, we will consider a classical harmonic oscillator, which was used in Ref., and calculate the GFE up to the third order in the variational perturbation expansion. Numerical comparisons between the first-, second- and third-order and exact results are made and indicate that the VPA method provides a better approximation than the variational method in Ref.

Nowadays, owing to the so-called “normalization” problem of Tsallis non-extensive thermostatistics, there have existed four versions for the TNESP. The first version with the usual constraint on the internal energy in Ref. was used, for some special sys-
tems, only a couple of times in the past, and the second version with the non-normalized constraint on the internal energy in Ref. [11] has been intensively studied and used, and furthermore the aforementioned variational and perturbation methods were developed in this version. The third version with the normalized constraint on the internal energy in Ref. [12] is a satisfactory version, but is very complicated for performing because there exist implied relations between relevant quantities, and so the fourth version with the non-normalized constraint on centered operators appears to unentangle the problem on the implied relations in the third version [13]. Happily, the four versions can be easily derived from just any one of them [12, 14]. Moreover, we notice that the second version has been applied to many systems with providing satisfactory theoretical and/or experimental results [1, 12]. Hence, here we will use the second version worked out in Ref. [11] to perform the VPA method.

Next, the Tsallis statistical mechanics with the canonical ensemble and the perturbation and variational methods in Ref. [5] will briefly be introduced for the convenience of our later investigations. In Sect. III, the VPA method will be stated and truncated expressions of the expansion series of the GFE in the second version in Ref. [11] for a system will be derived up to the third order. Sect. IV will contribute to investigating the classical harmonic oscillator, and conclusions will be made in Sect. V.

II. TSALLIS STATISTICAL MECHANICS

For a system with a non-extensive index \( q \), the Tsallis entropy is defined as [2]

\[
S_q = k \left( 1 - \sum_{i=1}^{W} p_i^q \right) / (q - 1),
\]

(1)

where \( k \) is the Boltzmann constant and \( W \) is the total number of microscopic possibilities \( p_i \) of the system. Note that \( q \) is a real number and characterizes the degree of non-extensiveness. When \( q = 1 \), Eq.(1) leads to the usual entropy \( S_1 = -k \sum_{i=1}^{W} p_i \ln p_i \). The three cases of \( q < 1 \), \( q = 1 \) and \( q > 1 \) characterize superextensiveness, extensiveness and subextensiveness of systems, respectively. Based on the Tsallis entropy, a generalized equilibrium thermostatistics can be established by making \( S_q \) extremal with appropriate constraints present. For the canonical ensemble, four possible candidates exist for the constraints and hence lead to the aforementioned four versions for Tsallis statistical mechanics. This section will use
the following non-normalized constraint on the internal energy $U_q$ \[11\]:

$$\sum_{i=1}^{W} p_i^q E_i = U_q,$$

where $E_i$ is the $i$th eigenvalue of the Hamiltonian of the system. (The corresponding constraint used in the first version of Tsallis statistical mechanics is $\sum_{i=1}^{W} p_i E_i = U_q$, and the one in the third version is the normalized one $\sum_{i=1}^{W} p_i^q E_i / \sum_{i=1}^{W} p_i^q = U_q$.) Thus, making $S_q$ extremal with present the constraint Eq.(2) and the normalization property of the probability yields the following power-law distribution \[11\]

$$p_i = p_i(E_i) = p_i(\beta^*) = \frac{[1 - (1 - q)\beta^* E_i]^{1/(1-q)}}{Z_q(\beta^*)},$$

with the generalized partition function

$$Z_q(\beta^*) = \sum_{i=1}^{W} [1 - (1 - q)\beta^* E_i]^{1/(1-q)},$$

where $\beta^*$ is the Lagrange multiplier associated with the internal-energy constraint, Eq.(2). In the case of $q < 1$, the summation in the distribution Eq.(2) will be cut off for those energy eigenvalues higher enough to give negative probabilities. It is easy to verify that when $q \to 1$, the power-law distribution Eq.(2) tends to the conventional exponential-law distribution.

From Eqs.(2), (3) and (4), one can easily read

$$U_q = -\frac{\partial}{\partial \beta^*} \frac{Z_q^{1-q} - 1}{1-q} = -\frac{\partial \ln_q(Z_q)}{\partial \beta^*},$$

where the $q$-logarithm function $\ln_q(x) \equiv (x^{1-q} - 1)/(1-q)$ is a generalization of the usual logarithm function. Through Legendre transform on $\ln_q(Z_q)$, which depends on $\beta^*$, one can find the relation $S_q = k(\ln_q(Z_q) + \beta^* U_q)$. Note that the relation between the generalized internal energy and Tsallis entropy takes the same form as in the conventional statistical mechanics. In fact, introducing $t \equiv 1/(k\beta^*)$, and defining generalized thermodynamic function in the same way as that in the conventional thermodynamics, one can find the same Legendre structure as in the conventional thermodynamics. For example, one can have the GFE

$$F_q \equiv U_q - t S_q = F_q(\beta^*) = -\frac{1}{\beta^*} \frac{Z_q^{1-q} - 1}{1-q} = -\frac{1}{\beta^*} \ln_q(Z_q).$$
Using the basic limit formula \( \lim_{x \to 0} (1 + ax)^{1/x} = e^a \), one can verify that the above generalized thermodynamic function and partition function are reduced to the usual ones in the limit of \( q \to 1 \).

From the above, one can see that although the usual thermodynamical Legendre structure remains valid in Tsallis statistical mechanics, it is evident that the original calculation techniques can not be directly borrowed into the generalized theory. One has to design calculation techniques for the generalized theory. As was stated in the introduction, a united presentation of the perturbation and variational methods for the TNESP has been given in Ref. [5]. Next, for convenience of later contrast, we give a brief introduction on them in the notations here.

Assume that the Hamiltonian can be written as

\[
H = H_0 + \lambda H_I, \tag{7}
\]

where, \( H_0 \) is the Hamiltonian of a soluble model, \( \lambda H_I \) is small enough so that it can be considered as a perturbation on \( H_0 \), and \( \lambda \) is the perturbation parameter. The GFE of the system with \( H, F_q(\lambda) \), is a function of \( \lambda \) and can be expanded as

\[
F_q(\lambda) = F_q(0) + \lambda F_q^{(1)} + \frac{\lambda^2}{2!} F_q^{(2)} + \cdots \tag{8}
\]

with \( F_q^{(1)} = \frac{\partial F_q(\lambda)}{\partial \lambda} \bigg|_{\lambda=0} \), \( F_q^{(2)} = \frac{\partial^2 F_q(\lambda)}{\partial \lambda^2} \bigg|_{\lambda=0} \), \cdots. Eq.(8) is a perturbation expansion series of \( F_q(\lambda) \) in powers of \( \lambda \), and to truncate it at some order, for example \( n \)th order, can provide an approximation to \( F_q(\lambda) \) up to the \( n \)th order. In Ref. [5], approximate expressions for \( F_q(\lambda) \) was derived up to the second order. Through analyzing the approximation expression of \( F_q(\lambda) \) up to the second order, Ref. [5] obtained the generalized Bogoliubov inequality

\[
F_q \leq F_q(0) + \sum_{i=1}^{W} p_i^q (E_i^{(0)}) \langle 0 | \hat{H}_I | i^{(0)} \rangle, \tag{9}
\]

where the symbol \( \hat{O} \) is the operator corresponding to the physical quantity \( O \) and \( | i^{(0)} \rangle \) (and \( < i^{(0)} | \)) is the \( i \)th eigenstate for \( \hat{H}_0 \). This inequality stems from the approximation expression of \( F_q(\lambda) \) up to the first order in the perturbation expansion, and affords a variational method.

According to Ref. [5], the approximate expression of \( F_q(\lambda) \) up to the \( n \)th order is valid only for the case of \( q > 1 - \frac{1}{n} \) because the derivation of the approximate expressions requires the interchangeability between the sum over the quantum numbers and the derivative with
respect to \( \lambda \). As was stated below Eq.(4), when \( q < 1 \), the sum in Eq.(4) and, accordingly, Eq.(6) has a cutoff and so its upper limit depends upon \( \lambda \), leading to the above limitation on the resultant expressions in Ref. [5]. Therefore, the variational method in Ref. [5] can be used only for \( q > 0 \).

We stop here for introducing the perturbation and variational methods in Ref. [5]. Next, we turn to our investigation in the present paper.

**III. VARIATIONAL PERTURBATION APPROXIMATION SCHEME**

For simplicity of the notation, \( k = 1 \) will be taken from now on.

To develop the VPA method, we consider calculating the GFE \( F_q \) (Of course, the method can be used to calculate other generalized thermodynamic potentials). We begin with modifying the Hamiltonian \( H \). Firstly, differently from Eq.(7) in the perturbation method, we add the zero term \( H_0(\mu) - H_0(\mu) \) to \( H \) and write it as

\[
H = H_0(\mu) + H_I(\mu)
\]

with \( H_I = H - H_0(\mu) \) and \( \mu \) an auxiliary parameter. In Eq.(10), \( H_0(\mu) \) is the Hamiltonian of some exactly soluble model which is originally not included in \( H \), and the exact solubility of the model is not affected by values of the auxiliary parameter \( \mu \). That is to say, for a value of \( \mu \), the energy eigenvalues \( E_n^{(0)} \) (non-degenerate, for simplicity), eigenstates \( |n^{(0)} \rangle \), the probability \( p_q(E_n^{(0)}) \), the generalized partition function \( Z_{q,0} \) and the GFE \( F_q^{(0)} \) for the model with \( H_0(\mu) \) are exactly known. Secondly, an artificial parameter \( \epsilon \) is inserted as a factor before \( H_I(\mu) \) in Eq.(10), that is, \( H \) in Eq.(10) is now modified as

\[
H_\epsilon = H_0(\mu) + \epsilon H_I(\mu).
\]

Thus, we have a new system with the Hamiltonian \( H_\epsilon \) which becomes \( H_0(\mu) \) and \( H \) in the cases of \( \epsilon = 0 \) and \( \epsilon = 1 \), respectively. Note that different from \( H \) in Eq.(10), \( H_\epsilon \) depends on \( \mu \) for \( \epsilon \neq 1 \). The above modification provides a possibility that we calculate \( F_q \) for the original system through considering the new system.

For the system with \( H_\epsilon \), suppose that the set of energy eigenvalues are the spectra \( E_{n,\epsilon} \), and the corresponding eigenfunctions is \( |n,\epsilon \rangle \). When the system is in thermal contact with a reservoir, i.e., when we adopt a generalized canonical ensemble, we have the probability
distributions $p_n(E_{n,\epsilon})$, and can calculate the GFE $F_q(\epsilon)$ in the presence of the constraint Eq.(2) according to the definition and expression Eq.(6). In analogy to Eq.(8), one can expand $F_q(\epsilon)$ as the following series

$$F_q(\epsilon) = F_q^{(0)} + \epsilon F_q^{(1)} + \frac{\epsilon^2}{2!} F_q^{(2)} + \frac{\epsilon^3}{3!} F_q^{(3)} + \cdots$$

(12)

with $F_q^{(k)} = \frac{\partial^k F_q(\epsilon)}{\partial \epsilon^k} \bigg|_{\epsilon=0}$ and $F_q^{(0)} = F_q(0)$. This is only a formal expansion, and the parameter $\epsilon$ acts as an expansion order index and needn’t be small. Taking $\epsilon = 1$ in the last equation, we obtain an expansion series of $F_q$ for the system with $H$ which is independent of $\mu$ if the resultant series is not truncated.

Now we have a simple discussion on the expansion Eq.(12). Of course, if $H_0(\mu)$ is naively one part of the original $H$ and $H_I$ can be regarded as a perturbation on $H_0(\mu)$ (in this case, $\mu$ is one of system parameters in $H$), then Eq.(12) with $\epsilon = 1$ is just the perturbation expansion series of $F_q$, Eq.(8). If $H_0(\mu)$ is not a naive part of $H$, as we assumed in Eq.(10), the truncated expression at the first order in $\epsilon$ can lead to a variational method, and substituting the value $\mu$ from the variational method into Eq.(12) with $\epsilon = 1$ will produce an expansion series of $F_q$ around the variational result. In this case, if the resultant variational method can provide a good approximation result for $F_q$, then it can be presumed that the expansion of $F_q$ around the variational result maybe afford a good non-perturbational approximation which will improve variational results. This is the original version of the variational perturbation theory, but the expansion series is possibly divergent [8]. If the variational method cannot provide a good approximation result for $F_q$, the expansion of $F_q$ around the variational result will make no senses. That is to say, in general, the above expansion series Eq.(12) seems to be useless.

However, as was mentioned in Sect.I, once the PMS is employed to single out an appropriate value of $\mu$, Eq.(12) can afford a presumably convergent, systematic non-perturbation approximation method, a modern version of the variational perturbation theory [8]. In Eq.(12), truncating the expansion series at some order in $\epsilon$ and then letting $\epsilon = 1$, the resultant truncated expression is a function of the parameter $\mu$, albeit Eq.(12) with $\epsilon = 1$ is independent of $\mu$. In principle, the value of the truncated expression can possibly take any value with variance of $\mu$, including the exact value of $F_q$. Since $F_q$ is a constant in the space of $\mu$ (the exact $F_q$ is independent of $\mu$), it should be believable that a requirement of the truncated result varying most slowly with the parameter $\mu$ can likely make the truncated
result provide a most reliable approximate result for the exact $F_q$. Employing this requirement to determine the parameter $\mu$ is the main spirit of the so called PMS \[10\]. Generally, the curve of a function varies more slowly near its extremum than in its slope part, and so a simple realization of the PMS is to require the first derivative of the truncated expression with respect to $\mu$ to be zero. Thus, substituting the appropriate value of $\mu$ determined at the truncated order into the corresponding truncated expression of $F_q$ will provide a reasonable and reliable approximation for $F_q$ up to the same order. Such a truncated result at some order is the approximate result of $F_q$ up to the same order in the VPA method.

In brief, the VPA method consists in only two crucial steps: one is to formally expand the quantity $F_q$ in consideration with an adjustable parameter $\mu$ entered, and the other is to determine the value of $\mu$ from the truncated expression of $F_q$ according to the PMS. Now, we continue to perform the first step, derive the first four terms in Eq.(12) (the derivations here are similar to those in Ref. \[5\]), and simultaneously indicate the VPA procedures up to the first, second and third orders, respectively.

The first term in Eq.(12) is straightforwardly

$$F_q^{(0)} \equiv F_q^{(0)}(\mu) = -\frac{1}{\beta^*} \frac{(Z_{q,0}(\beta^*))^{1-q} - 1}{1-q}$$

with

$$Z_{q,0}(\beta^*) = \sum_{n=1}^{W} \left[1 - (1-q)\beta^* E_n^{(0)}\right]^{1/(1-q)}.$$  \hspace{1cm} (14)

For deriving the other three terms, eigenstates of $\hat{H}_\epsilon$ are needed, and so we first consider the eigenequation, $\hat{H}_\epsilon |n, \epsilon \rangle = E_n, \epsilon |n, \epsilon \rangle$. By mimicking Rayleigh-Schrödinger perturbation theory, after substituting the expansions $|n, \epsilon \rangle = |n \rangle + \epsilon |n^{(1)} \rangle + \epsilon^2 |n^{(2)} \rangle + \cdots$  \hspace{1cm} (15)

and

$$E_n, \epsilon = E_n^{(0)} + \epsilon E_n^{(1)} + \epsilon^2 E_n^{(2)} + \cdots$$

into the eigenequation, one can formally have

$$|n^{(1)} \rangle = \sum_{m \neq n} \frac{H_{1, mn}}{E_n^{(0)} - E_m^{(0)}} |m^{(0)} \rangle,$$  \hspace{1cm} (17)
\[ |n^{(2)}> = \sum_{m \neq n} \left[ \sum_{l \neq n} \frac{H_{I,ml}H_{I,ln}}{(E_m^{(0)} - E_n^{(0)})(E_n^{(0)} - E_l^{(0)})} - \frac{H_{I,nn}H_{I,mn}}{(E_n^{(0)} - E_m^{(0)})^2} \right] m^{(0)}> \]
\[ - \frac{1}{2} \sum_{m \neq n} \frac{(H_{I,nn})^2}{(E_n^{(0)} - E_m^{(0)})^2} n^{(0)}> \]

(18)

and so on. Here, \( H_{I, mn} = \langle m | \hat{H}_I(\mu) | n > \). By the way, the expansion expressions, Eqs.(15) and (16), together with the PMS can lead to a VPA method to solve Schrödinger equation \([9\text{ (PRD)}]^{[15]}\).

For the second term of Eq.(12), \( F_q^{(1)} = \frac{\partial F_q(\epsilon)}{\partial \epsilon} \bigg|_{\epsilon=0} \) can be calculated as

\[
F_q^{(1)} = \left[ \frac{\partial}{\partial \epsilon} \frac{1 - Z_{q,\epsilon}^{-1}}{\beta^*(1-q)} \right]_{\epsilon=0} = Z_{q,\epsilon}^{-q} \sum_n \left[ 1 - (1-q) \beta^* E_n \right] \frac{\partial E_n, \epsilon}{\partial \epsilon} \bigg|_{\epsilon=0}
\]

(19)

with \( Z_{q,\epsilon} \) the generalized partition function for the system with \( H_\epsilon \). From Hellmann-Feynman theorem \( \frac{\partial E_n}{\partial \epsilon} = \langle \epsilon, n | \frac{\partial \hat{H}}{\partial \epsilon} | n, \epsilon > \), we have

\[
F_q^{(1)} = \left[ Z_{q,\epsilon}^{-q} \sum_n \left[ 1 - (1-q) \beta^* E_n \right] \frac{\partial E_n, \epsilon}{\partial \epsilon} \bigg|_{\epsilon=0} \right] = \sum_n p_n^0(E_n^0) H_{I, nn} = < H_I >_q^0.
\]

(20)

which takes the same form as Eq.(5) in Ref. [3]. Thus, the truncated expression for \( F_q \) at the first order, \( F_q^I(\mu) \), is

\[
F_q^I(\mu) = F_q^0 + F_q^{(1)} = \frac{1 - Z_{q,0}^{-1}}{\beta^*(1-q)} + < H_I >_q^0.
\]

(21)

The right hand side of last equation has the same form as that in the right hand side of the inequality, Eq.(9). \( F_q^I(\mu) \) is a function of \( \mu \) and a different value of \( \mu \) produces a different approximation for \( F_q \) which maybe have nothing to do with the exact value of \( F_q \). However, if the value of \( \mu \) in Eq.(21) is chosen from roots of the following condition

\[
\frac{\partial F_q^I(\mu)}{\partial \mu} = 0
\]

(22)

according to the PMS, then \( F_q^I(\mu) \) in Eq.(21) would produce a most reliable approximation for \( F_q \) up to the first order. Since \( F_q \) has the same form as the right hand side of the inequality, Eq.(9), the VPA procedure up to the first order for the case of \( q > 0 \) is consistent with the variational method based on the Bogoliubov inequality in Ref. [3], and so the appropriate root of Eq.(22) for \( \mu \) makes \( F_q^I(\mu) \) minimal. For the case of \( q \leq 0 \), an example
in next section shows that the appropriate root of Eq.(22) for $\mu$ also makes $F_q^I(\mu)$ minimal. This suggests that the VPA procedure up to the first order is generally a variational method which provides a reliable upper limit for the exact $F_q$.

In order to give the truncated expression for the GFE at the second order $F_q^{II}(\mu) = F_q^I(\mu) + F_q^{(2)}/2!$, we calculate $F_q^{(2)}$ as follows. A straightforward differentiation gives

$$F_q^{(2)} = \frac{\partial^2 F_q}{\partial \epsilon^2} \bigg|_{\epsilon=0} = \beta^2 q Z_{q,0}^q \left[ (< H_I >_q)_0^2 \right] - \sum_n \left( p_q(E_n^{(0)}) \right)^{2q-1} \left( H_I, nn \right)^2 \right] + \sum_n \left( p_q(E_n^{(0)}) \right)^n \frac{\partial < \epsilon, n > H_I | n, \epsilon >}{\partial \epsilon} \bigg|_{\epsilon=0}. \quad (23)$$

From Eq.(15), we have $\frac{\partial n, \epsilon >}{\partial \epsilon} \bigg|_{\epsilon=0} = |n>^{(1)}$. Consequently, Eq.(23) becomes

$$F_q^{(2)} = \beta^2 q Z_{q,0}^q \left[ (< H_I >_q)_0^2 \right] - \sum_n \left( p_q(E_n^{(0)}) \right)^{2q-1} \left( H_I, nn \right)^2 \right] + 2 \sum_n \left( p_q(E_n^{(0)}) \right)^n \sum_{m \neq n} \frac{|H_{I, nm}|^2}{E_n^{(0)} - E_m^{(0)}}. \quad (24)$$

Formally, the right hand side of Eq.(24) can be rewritten as Eq.(6) in Ref. [2]. According to the PMS, using the reasonable root of the condition

$$\frac{\partial F_q^{II}(\mu)}{\partial \mu} = 0 \quad (25)$$

as the value of $\mu$, one can give the approximation result for $F_q$ up to the second order from $F_q^{II}(\mu)$. The approximation result up to the second order would improve the approximation result up to the first order.

Similarly, one can calculate $F_q^{(3)}$. In the calculation, we need the additional relation $\frac{\partial^3 |n, \epsilon >}{\partial \epsilon^2} \bigg|_{\epsilon=0} = 2 |n>^{(2)}$, which can be easily obtained from Eqs.(15), (17) and (18). Thus, $F_q^{(3)}$ can be written as

$$F_q^{(3)} = \beta^2 q (q + 1) Z_{q,0}^{2q-2} (< H_I >_q)_0^3 - 3 \beta^2 q^2 Z_{q,0}^{2q-2} \sum_n \left( p_q(E_n^{(0)}) \right)^{2q-1} \left( H_I, nn \right)^2 < H_I >_q^0$$

$$+ \beta^2 q (2q - 1) Z_{q,0}^{2q-2} \sum_n \left( p_q(E_n^{(0)}) \right)^{3q-2} \left( H_I, nn \right)^3$$

$$+ 6 \beta^2 q Z_{q,0}^{q-1} \sum_n \left( p_q(E_n^{(0)}) \right)^q < H_I >_q^0 - \left( p_q(E_n^{(0)}) \right)^{2q-1} \left( H_I, nn \right) \sum_{m \neq n} \frac{|H_{I, nm}|^2}{E_n^{(0)} - E_m^{(0)}}$$

$$+ 6 \sum_n \left( p_q(E_n^{(0)}) \right)^q \left[ \sum_{l \neq n} \sum_{m \neq n} \frac{H_{I, ml} H_{I, lm} H_{I, nm}}{(E_n^{(0)} - E_m^{(0)})(E_n^{(0)} - E_l^{(0)})} - \sum_{m \neq n} \frac{|H_{I, nm}|^2 H_{I, nn}}{(E_n^{(0)} - E_m^{(0)})^2} \right]. \quad (26)$$
Then one can have the truncated expression for $F_q$ at the third order, $F_{q}^{III}(\mu) = F_{q}^{II}(\mu) + \frac{1}{3!}F_{q}^{(3)}$. Furthermore, using the reasonable root of the condition

$$\frac{\partial F_{q}^{III}(\mu)}{\partial \mu} = 0 \quad (27)$$

as the value of $\mu$, one can give the approximation result for $F_q$ up to the third order from $F_{q}^{III}(\mu)$.

In the same way, one can consider VPA results for $F_q$ up to higher orders. Obviously, the VPA results up to various orders constitute a sequence of the approximation results of $F_q$. Owing to the employment of the PMS, the values of $\mu$ determined depend upon the truncated orders, and the value of $\mu$ at a given order is different from values of $\mu$ at other orders. Presumably, it is the dependence of $\mu$ upon the truncated order that makes the sequence of the VPA results of $F_q$ up to various orders converge to the exact $F_q$. Although we cannot verify this convergent property of the variational perturbation theory, investigations in other fields have provided such a few examples [8, 17]. Additionally, in the example of next section, generally, the VPA result up to the third order approaches more closely the exact $F_q$ than the approximations up to the lower orders.

The second crucial step plays a vital role in the VPA method, and one have to perform it very carefully. Sometimes, Eqs.(22), (25) and (27) can not provide appropriate roots for $\mu$, and in those cases one should render the second derivative of the truncated expressions for $F_q$ with respect to $\mu$ zero to determine $\mu$. This can be understandable because the curve of a function varies more slowly near its knee than in its slope part (As a matter of fact, when there exist both an extremum and a knee, one should analyze behaviors of the truncated expressions as a function of $\mu$ near the extremum and knee to determine $\mu$ according to the PMS). In case the second derivative condition can not provide an appropriate root for $\mu$, too, then the VPA method cannot provide an approximation result for $F_q$ up to the truncated order in consideration, and one should further consider VPA result up to the next order. Furthermore, when there exist multi-roots of the vanishing derivatives for $\mu$, one should choose to adopt the root near which the truncated result varies most slowly with $\mu$. Next section, we will show how to determine $\mu$ according to the PMS in a concrete example.

In concluding this section, we intend to emphasize one point. In the above calculations, the interchange between the differentiation with respect to $\epsilon$ and the sum over eigenstates was involved. As was mentioned in last section, the interchangeability between the differentiation
and the sum leads to a limitation for the variational and perturbation methods in Ref. [5]. Nevertheless, for the VPA method developed here, the relevant calculations are only formal calculations and the resultant expressions are independent of $\varepsilon$, and presumably, we suggest that the VPA method needn’t suffer those limitations on the methods in Ref. [5]. At least, this point yields no problem in the example of next section.

IV. A CLASSICAL HARMONIC OSCILLATOR

For a one-dimensional classical harmonic oscillator with mass $M$ and an angular frequency $\omega$, the Hamiltonian is $H = p^2/(2M) + M\omega^2x^2/2$ with $x$ the coordinate and $p$ the momentum. In a manner analogous to the one used for the quantum oscillator, we can associate with the oscillator a continuous energy spectra $E_n = \delta_o n$, where $\delta_o$ is an arbitrary positive constant with the dimension of energy and $n$ any positive real number including 0 [12]. Then, from Eq.(4), the generalized partition function can be written and calculated as

$$Z_q = \int_0^N [1 - (1 - q)\beta^* n\delta_o]^{1/(1-q)}dn = \frac{1}{(2 - q)\beta^* \delta_o}$$

(28)

with $N \to \infty$ for the case of $q > 1$ and $N = 1/[(1 - q)\beta^* \delta_o]$ for the case of $q < 1$ (In this section, we suppose that $\beta^* > 0$.). The right hand side of Eq.(28) is valid only for $q < 2$ and $Z_q$ is divergent for $q > 2$. So, Eq.(6) leads to the GFE for the classical harmonic oscillator

$$F_q = -\frac{1}{(1 - q)\beta^*}[(\frac{1}{(2 - q)\beta^* \delta_o})^{1-q} - 1].$$

(29)

Last equation with $\delta_o = \hbar\omega$ is just Eq.(14) in Ref. [5].

On the other hand, for a particle with mass $M$ which moves in a one-dimensional box, the Hamiltonian $H_0(L) = p^2/(2M) + V_0$ with $V_0 = 0$ for $|x| < \frac{L}{2}$ and $V_0 \to \infty$ for $|x| \geq \frac{L}{2}$. In analogy to what we did for the oscillator, we can associate with the particle a continuous energy spectra $E_n^{(0)} = \delta_b n^2/(2ML^2)$, where $\delta_b$ is an arbitrary positive constant with the dimension of action and $n$ any positive real number including 0. So the generalized partition function for the particle in the box can be written and calculated as

$$Z_{q,0} = \int_0^N [1 - (1 - q)\beta^* \frac{n^2\delta_b}{2ML^2}]^{1/(1-q)}dn = \begin{cases} \frac{L}{2\delta_b} \sqrt{\frac{2M}{(1-q)\beta^*}} B(\frac{1}{2}, \frac{2-q}{2-q-1}), & q < 1 \\ \frac{L}{2\delta_b} \sqrt{\frac{2M}{(q-1)\beta^*}} B(\frac{1}{2}, \frac{3-q}{2(q-1)}), & q > 1 \end{cases}$$

(30)

with $N \to \infty$ for the case of $q > 1$ and $N = L\sqrt{2M/((1 - q)\beta^*/\delta_b}$ for the case of $q < 1$. In Eq.(30), $B(x, y)$ is the Beta function. Note that $Z_{q,0}$ is convergent only for the case of $q < 3$. 

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In the calculation of the above equation, the formulae 8.380(1) and 8.380(3) in Ref. [18] were employed. Owing to 

\[ B(x, y) = \Gamma(x)\Gamma(y)/\Gamma(x+y) \]

with \( \Gamma(x) \) the gamma function (8.384(1) in Ref. [18]), Eq.(30) with \( \delta_b = \hbar\pi \) is nothing but Eq.(11) in Ref. [5]. From Eqs.(6) and (30), the GFE for the classical particle in the box is easily calculated as

\[ F_q^0(L) = \frac{1}{\beta^*(1-q)} - \frac{1}{\beta^*(1-q)}C_q, \]

where

\[ C_q = \begin{cases} 
\left( \frac{L}{\delta_b(3-q)} \right)^{1/2} \frac{\Gamma(\frac{1}{2})}{\beta^*(1-q)\Gamma(\frac{1}{2}+\frac{1}{2})}^{1-q}, & q < 1 \\
\left( \frac{L}{2\delta_b} \right)^{1/2} \frac{\Gamma(\frac{1}{2}-\frac{1}{2})}{\beta^*(q-1)\Gamma(\frac{1}{2})}^{1-q}, & q > 1 
\end{cases} \]

Since the above two systems are exactly solved, Ref. [5] employed them to illustrate the variational method there. In the present paper, we will use them to illustrate the VPA method. That is, by regarding the Hamiltonian of the classical particle in the box as \( H_0(\mu) \) in eq.(10) and using the VPA scheme in last section, we will calculate the GFE for the classical harmonic oscillator up to the third order and then make comparisons among the results up to the various orders and the exact result for the oscillator. Next, the present section will be divided into three subsections. In subsection A, the truncated variational perturbation expressions for the classical harmonic oscillator will be given up to the third order. The values of \( \mu \) in the truncated expressions will be determined according to the PMS in subsection B, and the approximated values of the GFE will be calculated and compared with the exact result in subsection C.

### A. Truncated Expressions

Take the width \( L \) of the box as the adjustable parameter \( \mu \) in our VPA scheme. Then, \( H_1(\mu) \) in last section is now

\[ H_1(L) = \begin{cases} 
\frac{M\omega^2x^2}{2}, & |x| < \frac{L}{2} \\
\frac{M\omega^2x^2}{2} - \infty, & |x| \geq \frac{L}{2} 
\end{cases} \]  

(32)

For the classical particle in the box, the speed \( v_n = n\delta_b/(ML) \) corresponds to the particle energy \( E_n^{(0)} \). In a state with the energy \( E_n^{(0)} \), the particle moves in the box back and forth at the constant speed \( v_n \), and so the probability of finding the particle in one of the directions near \( x \) (\(|x| < L/2\)) is \( dx/(v_nT) \) with \( T = 2L/v_n \) (except for \( n = 0 \)), but zero out of the box.
Thus, in the present case, the matrix elements $H_{I,nm}$ appeared in Eqs. (20), (24) and (26) can be straightforwardly calculated as

$$H_{I,nm} = \delta_{nm} 2 \int_{-L/2}^{L/2} \frac{M \omega^2 x^2}{2} dx = \delta_{nm} \frac{M \omega^2 L^2}{24},$$

where $\delta_{nm} = 0$ for $m \neq n$ and $\delta_{nn} = 1$.

Now we are at the position to calculate the truncated expressions for $F_q$ of the classical harmonic oscillator up to the third order from Eqs. (13), (20), (24) and (26). The zeroth-order expression is Eq. (31). At the first order, one can have, from Eq. (20),

$$F_q^{(1)} = \sum_n p_q^e (E_n^0) H_{I,nm} = \frac{M \omega^2 L^2}{24} (Z_q,0)^{-q} \int_0^N [1 - (1 - q) \beta^* \frac{n^2 \delta^2}{2ML^2}]^{q/(1-q)} dn$$

$$= \frac{M \omega^2 L^2}{24} (Z_q,0)^{-q} \left\{ \begin{array}{ll} \frac{L}{2M} \sqrt{\frac{2M}{(1-q) \beta^*}} B\left(\frac{1}{2}, \frac{1}{1-q}\right), & q < 1 \\ \frac{L}{2M} \sqrt{\frac{2M}{(q-1) \beta^*}} B\left(\frac{1}{2}, \frac{q+1}{2(q-1)}\right), & q > 1 \end{array} \right.$$$$= \frac{M \omega^2 L^2}{24} \left[ 3 - q \frac{2}{2} C_q \right].$$

The right hand side of last equation is identical to Eq. (12) in Ref. [5].

At the second order in $\epsilon$, Eq. (24) leads to

$$F_q^{(2)} = \beta^* q Z_{q,0}^{-1} \left[ (H_I)^0 q^0 \sum_n (p_q^e (E_n^0)))^{2q-1} (H_{I,nm})^2 \right]$$

$$= \beta^* q Z_{q,0}^{-1} \left[ (F_q^{(1)})^2 - \frac{M^2 \omega^4 L^4}{(24)^2} (Z_q,0)^{1-2q} \int_0^N [1 - (1 - q) \beta^* \frac{n^2 \delta^2}{2ML^2}]^{(2q-1)/(1-q)} dn \right]$$

$$= \beta^* q Z_{q,0}^{-1} (F_q^{(1)})^2 - \beta^* q Z_{q,0}^{-1} \frac{M^2 \omega^4 L^4}{(24)^2} (Z_q,0)^{1-2q} \left\{ \begin{array}{ll} \frac{L}{2M} \sqrt{\frac{2M}{(1-q) \beta^*}} B\left(\frac{1}{2}, \frac{1}{1-q}\right), & q < 1 \\ \frac{L}{2M} \sqrt{\frac{2M}{(q-1) \beta^*}} B\left(\frac{1}{2}, \frac{3q-1}{2(q-1)}\right), & q > 1 \end{array} \right.$$$$= \beta^* \frac{M^2 \omega^4 L^4}{(24)^2} \left[ q^2 (1-q)^2 \frac{4}{4} C_q \right].$$

(35)
Finally, we consider the third order. Eq.(26), in the present case, is reduced to

\[ F_q^{(3)} = \beta^* q (q + 1) Z_{q,0}^{2q-2} \left( < H_I >_{q}^{0} - 3 \beta^* (q-1) Z_{q,0}^{2q-2} \sum_{n} (p_{q}(E_{n}^{(0)}))^{2q-1} (H_{I,n})^2 < H_I >_{q}^{0} \right) + \beta^* q (2q - 1) Z_{q,0}^{2q-2} \sum_{n} (p_{q}(E_{n}^{(0)}))^{3q-2} (H_{I,n})^3 \]

\[ = \beta^* q (q + 1) Z_{q,0}^{2q-2} (F_{q}^{(1)})^3 - 3 \beta^* q (q-1) Z_{q,0}^{2q-2} \sum_{n} (p_{q}(E_{n}^{(0)}))^{2q-1} (H_{I,n})^2 \int_{0}^{1} \left[ 1 - (1 - q) \beta^* \frac{n^2 \delta_{n}^2}{2ML^2} \right]^{3q-2} dn \]

\[ + \beta^* q (2q - 1) Z_{q,0}^{2q-2} \sum_{n} (p_{q}(E_{n}^{(0)}))^{3q-2} (H_{I,n})^3 \int_{0}^{1} \left[ 1 - (1 - q) \beta^* \frac{n^2 \delta_{n}^2}{2ML^2} \right]^{3q-2} dn \]

\[ = \beta^* q (q + 1) Z_{q,0}^{2q-2} (F_{q}^{(1)})^3 - 3 \beta^* q (q-1) Z_{q,0}^{2q-2} \sum_{n} (p_{q}(E_{n}^{(0)}))^{2q-1} (H_{I,n})^2 \int_{0}^{1} \left\{ \frac{L}{2 \delta_{b} \sqrt{q}} \left[ B \left( \frac{1}{2}, \frac{3q}{2q-1} \right) \right] \right\} \]

\[ + \beta^* q (2q - 1) Z_{q,0}^{2q-2} \sum_{n} (p_{q}(E_{n}^{(0)}))^{3q-2} (H_{I,n})^3 \int_{0}^{1} \left\{ \frac{L}{2 \delta_{b} \sqrt{q}} \left[ B \left( \frac{1}{2}, \frac{5q-3}{2q-1} \right) \right] \right\}, \quad q > 1 \]

\[ = \beta^* \frac{3 \omega^6 L^6}{(24)^3} \left( 1 + q \right) \left( 3 - q \right) (q - 1)^3 C_q \]. \quad (36) \]

Thus, collecting Eqs.(31),(34),(35) and (36), one can get \( F_q^{I} \), \( F_q^{II} \) and \( F_q^{III} \), the truncated expressions for \( F_q \) of the classical oscillator at the first, second and third orders. When \( q < 1 \), the truncated expression for \( F_q \) at the third order is

\[ F_{q,\text{sup}}^{III}(L) = \frac{1}{\beta^* (1 - q)} + \left( \frac{L}{2 \delta_{b} \sqrt{q}} \sqrt{\frac{2M \pi}{\beta^* (1 - q)}} \right) \left[ \frac{1}{\beta^* (1 - q)} \right]^{-q} \left[ \frac{2}{\beta^* (1 - q)} \right] (3 - q) \]

\[ + \frac{M \omega^2 L^2}{24} - \frac{\beta^* M^2 \omega^4 L^4 (1 - q)^2}{(24)^2} + \frac{\beta^* M^3 \omega^6 L^6}{(24)^4} (q + 1)(q - 1)^3 \], \quad (37) \]

and when \( 3 > q > 1 \), it is

\[ F_{q,\text{sub}}^{III}(L) = \frac{1}{\beta^* (1 - q)} + \left( \frac{L}{2 \delta_{b} \sqrt{q}} \sqrt{\frac{2M \pi}{\beta^* (1 - q)}} \right) \left[ \frac{1}{\beta^* (1 - q)} \right]^{-q} \left[ \frac{2}{\beta^* (1 - q)} \right] (3 - q) \]

\[ + \frac{M \omega^2 L^2}{24} - \frac{\beta^* M^2 \omega^4 L^4 (1 - q)^2}{(24)^2} + \frac{\beta^* M^3 \omega^6 L^6 (q + 1)(q - 1)^3 (3 - q)}{2} \]. \quad (38) \]

For the case of \( q > 3 \), \( F_{q,\text{sub}}^{III}(L) \) in Eq.(38) is divergent. In Eqs.(37) and (38), all the terms in which the powers in \( \omega^2 \) are lower than the second and the third powers give the truncated expressions for \( F_q \) at the first and second orders, respectively. Next subsection, we will determine \( L \) in them according to the PMS to get approximations for \( F_q \).
In the following subsections, when a numerical calculation is performed, we will take \( M = 1, \omega = 1, \delta_b = 1/2 \), and we will consider only the case of \( q < 2 \) which is the convergent range of \( F_q \) for the oscillator. \((\delta_b = 1/2 \text{ corresponds to the case } \hbar = 1 \text{ in Ref. [5].})\)

B. Determining \( L \)

\( L \) must be positively real.

Up to the first order in \( \epsilon \), for the cases of both superextensiveness and subextensiveness, Eq.(22) leads to the equation

\[- \frac{48}{\beta^*} + M\omega^2(-3 + q)^2L^2 = 0. \tag{39}\]

To see whether \( F_q^I(L) \) is most insensitive to \( L \) near the positive root of Eq.(39) or not, one can analyze varying property of \( F_q^I(L) \) as a function of \( L \). For illustration, the function \( F_q^I(L) \) is depicted for \( \beta^* = 1 \) and some values of \( q \) in Fig.1. Fig.1 indicates that the positive root of Eq.(39) for \( L \) makes \( F_q^I(L) \) reach a minimum and simultaneously be most insensitive to \( L \). So, we should choose this positive root as the value of \( L \)

\[ L^I = \frac{4}{3} q\left( \frac{3}{M\omega^2\beta^*}\right)^{1/2}, \tag{40} \]
which is identical to Eq.(13) in Ref. [5]. The minimum \( F_I^q(L) \) provides an upper limit for \( F_q \). Thus, the VPA up to the first order is really a variational method and it, in the case of \( q > 0 \), is consistent with the variational method in Ref. [5] which is based on the generalized Bogoliubov inequality, Eq.(9) in Ref. [5].

Up to the second order, for the cases of both superextensiveness and subextensiveness, Eq.(25) leads to the equation

\[
4608\beta^*-2 - 96L^2M(q - 3)^2\beta^{*-1}\omega^2 + L^4M^2(q - 1)^2(15 - 8q + q^2)\omega^4 = 0. \tag{41}
\]

Last equation produces four roots for \( L \). The roots are real only when \(-1.96239 < q < 1.62222 \) and \( 3 < q < 5.34017 \), and two of them are positive as well as the other roots are negative. To choose an appropriate root as \( L \), \( F_{q}^{II}(L) \), as a function of \( L \), is representatively illustrated for \( \beta^* = 1 \) and some values of \( q \) in Fig.2. In Fig.2, horizontal lines represent exact values of \( F_q \), and every pair of curve and horizontal line with an identical line-type is for the same value of \( q \). In the figure, every curve has a minimum and a maximum.

![FIG. 2: The dependence of \( F_{q}^{II}(L) \) upon \( L \) for some values of \( q \) and at \( \beta^* = 1 \). The dot-dashed and dotted curves are for \( q = 1.25 \) and \( 0.1 \), respectively, and the solid and dashed curves in the image are for \( q = -0.5 \) and \( -1.5 \), respectively. Horizontal lines represent exact values of \( F_q \), and every pair of curve and horizontal line with an identical line-type is for the same value of \( q \). In the figure, every curve has a minimum and a maximum.](image)

values of \( F_q \), and every pair of curve and horizontal line with an identical line type is for the same value of \( q \). From curves in Fig.2, one can see that the smaller positive root makes \( F_{q}^{II}(L) \) minimal whereas the larger positive root makes \( F_{q}^{II}(L) \) maximal. Hence, \( F_{q}^{II}(L) \) is more insensitive to \( L \) near the smaller positive root than near the other positive root, and so the smaller root should be chosen as the value of \( L \), \( L^{II} \), for \(-1.96239 < q < 1.62222 \).
For the other values of $q$, Eq.(25) cannot produce reasonable values for $L$. In this case, the vanishing requirement for the second derivative of $F_{II}^q(L)$ with respect to $L$ should be considered and yields the following equation for $L$

$$
-14L^4M^2q^4\omega^4 + L^4M^2q^5\omega^4 + 2L^2Mq^2\omega^2(384\beta^{* -1} - 83L^2M\omega^2)
+12L^2M\omega^2(144\beta^{* -1} - 5L^2M\omega^2) + 24L^2Mq^2\omega^2(-4\beta^{* -1} + 3L^2M\omega^2)
+q(4608\beta^{* -2} - 2016L^2M\beta^{* -1}\omega^2 + 167L^4M^2\omega^4) = 0,
$$

(42)

which is valid for the cases of both superextensiveness and subextensiveness. Eq.(42) produces four roots for $L$. There exist real roots only when $-3.02227 < q < 3$ and $3.95406 < q < 5.601$, and for $q < 0$, two of them are positive as well as the other roots are negative, and for $q > 0$, only one positive root exists. To choose an appropriate root as $L$ for the case of $-3.02227 < q < -1.96239$, $F_{II}^q(L)$, as a function of $L$, is typically illustrated for $\beta^{*} = 1$ and $q = -2$ in Fig.3. For completeness, we also depict $F_{II}^q(L)$ for $q = 1.8$ (which is involved in the range of $1.62222 < q < 2$) in Fig.3 as an image. In this figure, the solid curve for $q = -2$ has two knees which correspond to the two positive roots of Eq.(42) for $L$: 1.13365 and 1.94787. Obviously, $F_{II}^q(L)$ is more insensitive to $L$ near the larger positive root than near the other positive root. The same situation occurs for other negative values of $q$ ($-3.02227 < q < -1.96239$), and so the larger positive root of Eq.(42) should be chosen as the value of $L$, $L_{II}$, for $-3.02227 < q < -1.96239$. Furthermore, as is
illustrated in the image of Fig.3, for the case of $2 > q > 1.62222$, $F_q^{II}(L)$ is most insensitive to $L$ near the positive root of Eq.(42), and so the positive root of Eq.(42) should be chosen as the value of $L$, $L^{II}$, for $1.62222 < q < 2$. By the way, for the case of $q < -3.02227$, there exists not any appropriate root of Eq.(41) or Eq.(42) for $L$ and so the VPA method cannot provide an approximation for $F_q$ up to the second order in this case.

Finally, we determine $L$ so as to approximate $F_q$ up to the third order. For the cases of both superextensiveness and subextensiveness, Eq.(27) leads to the equation

$$-66352 \beta^{*-3} + 13824 L^2 M (-3 + q)^2 \beta^{*-2} \omega^2 - 144 L^4 M^2 (-1 + q^2)(15 - 8q + q^2) \beta^{-1} \omega^4$$

$$+ L^6 M^3 (-1 + q)^3 (21 + 11q - 9q^2 + q^3) \omega^6 = 0$$

(43)

Last equation produces six roots for $L$. Among the six roots, there exist three positive roots for $-3 < q < -1$, two positive roots for $-1 < q < 1$ and only one positive root for $q < -3$, $1 < q < 3$ and $q > 7$. In Fig.4, $F_q^{III}(L)$, as a function of $L$, is typically depicted for some values of $q$ and $\beta^*$. In Fig.4, the dotted curve is for $\{q, \beta^*\} = \{-2.9, 1\}$, and has two minima and a maximum, which corresponds to the case of having three positive roots. In this case, it is evident, from Fig.4, that $F_q^{III}(L)$ is most insensitive to $L$ near the smallest
positive root of Eq.(43) (the curvature of the curve at the smallest positive root is smaller than that at the largest positive root), and so the smallest positive root should be chosen as the value of \( L \), \( L^{III} \), for \(-3 < q < -1\). The short-dashed and the dot-dashed curves are for \( \{q, \beta^*\} = \{0.5, 10\} \) and \( \{-0.5, 1.9608\} \) and have a minimum at the smaller positive root and a maximum at the other positive root. So, for the case of having two positive roots, the smaller positive root is appropriate for \( L \) when \(-1 < q < 1\). As for the cases of \( q < -3 \) and \( 1 < q < 2 \), the solid and the long-dashed curves indicate that \( F^{III}_q(L) \) reaches an extremum, the minimum at the positive root, and so it can be taken as the value of \( L \), \( L^{III} \).

According to the PMS, we have determined \( L \) for all cases which we are interested in. In the above, analytical and numerical discussions are done with Mathematica, and we do not list all expressions of roots of Eqs.(41), (42) and (43) because they are too lengthy. Note that although \( L \) is determined as \( L^I, L^{II} \) and \( L^{III} \) for approximating \( F_q \) up to the first, second and third orders, respectively, it is not meant that \( L \) is being expanded as a series.

C. Generalized Free energy and Comparisons

From analysis and results in last subsection, employing Mathematica package, one can get, for various ranges of \( q \), the expressions of \( F^I_q(L = L^I) \), \( F^{II}_q(L = L^{II}) \) and \( F^{III}_q(L = L^{III}) \), the approximations of the GFE \( F_q \) up to the first, second and third orders. Regarding them as functions of \( t \) (\( t = 1/\beta^* \)) and the non-extensiveness index \( q \), respectively, we can numerically calculate and compare them with the exact \( F_q \), Eq.(29).

The exact free energy, \( F_q \) in Eq.(29), reaches a maximum at \( t = \delta_0(2 - q)^{q/(q-1)} \) for any given value of \( q < 2 \). As a function of \( q \), \( F_q \) in Eq.(29) has a maximum for any \( t < 0.17 \) or so, and, otherwise, reaches first a maximum and then a minimum when \( q \) increases up to \( q = 2 \).

In Ref. [5], the approximate GFE from variational method there was considered for \( 0 < q < 2 \), and when \( t \) increases or when \( q \) decreases, the discrepancies between the approximate values and the exact values become more and more evident. Here, we consider the VPA GFE up to the first order, \( F^I_q(L = L^I) \), for all values of \( q < 2 \), which with \( 0 < q < 2 \) is identical to that in Ref. [5]. Basically, \( F^I_q(L = L^I) \), as a function of \( t \) or \( q \), mimics the feature of the exact free energy, and for a given value of \( t \), when \( q \) approaches 2 or is sufficiently negative, the error \( \Delta F \equiv F^I_q(L = L^I) - F_q \) is very small whereas \( \Delta F \) is not small for intermediate
values of $q$. Interestingly, the dependent feature of $\Delta F$ upon $q$ is similar to that of curvature of $F_q^I(L)$ at $L = L^I$, $F'' \equiv \frac{d^2F_q^I(L)}{dL^2}|_{L=L^I}$, upon $q$ (For subextensiveness case, when $t$ is small, there exists not such a similarity.). For an illustration of this similarity, in Fig.5, we depict the dependence of $\Delta F$ (dashed curve) and $F''$ (solid curve) upon $q$ at $t = 3$. In Fig.5, the

![Graph](image_url)

FIG. 5: The dependence of $\Delta F$ (dashed curve) and $F''$ (solid curve) upon $q$ at $t = 3$.

image is drawn for the range of $-12 < q < 0$, and evidently indicates that while the solid curve reaches the maximum, the dashed curve also gets to its maximum. This similarity can be understood from the PMS. Smaller the curvature at $L = L^I$ is, more slowly $F_q^I(L)$ varies near $L = L^I$, and so, closer $F_q^I(L = L^I)$ approaches $F_q$ according to the spirit of the PMS, yielding the similarity.

The approximation of $F_q$ up to the second order, $F_q^{II}(L = L^{II})$, improves the approximation of $F_q$ up to the first order, $F_q^I(L = L^I)$, the variational result for the range of $-3.02 < q < 2$ where $F_q^{II}(L = L^{II})$ makes senses, and the approximation of $F_q$ up to the third order, $F_q^{III}(L = L^{III})$, generally further improves the variational result. For a comparison and an illustration, the exact and various approximate results are shown at $t = 1$ in Fig.6. In Fig.6, the solid, short-dashed, dot-dashed and dotted curves are $F_q$, $F_q^I(L = L^I)$, $F_q^{II}(L = L^{II})$ and $F_q^{III}(L = L^{III})$, respectively (note that the dot-dashed curve, $F_q^{II}(L = L^{II})$, interrupts at $q = -3.02$ or so, and almost coincides with the dotted curve, $F_q^{III}(L = L^{III})$, when $q > -1$ or so). Additionally, the long-dashed curve in Fig.6 is $F_q^{III}(L = L^I)$, and obviously it is a bad approximation for $F_q$ when $q > -2$ or so, albeit $F_q^{II}(L = L^I)$ can produce as a good approximation for $F_q$ as $F_q^{III}(L = L^{II})$ does. Fig.6
FIG. 6: The dependence of \( F_q \) and its approximations up to various orders upon \( q \) at \( t = 1 \).

The solid, short-dashed, dot-dashed and dotted curves are the exact \( F_q \) and its approximations \( F_q^I(L = L^I) \), \( F_q^{II}(L = L^{II}) \) and \( F_q^{III}(L = L^{III}) \), respectively. The dot-dashed curve interrupts at \( q = -3.02 \) or so, and almost coincides with the dotted curve when \( q > -1 \) or so. The long-dashed curve is \( F_q^{III}(L = L^I) \), and goes up quickly when \( q > -2 \) or so.

indicates that the improvement of \( F_q^{II}(L = L^{II}) \) to the variational result is substantial when \(-3.02 < q < 0\). Furthermore, the approximation of \( F_q \) up to the third order mimics the exact \( F_q \) better than \( F_q^{II}(L = L^{II}) \), and substantially improves the variational result for the range of \(-6 < q < -3.02\) where \( F_q^{II}(L = L^{II}) \) is invalid. For the cases of both \( q < -6 \) and \( q > 0 \), \( F_q^{II}(L = L^{II}) \) and/or \( F_q^{III}(L = L^{III}) \) only slightly improve the variational result.(By the way, because \( F_q \) and its various approximations here vary slowly with \( q \) near their maxima, the humps of those curves in Fig.6 are not evident.)

For further and more clear illustration and comparison, we also consider the dependence of the various approximations here upon \( t \). In Figs.7,8,9 and 10, \( F_q \), \( F_q^I(L = L^I) \), \( F_q^{II}(L = L^{II}) \) and \( F_q^{III}(L = L^{III}) \) are depicted for some typical values of \( q \) as the solid, short-dashed, dot-dashed and dotted curves, respectively, and, for the sake of clearness, we redraw them for the range of \( 0 < t < 2 \) in the image.

Fig.7 is drawn for \( q = -7 \), and so there is not a dot-dashed curve owing to the invalidness of \( F_q^{II}(L = L^{II}) \) for this case. In this figure, the long-dashed curve is \( F_q^{III}(L = L^I) \) which goes up when \( t > 5 \) or so, and is not given in Fig.8, 9 and 10 because it behaves too badly. Fig.7 indicates that although \( F_q^{II}(L = L^{II}) \) does not exist, \( F_q^{III}(L = L^{III}) \) substantially
FIG. 7: The dependence of $F_q$ and its approximations up to various orders upon $t$ at $q = -7$. The solid, short-dashed and dotted curves are the exact $F_q$ and its approximations $F^I_q(L = L^I)$ and $F^{III}_q(L = L^{III})$, respectively. The long-dashed curve is $F^{III}_q(L = L^I)$, going up when $t > 5$ or so. They are redrawn for the range of $0 < t < 2$ in the image.

FIG. 8: Similar to Fig.7, but $q = -2.5$, and the dot-dashed is $F^{II}_q(L = L^{II})$.

improves the variational result and provide a better approximation for $F_q$. Fig.8 is depicted for $q = -2.5$. In this figure, although the dot-dashed and dotted curves are lower than the solid curve, they indicate that in this case, the approximations up to the first, second and third orders are distinct from each other, and evidently the second- and third-order approximations more closely approach the exact value than the variational result. Fig.9 and 10 are drawn for $q = 0.5$ and $1.5$, respectively, which was considered in Fig.1 in Ref. [5]. For these
cases, the short-dashed, dot-dashed and dotted curves almost coincide and suggests that the approximations up to the second and third orders provide only a very small corrections to the variational results.

V. CONCLUSION

By considering the GFE for a system, this paper proposed a VPA scheme for the generalized statistical mechanics based on the Tsallis entropy. For approximating the GFE, we derived the truncated expressions for $F_q$ up to the third order in the variational perturbation expansion, and the classical harmonic oscillator was considered in detail for an illustration.
The model investigation, albeit being a little academic, illustrates that the approximation up to the first order amounts to a variational method and covers the variational method in Ref. \[5\], and the approximations up to the second and third orders improve the variational result and tend to approach the exact result.

Frankly, the variational perturbation expansion technique is formally similar to the perturbation expansion in Ref. \[5\], the work in the present paper is to introduce the variational perturbation idea into the perturbation expansion and use the PMS for determining the auxiliary parameter in the VPA scheme. It is these revisions that make the variational perturbational approximation method be non-perturbational, take the variational result as the first-order approximation and systematically improve the variational result. We believe that the investigation in the present paper is useful, at least, for calculating the generalized thermodynamical functions based on the Tsallis statistics. Finally, we intend to point out that since path-integral formalism has been developed \[1\], it is worth while developing VPA method within the formalism of the generalized thermodynamics.

[1] S. Abe and Y. Okamoto, Eds., *Nonextensive Statistical Mechanics and Its Applications*, Lectures Notes in Physics, Vol. 560, (Springer, Berlin, 2001). A full and timely list of references can be found in the following Webpage: http://tsallis.cat.cbpf.br/biblio.htm.

[2] C. Tsallis, J. Stat. Phys. 52, 479 (1988).

[3] R. P. Feynman, *Statistical Mechanics : A Set of Lectures*, (Addison-Wesley Publishing Company, Inc., Reading, Massachusetts, 1972).

[4] A. Plastino and C. Tsallis, J. Phys. A 26, L893 (1993).

[5] E. K. Lenzi, L. C. Malacarne and R. S. Mendes, Phys. Rev. Lett. 80, 218 (1998).

[6] R. S. Mendes, C. A. Lopes, E. K. Lenzi and L. C. Malacarne, Physica A, 344, 562 (2004).

[7] E. Hylleraas, Z. Phys. 65, 209 (1930); L. Cohen, Proc. Phys. Soc. A 68, 419 (1955); A 68, 425 (1955).

[8] H. Kleinert and V. Schulte-Frohlinde, *Critical Properties of φ^4-Theories*, World Scientific, Singapore, 2001, Chapter 19; H. Kleinert, *Path Integrals in Quantum Mechanics, Statistics, Polymer Physics, and Financial Markets*, 3rd Ed., World Scientific, Singapore, 2004.

[9] W. F. Lu, C. K. Kim, J. H. Yee, K. Nham, Phys. Rev. D 64, 025006 (2001); W. F. Lu, S. K.
You, Jino Bak, C. K. Kim and K. Nham, J. Phys. A 35, 21 (2002); W. F. Lu, C. K. Kim, Jae Hyung Yee, K. Nham, Phys. Lett. B 540, 309 (2002); W. F. Lu, C. K. Kim, K. Nham, Phys. Lett. B 546, 177 (2002); W. F. Lu, Phys. Lett. B 602, 261 (2004).

[10] P. M. Stevenson, Phys. Rev. D 23, 2916 (1981); Phys. Lett. B 100 (1981) 61; Phys. Rev. D 24, 1622 (1981); S. K. Kaufmann and S. M. Perez, J. Phys. A 17, 2027 (1984); P. M. Stevenson, Nucl. Phys. B 231, 65 (1984).

[11] E. M. F. Curado and C. Tsallis, J. Phys. A 24, L69 (1991); Corrigendum, J. Phys. A 24, 3187 (1991); Corrigendum, J. Phys. A 25, 1019 (1992).

[12] C. Tsallis, R. S. Mendes and A. R. Plastino, Physica A 261, 534 (1998).

[13] S. Martínez, F. Nicolás, F. Pennini and A. R. Plastino, Physica A 286, 489 (2000); G. L. Ferri, S. Martínez and A. R. Plastino, Physica A 347, 205 (2005).

[14] G. L. Ferri, S. Martínez and A. R. Plastino, J. Stat. Mech. P04009 (2005).

[15] P. M. Stevenson, Phys. Rev. D 30, 1712 (1984).

[16] R. P. Feynman, Phys. Rev. 56, 340 (1939); D. B. Lichtenberg, Phys. Rev. D 40, 4196 (1989); W. Namgung, J. Kr. Phys. Soc. 32, 649 (1998).

[17] A. Duncan and H. F. Jones, Phys. Rev. D 47, 2560 (1993); C. M. Bender, A. Duncan, and H. F. Jones, Phys. Rev. D 49, 4219 (1994); R. Guida, K. Konishi, and H. Suzuki, Ann. Phys. (N.Y.) 241, 152 (1995); R. Guida and K. Konishi, Ann. Phys. 249, 109 (1996); E. Braaten and E. Radescu, Phys. Rev. Lett. 89, 271602 (2002); J.-L. Kneur, M. B. Pinto and R. O. Ramos, Phys. Rev. Lett. 89, 210403 (2002).

[18] I. S. Gradshteyn and I. M. Ryzhik, Table of Integrals, Series, and Products (Academic Press, New York, 1980).