Generalized Statistics Variational Perturbation Approximation using q-Deformed Calculus

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Abstract

A principled framework to generalize variational perturbation approximations (VPA’s) formulated within the ambit of the nonadditive statistics of Tsallis statistics, is introduced. This is accomplished by operating on the terms constituting the perturbation expansion of the generalized free energy (GFE) with a variational procedure formulated using q-deformed calculus. A candidate q-deformed generalized VPA (GVPA) is derived with the aid of the Hellmann-Feynman theorem. The generalized Bogoliubov inequality for the approximate GFE are derived for the case of canonical probability densities that maximize the Tsallis entropy. Numerical examples demonstrating the application of the q-deformed GVPA are presented. The qualitative distinctions between the q-deformed GVPA model vis-à-vis prior GVPA models are highlighted.

Key words: Generalized Tsallis statistics, additive duality, variational perturbation approximations, q-deformed calculus, Hellman-Feynman theorem, generalized Bogliubov inequality.
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1 Introduction

The generalized (nonadditive) statistics of Tsallis’ [1,2] has recently been the focus of much attention in statistical physics, and allied disciplines. Nonad-

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ditive statistics\(^1\), which generalizes the extensive Boltzmann-Gibbs-Shannon (B-G-S) statistics, has much utility in a wide spectrum of disciplines ranging from complex systems and condensed matter physics to financial mathematics\(^2\). Recent works have extended the scope of Tsallis statistics, by demonstrating its efficacy in lossy data compression in communication theory \([3]\) and machine learning \([4]\).

Variational perturbation approximations (VPA’s) \([5]\) are extensively employed in quantum mechanics and statistical physics \([6]\). The first attempt to generalize VPA’s to the case of Tsallis statistics was performed by Plastino and Tsallis \([7]\). This proof-of-principle analysis for generalized VPA (GVPA) models \([7]\) established the predominance of concavity of the measure of uncertainty over extensivity (as defined within the context of B-G-S statistics). Further work by Lenzi, Malacarne, and Mendes \([8]\) and Mendes et. al. \([9]\) demonstrated the workings of a GVPA model for the GFE expanded to include second-order terms, using a classical harmonic oscillator as an example. More recently, Lu, Cai, and Kim \([10]\) demonstrated that the inclusion of higher-order terms can significantly improve the results of a GVPA.

The generic procedure for GVPA’s is as follows: (i) evaluation the canonical probability distribution \(p_n\) that maximizes the Tsallis entropy, and, formulation of the generalized free energy (GFE) \([11]\)

\[
F_q = U_q - \frac{1}{\beta} S_q = -\frac{1}{\beta} \frac{\tilde{Z}^{1-q} - 1}{1-q} = -\frac{1}{\beta} \ln \tilde{Z},
\]

where, \(S_q\) is the Tsallis entropy (defined in Section 2), \(U_q\) is the generalized internal energy, \(\beta\) (the energy Lagrange multiplier) is the “inverse thermodynamic temperature”\(^3\), and \(\tilde{Z}\) is canonical partition function, (ii) assuming a Hamiltonian of the system as

\[
H = H_0 + \lambda H_1,
\]

where, \(H_0\) is a Hamiltonian of a soluble system and \(\lambda H_1\) is a perturbation to \(H_0\). Here, \(\lambda \in [0, 1]\) is a perturbation parameter, (iii) perturbation expansion of the GFE

\[
F_q(\lambda) = F_q^{(0)} + \lambda \delta^{(1)} F_q\bigg|_{\lambda=0} + \frac{\lambda^2}{2!} \delta^{(2)} F_q\bigg|_{\lambda=0} + \ldots .\ldots .\ldots .
\]

\(^1\) The terms generalized statistics, nonadditive statistics, and nonextensive statistics are used interchangeably.

\(^2\) A continually updated bibliography of works related to nonextensive statistics may be found at [http://tsallis.cat.cbpf.br/biblio.htm](http://tsallis.cat.cbpf.br/biblio.htm).

\(^3\) Note that for constraints expressed in the form of normal averages, \(\beta\) is replaced by \(\tilde{\beta} = \beta/q\) as is discussed in Section 3.2 and Appendix A of this paper.
where: \( \delta^{(k)} F_q = \frac{d^k F_q}{d\lambda^k}; k = 1, ..., \) and, (iv) solving (2) with the aid of the Hellmann-Feynman theorem [12]

\[
dE_n = \langle n | \frac{dH}{d\lambda} | n \rangle = \langle n | H_1 | n \rangle,
\]

(4)

where, \( E_n \) is the \( n^{th} \) energy eigenvalue of the Hamiltonian \( H \), and, (v) evaluating the generalized Bogoliubov inequality [7-10]

\[
F_q \leq F_q^{(0)} + \langle H_1 \rangle^{(0)},
\]

where, \( \langle H_1 \rangle^{(0)} \) is the generalized expectation of \( H_1 \) in (2) evaluated with \( \lambda = 0 \). Note that while the proof-of-principle analysis in [7] implicitly assumed the above steps (i) – (v) to have been performed, their explicit implementation was demonstrated in [8-10]. Further, the expression for the GFE (1) has recently been the object of much research and debate. Most generally, the inverse temperature \( \beta \), which in essence is the Lagrange multiplier associated with the internal energy relates to the thermodynamic temperature \( T \) as: \( \beta = \frac{1}{k_B T} \), where \( k_B \) is the Boltzmann constant (sometimes set to unity for the sake of convenience) only in the limiting case \( q \to 1 \). Prominent attempts to mitigate this issue are those by Abe et. al. [13], Abe [14], amongst others.

Generalized statistics and the problem of obtaining maximum Tsallis entropy canonical probability distributions has been associated with many forms of constraints. These include the linear constraints originally employed by Tsallis [1] (also known as normal averages) of the form: \( \langle A \rangle = \sum_i p_i A_i \), the Curado-Tsallis (C-T) constraints [15] of the form: \( \langle A \rangle_q = \sum_i p_i^q A_i \), and, the normalized Tsallis-Mendes-Plastino (T-M-P) constraints [11] (also known as \( q \)-averages) of the form: \( \langle \langle A \rangle \rangle_q = \sum_i \left( \frac{p_i}{\sum_i p_i^q} \right) A_i \). The normalized T-M-P constraints render the canonical probability distribution to be self-referential, owing to the dependence of the expectation value on the normalized pdf. A fourth form of constraints are the optimal Lagrange multiplier (OLM) constraints [16, 17]. A work by Ferri, Martinez, and Plastino [18] introduces a methodology to "rescue" the normal averages constraints, and, seamlessly relates canonical probability distributions obtained using the normal averages, C-T, \( q \)-averages, and OLM constraints.

The normal averages constraints [1] were initially abandoned because of difficulties encountered in obtaining an acceptable form for the partition function, and, the nonextensive statistics community have largely utilized \( q \)-averages constraints instead of the C-T constraints, since \( \langle 1 \rangle_q \neq 1 \). Recent studies by Abe [19,20] suggest that unlike \( q \)-averages, normal averages are physical and consistent with both the generalized H-theorem and the generalized Stosszahlansatz (molecular chaos hypothesis).
Despite this physics-related deficiency prominently cited prior works on GVPA’s [8-10] utilized the C-T constraints as a consequence of mathematical necessity. For C-T constraints, the generalized internal energy: \( U_q = \langle E_n \rangle_q \). The canonical distribution that maximizes the Tsallis entropy is

\[ p_n = \frac{1 - (1 - q) \beta E_n}{Z(\beta)} \]

The partition function is:

\[ Z(\beta) = \sum_n \left[ 1 - (1 - q) \beta E_n \right]^{\frac{1}{1-q}} \]

where, \( \beta \) is the Lagrange multiplier associated with the generalized internal energy \( U_q \).

From (1), the GFE is:

\[ F_q = -\frac{1}{\beta} \frac{\dd Z(\beta)}{\dd \beta} \left( \frac{1}{1-q} \right) \sum_n \left[ 1 - (1 - q) \beta E_n \right]^{\frac{1}{1-q}} \frac{\dd E_n}{\dd \lambda} \]

The first-order Newtonian derivative of the GFE naturally yields:

\[ \frac{\dd F_q}{\dd \lambda} = \sum_n p_n^{\dd} \frac{\dd E_n}{\dd \lambda} = \left\langle \frac{\dd E_n}{\dd \lambda} \right\rangle_q \]

The exponential: \( \exp_q x = [1 + (1 - q) x]^{\frac{1}{1-q}} \)

satisfies the differential equation:

\[ \frac{\dd y}{\dd x} = y^q \]

mandates that Newtonian derivatives of the GFE (1) results in expectations defined in the C-T form. These strictures severely constrain the scope and generality of the GVPA analyses described in [8-10].

The primary leitmotif of this paper is to derive a candidate \( q \)-deformed GVPA employing the \( q \)-deformed derivatives defined by [21]:

\[ D^x_q y = [1 + (1 - q) x] \frac{\dd y}{\dd x} \]

where the \( q \)-deformed exponential satisfies:

\[ D^x_q y = y \]

One of the significant consequences of such a generalization is the ability to define expectations defined in terms of normal averages, when taking derivatives of the GFE.

It has been suggested [10] that the results of Ref. [18] could be employed to transform GVPA’s derived using C-T constraints to equivalent forms described by either normal averages or \( q \)-averages. While such a suggestion may be true in principle for simple cases, its practical tractability is questionable when applied to studies in communication theory and machine learning, where the variational extremization of the maximum Tsallis entropy problem is done with respect to conditional (transition) probabilities. Furthermore, this prescription does not result in a true generalization of the variational procedure employed in GVPA’s, within the framework of \( q \)-deformed calculus [21].

In accordance with [18], a generic form of the canonical probability distribution that maximizes the Tsallis entropy is

\[ p_n = \frac{[1 - (1 - q^*) \beta^* E_n]^{\frac{1}{1-q^*}}}{\tilde{Z}(\beta^*)} ; \sum_n p_n = 1, \]

\[ \tilde{Z}(\beta^*) = \sum_n \left[ 1 - (1 - q^*) \beta^* E_n \right]^{\frac{1}{1-q^*}} \]
For normal averages constraints

\begin{equation}
q^* = 2 - q
\end{equation}

\begin{equation}
\beta^* = \left( \frac{\beta}{\bar{\beta}} \right)_{q*} = \frac{\bar{\beta}}{\sum_{q+1} p_n E_n} ; \text{ where } \bar{\beta} = \beta/q.
\end{equation}

\( \bar{\beta} = \frac{\beta}{q} \), \( \bar{\beta} = \frac{\beta}{q} \) and, \( U_q = \sum_n p_n E_n \).

For the C-T constraints

\begin{equation}
q^* = q \quad \beta^* = \beta, \quad U_q = \sum_n p_n E_n.
\end{equation}

For normal averages constraints, (6) and (7) employ the additive duality of generalized statistics (see [1] and the references therein). Specifically, \( q \to 2 - q = q^* \) here, (6) is subjected to the Tsallis cut-off condition [1]: \( [1 - (1 - q^*) \beta^* E_n] \leq 0 \). The rationale for denoting the generalized internal energy as: \( U_q \), is to highlight its nonextensive nature irrespective of the form of expectation involved in its definition. Note that even for expectations defined by normal averages, \( U_q \) has an implicit \( q \)-dependency facilitated by the canonical probability (6).

While replacing the Shannon entropy with the Tsallis entropy yielding GVPA’s [8-10] represents an initial level of generalization, the \( q \)-deformed GVPA model described in this paper achieves a further level of generalization by replacing the Newtonian derivative with the \( q \)-deformed derivative in the variational procedure. Specifically, given a function: \( F(\tau) = \sum_n F(\tau_n) \), the chain rule yields: \( \frac{dF(\tau)}{d\lambda} = \frac{dF(\tau)}{d\tau} \frac{d\tau}{d\lambda} \). Replacing the Newtonian derivative: \( \frac{dF(\tau)}{d\tau} \) by the \( q \)-deformed derivative defined by [21]: \( D_{\tau}^q F(\tau) = [1 + (1 - q) \tau] \frac{dF(\tau)}{d\tau} \) (see Section 2) and defining: \( D_{\tau}^q F(\tau) \frac{d\tau}{d\lambda} = \delta_{(q),\tau} F(\tau) \), facilitates the transformation: \( \frac{dF(\tau)}{d\lambda} \to \delta_{(q),\tau} F(\tau) \). Note that the \( q \)-deformed derivative \( D_{\tau}^q \) operates only on the term \( F(\tau) \), which in this paper is a thermodynamic function expressed as a \( q \)-deformed exponential. Within the scope of this paper, \( F(\tau) \) comprises the GFE. Thus the increasing order to derivatives acquire the form

\begin{equation}
\begin{aligned}
\delta_{(q),\tau}^1 F(\tau) &= D_{\tau}^q F(\tau) \frac{d\tau}{d\lambda}, \\
\delta_{(q),\tau}^2 F(\tau) &= D_{\tau}^q F(\tau) \frac{d\tau}{d\lambda} \delta_{(q),\tau} F(\tau), \\
&\vdots \\
\delta_{(q),\tau}^{k+1} F(\tau) &= D_{\tau}^q F(\tau) \frac{d\tau}{d\lambda} \delta_{(q),\tau}^k F(\tau); \ k = 1, \ldots
\end{aligned}
\end{equation}

This results in \( q \)-deformed GVPA models that simultaneously exhibit generalization within the context of the generalized statistics framework employed.

4 Note that \( q \to q^* \) denotes re-parameterization from \( q \) to \( q^* \).
and, in their underlying mathematical structure. The commutation relations: 
\[ D_{(q)}^\tau F(\tau) = \sum_n D_{(q)}^n F(\tau_n), \text{ and, } \delta_{(q),\tau} F(\tau) = D_{(q)}^\tau F(\tau) \frac{\partial}{\partial \lambda} = \sum_n D_{(q)}^n F(\tau_n) \frac{\partial}{\partial \lambda} = \sum_n \delta_{(q),\tau_n} F(\tau_n) \] are established in Theorem 1. These relations are critical to the correctness and admissability of the \( q \)-deformed GVPA model, and are derived in Section 2 of this paper.

Section 3 derives a \( q \)-deformed GVPA model employing the \( q \)-deformed derivative in the variational procedure. This is accomplished with the aid of the Hellmann-Feynman theorem \[12\]. Section 3 also analyzes the commutation between the Newtonian derivative \( \frac{d}{d\lambda} \) and the summation sign, and the contribution of the cut-off in the variational and perturbation methods for higher-order perturbation terms. It is noteworthy to mention that expectations in terms of normal averages are achieved by relating the "inverse thermodynamic temperature" \( \beta \) (the energy Lagrange multiplier) to the "physical inverse temperature": \( \beta^* [13] \) via \( \beta = \beta^* \hat{Z}(\beta^*)^{q-1} \), where: \( \beta = \beta/q \) is the scaled "inverse thermodynamic temperature".

Section 4 formulates the generalized Bogoliubov inequality \[5,7-10\] truncated at first-order terms for the case of the classical harmonic oscillator. Numerical examples demonstrating the results for the \( q \)-deformed GVPA are presented in Section 5. The ability of the \( q \)-deformed GVPA model presented in this paper to demonstrate both sub-extensivity (sub-additivity) and super-extensivity (super-additivity) within the context of the generalized Bogoliubov inequality truncated at first-order terms is demonstrated. This feature is not possessed by existing GVPA models \[8, 10\]. Section 6 concludes this paper.

2 Theoretical preliminaries

2.1 Tsallis entropy

The \( q \)-deformed logarithm and exponential are defined as \[21\]

\[
\ln_q(x) = \frac{x^{1-q}-1}{1-q},
\]

and,

\[
\exp_q(x) = \begin{cases} 
[1 + (1 - q) x]^{1/q} ; & 1 + (1 - q) x \geq 0 \\
0 ; & \text{otherwise},
\end{cases}
\]
respectively. By definition, the un-normalized Tsallis entropy, is defined in terms of discrete variables as \[1, 2\]

\[
S_q = -\frac{1 - \sum_n p_n q^n}{1 - q} = -\sum_n p_n \ln_q p_n; \sum_n p_n = 1.
\] (11)

The constant \(q\) is referred to as the nonadditivity parameter.

2.2 Results from \(q\)-algebra and \(q\)-calculus

The \(q\)-deformed addition \(\oplus_q\) and the \(q\)-deformed subtraction \(\ominus_q\) are defined as

\[
x \oplus_q y = x + y + (1 - q) xy,
\]

\[
\ominus_q y = \frac{-y}{1 + (1 - q)y}; 1 + (1 - q)y > 0 \Rightarrow x \ominus_q y = \frac{x - y}{1 + (1 - q)y} \tag{12}
\]

The \(q\)-deformed derivative, is defined as

\[
D^\tau_{(q)} F (\tau) = \lim_{\nu \to \tau} \frac{F (\tau) - F (\nu)}{\tau \ominus_q \nu} = [1 + (1 - q) \tau] \frac{dF (\tau)}{d\tau} \tag{13}
\]

2.3 Deformed calculus framework for \(q\)-deformed GVPA

Consider a function: \(F (g (E)) = \sum_n (1 - (1 - q) \beta g (E_n)]^{\frac{1}{1-q}} = \sum_n F (g (E_n))\). On comparison with (6), \(F (\tau)\) may be construed as a generic form of the canonical partition function \(\tilde{Z} (\beta)\). Substituting \(-\beta g (E) = \tau\), yields \(F (\tau) = \sum_n [1 + (1 - q) \tau_n]^{\frac{1}{1-q}} = \sum_n F (\tau_n)\).

**Theorem 1**: Given a function \(F (\tau) = \sum_n [1 + (1 - q) \tau_n]^{\frac{1}{1-q}} = \sum_n F (\tau_n)\), where \(\tau = \{\tau_1, \ldots, \tau_N\}\) are \(N\) separate instances of \(\tau_n; n = 1, \ldots, N\). The following relation involving action of the \(q\)-deformed derivative

\[
D^\tau_{(q)} F (\tau) = \sum_n D^\tau_{(q)} \left[1 + (1 - q) \tau_n\right]^{\frac{1}{1-q}} = \sum_n D^\tau_{(q)} F (\tau_n), \tag{14}
\]

and,

\[
D^\tau_{(q)} F (\tau) \frac{dx}{d\tau} = \sum_n D^\tau_{(q)} \left[1 + (1 - q) \tau_n\right]^{\frac{1}{1-q}} \frac{d\tau_n}{d\tau} = \sum_n D^\tau_{(q)} F (\tau_n) \frac{d\tau_n}{d\tau}. \tag{15}
\]

hold true.
Proof: Employing (13) yields

\[
D_{(q)}^\tau F(\tau) = \left[1 + (1 - q) \tau\right] \frac{dF(\tau)}{d\tau} = \left[1 + (1 - q) \tau_1\right] \frac{dF(\tau_1)}{d\tau_1} + ... + \left[1 + (1 - q) \tau_N\right] \frac{dF(\tau_N)}{d\tau_N}
\]

(16)

Similarly,

\[
D_{(q)}^\tau F(\tau) \frac{dF}{d\lambda} = \left[1 + (1 - q) \tau_1\right] \frac{dF(\tau_1)}{d\tau_1} \frac{d\tau_1}{d\lambda} + ... + \left[1 + (1 - q) \tau_N\right] \frac{dF(\tau_N)}{d\tau_N} \frac{d\tau_N}{d\lambda} = \sum_n \left[1 + (1 - q) \tau_n\right] \frac{dF(\tau_n)}{d\tau_n} \frac{d\tau_n}{d\lambda}.
\]

(17)

Note that (17) assumes that the Newtonian derivative \(\frac{d}{d\lambda}\) commutes with the summation sign [8]. The results of Theorem 1 form the basis for the \(q\)-deformed GVPA model presented in this paper, which extends earlier GVPA studies [8-10]. Note that (17) may be extended to obtain expressions for higher order derivatives with the aid of (9), which is demonstrated in Section 3. Setting:

\[
F(\tau) = \left[1 + (1 - q) \tau\right]^{\frac{1}{1-q}} = \sum n \left[1 + (1 - q) \tau_n\right]^{\frac{1}{1-q}}, D_{(q)}^\tau F(\tau) \text{ yields with the aid of (16)}
\]

\[
D_{(q)}^\tau F(\tau) = \left[1 + (1 - q) \tau\right] \frac{dF(\tau)}{d\tau} = \sum n \left[1 + (1 - q) \tau_n\right] \frac{dF(\tau_n)}{d\tau_n}.
\]

(18)

Analogously

\[
\frac{dF(\tau)}{d\tau} = \sum n \left[1 + (1 - q) \tau_n\right]^{\frac{q}{1-q}}.
\]

(19)

Setting \(\tau = -\beta E \Rightarrow \frac{dF(\tau)}{dE} = -\beta, \delta_{(q),\tau} F(\tau) = D_{(q)}^\tau F(\tau) \frac{dF}{d\tau} = D_{(q)}^\tau F(\tau) \frac{dF}{d\tau} \frac{d\tau}{dE} = -\beta D_{(q)}^\tau F(\tau) \frac{dF}{d\lambda}. \) Thus, (17) and (18) yield

\[
\delta_{(q),\tau} F(x)|_{\lambda=0} = \left[1 - (1 - q) \beta E\right] \frac{dF(E)}{d\lambda} \bigg|_{\lambda=0}
\]

(20)

Analogously

\[
\frac{dF(\tau)}{d\lambda} \bigg|_{\lambda=0} = -\beta \sum n \left[1 - (1 - q) \beta E_n\right]^{\frac{q}{1-q}} \frac{dE_n}{d\lambda} \bigg|_{\lambda=0}.
\]

(21)
Comparison between (20) and (21) provides initial evidence that optimality conditions obtained using the $q$-deformed derivative qualitatively differ from those obtained using the Newtonian derivative.

3 $q$-Deformed generalized variational perturbation approximation

3.1 Overview of the Rayleigh-Schrödinger perturbation method

Consider the eigenvalue equation

$$H |n\rangle = E_n |n\rangle,$$  \hspace{1cm} (22)

where $H$ is the Hamiltonian, $E_n$ is the energy eigenvalue, $n$ is the quantum number, and, $|n\rangle$ is the eigenfunction (eigenvector). Note that the non-degenerate case is considered herein. The eigenfunctions and the eigenvalues are written as [22]

$$|n\rangle = |n\rangle^{(0)} + \lambda |n\rangle^{(1)} + \lambda^2 |n\rangle^{(2)} + ..., \hspace{1cm} (23)$$

$$E_n = E^{(0)}_n + \lambda E^{(1)}_n + \lambda^2 E^{(2)}_n + ..., \hspace{1cm} (24)$$

where $\lambda \in [0, 1]$. In (23), $E^{(k)}_n$ and $|n\rangle^{(k)}$ are the $k^{th}$ corrections to the energy eigenvalues and eigenfunctions, respectively. Note that the non-degenerate theory is valid only when: $|\langle m | H_1 | n^{(0)} \rangle | << |E^{(0)}_n - E^{(0)}_m|$. Substituting (23) into the time-independent Schrödinger equation, and comparing the coefficients of the powers of $\lambda$ on either side, the first two eigenfunction corrections are

$$|n\rangle^{(1)} = \sum_{m \neq n} \frac{\langle m | H_1 | n^{(0)} \rangle}{E^{(0)}_n - E^{(0)}_m} |m\rangle^{(0)} = \sum_{m \neq n} \frac{H_{1mn}}{E^{(0)}_n - E^{(0)}_m} |m\rangle^{(0)}$$

$$|n\rangle^{(2)} = \sum_{m \neq n} \left[ \sum_{l \neq n} \frac{H_{1mn} H_{1ml} H_{1ln}}{(E^{(0)}_n - E^{(0)}_m)(E^{(0)}_n - E^{(0)}_l)(E^{(0)}_n - E^{(0)}_l)} - \frac{H_{1mn} H_{1mn}}{(E^{(0)}_n - E^{(0)}_m)^2} \right] |m\rangle^{(0)} - \frac{1}{2} \sum_{m \neq n} \frac{(H_{1mn})^2}{E^{(0)}_n - E^{(0)}_m} |n\rangle^{(0)}.$$

9
3.2 Generalized free energy correction terms

Setting $\tau_n = -\beta^* E_n$, (6) acquires the form

$$p_n = \frac{[1+(1-q^*(\beta)^*E_n)\tau_n]}{Z(\tau)}^{1-q^*},$$

$$\tilde{Z}(\tau) = \sum_n \left[1 + (1-q^*)\tau_n\right]^{-\frac{1}{1-q^*}}.$$  \hspace{1cm} (25)

For expectations defined by normal averages, the GFE (1) is defined by:

$$F_q = U_q - \frac{1}{\beta^*} S_q = -\frac{1}{\beta^*} \ln \tilde{Z}(\beta^*),$$

where $\beta^* = \beta / q$. Note that the scaled energy Lagrange multiplier $\tilde{\beta}$ is introduced in order to achieve consistency between the two forms of the GFE. The $q^*$-deformed GFE is defined as

$$\mathfrak{F}_{q^*} = -\frac{1}{\tilde{\beta}} \tilde{Z}_q(\tau) q^* - \frac{1}{q^* - 1}.$$  \hspace{1cm} (26)

The derivation of (26) is provided in Appendix A of this paper. Defining

$$\delta(_{(q^*)},\tau) \tilde{Z}(\tau) = D_{(q^*)} \tilde{Z}(\tau) \frac{d\tau}{d\lambda},$$

a perturbation expansion of the $q^*$-deformed GFE, analogous to (3), is

$$\mathfrak{F}_{q^*}(\lambda) = \mathfrak{F}_{q^*}^{(0)} + \lambda \mathfrak{F}_{q^*}^{(1)}|_{\lambda=0} + \frac{\lambda^2}{2!} \mathfrak{F}_{q^*}^{(2)}|_{\lambda=0} + \ldots$$

$$\mathfrak{F}_{q^*}^{(1)} = \delta(_{(q^*)},\tau) \mathfrak{F}_{q^*},$$

$$\mathfrak{F}_{q^*}^{(2)} = \delta(_{(q^*)},\tau) \mathfrak{F}_{q^*}^{(1)},$$

$$\ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \l
tion in (25), (28) yields

\[ \mathfrak{S}_{q^*}^{(1)} = \delta_{(q^*)} \mathcal{S}_{q^*} = D_{q^*} \mathfrak{S}_{q^*} \left( \tilde{Z} (\tau) \right) \frac{d\tau}{d\lambda} \]

\[ = \left[ 1 + (1 - q^*) \right] \left[ 1 + \left( 1 - q^* \right) \tau_n \right] \left[ 1 + (1 - q^*) \right] \left( \frac{dF_{n}(\tilde{Z}(\tau))}{d\tau} \right) \frac{d\tau}{d\lambda} \]

\[ = \left[ 1 + (1 - q^*) \right] \left[ 1 + \left( 1 - q^* \right) \tau_n \right] \left( \frac{dF_{n}(\tilde{Z}(\tau))}{d\tau} \right) \frac{d\tau}{d\lambda} \]  \hspace{1cm} (30)

Substituting (25) and (26) into (30), and employing (15), yields

\[ \mathfrak{S}_{q^*}^{(1)} = -\frac{1}{\beta} \tilde{Z} (\tau)^{q^* - 2} \sum_n \left[ 1 - (1 - q^*) \right] \frac{dE_n}{d\lambda} \]

Setting: \( \tau_n = -\beta^* E_n \), employing the chain rule: \( \frac{d\tau_n}{d\lambda} = \frac{dE_n}{d\lambda} \), and substituting: \( \tilde{\chi} = \beta^* \tilde{Z}(\beta^*)^{q^* - 1} \) from (7) into (31) yields

\[ \mathfrak{S}_{q^*}^{(1)} = \frac{1}{\tilde{Z}(\beta^*)} \sum_n \left[ 1 - (1 - q^*) \right] \beta^* E_n \left( \frac{1}{1 - q^*} \right) \frac{dE_n}{d\lambda} \]  \hspace{1cm} (32)

Employing the Hellmann-Feynman theorem (4), the first-order perturbation term in (28) is defined as

\[ \mathfrak{S}_{q^*}^{(1)} \bigg|_{\lambda = 0} = \frac{1}{\tilde{Z}(\beta^*)} \sum_n \left[ 1 - (1 - q^*) \right] \beta^* E_n \left( \frac{1}{1 - q^*} \right) \frac{dE_n}{d\lambda} \bigg|_{\lambda = 0} \]

\[ = \frac{1}{\tilde{Z}(\beta^*)} \sum_n \left[ 1 - (1 - q^*) \right] \beta^* E_n \left( \frac{1}{1 - q^*} \right) H_{1n} \bigg|_{\lambda = 0} \]

\[ = \sum_n p_n \left( E_n^{(0)} \right) H_{1n} = \langle H_1 \rangle_{q^*}^{(0)} \]  \hspace{1cm} (33)

where, \( \langle H_1 \rangle_{q^*}^{(0)} \) denotes the expectation of \( H_1 \) in normal averages form, defined with respect to the probability \( p(E_n^{(0)}) \) parameterized by \( q^* \).

Note that \( \mathfrak{S}_{q^*}^{(1)} \) in (32) is obtained by operating on the \( q^* \)-deformed GFE in (26) with \( \delta_{(q^*)} \tau_n \), where \( \tau_n = -\beta^* E_n \). Thus, the ”inverse thermodynamic temperature” \( \beta \) (the energy Lagrange multiplier) is related to the ”physical inverse temperature” \( \beta^* \) by the relation: \( \beta/q = \tilde{\chi} = \beta^* \tilde{Z}(\beta^*)^{q^* - 1} \), employing the results of Theorem 1. In (33), \( \mathfrak{S}_{q^*}^{(1)} \bigg|_{\lambda = 0} \) is tantamount to specifying the \( E_n = E_n^{(0)} \) as defined in (4) and (23). Thus, \( \beta \neq \beta^* \tilde{Z}_{(q^*)0}(\beta^*)^{q^* - 1} \), where \( \tilde{Z}_{(q^*)0}(\beta^*) \) is defined in (29).
Setting $\tau_n = -\beta^* E_n$, (32) is re-expressed as

$$S_{q^n}^{(1)} = -\frac{1}{\beta^*} \left\{ \tilde{Z} (\tau)^{-1} \sum_n [1 + (1 - q^*) \tau_n] \frac{1}{1 - q^*} \frac{d\tau_n}{d\lambda} \right\}. \quad (34)$$

Operating on (34) with $\delta (q^*) \tau$ defined in (28), yields

$$S_{q^n}^{(2)} = \delta (q^*) \tau \cdot S_{q^n}^{(1)} = D^\tau_{(q^*)} S_{q^n}^{(1)} \frac{d\tau}{d\lambda}$$

$$= -\frac{1}{\beta^*} D^\tau_{(q^*)} \left\{ \tilde{Z} (\tau)^{-1} \sum_n [1 + (1 - q^*) \tau_n] \frac{1}{1 - q^*} \frac{d\tau_n}{d\lambda} \right\} \frac{d\tau}{d\lambda}. \quad (35)$$

Employing the Leibnitz rule for deformed derivatives [21]

$$D^\tau_{(q^*)} [A (\tau) B (\tau)] = B (\tau) D^\tau_{(q^*)} A (\tau) + A (\tau) D^\tau_{(q^*)} B (\tau), \quad (36)$$

and defining: $A (\tau) = \sum_n [1 + (1 - q^*) \tau_n] \frac{1}{1 - q^*} \frac{d\tau_n}{d\lambda}$ and $B (\tau) = \tilde{Z} (\tau)^{-1}$, yields

$$S_{q^n}^{(2)} = -\frac{1}{\beta^*} \left\{ \tilde{Z} (\tau)^{-1} D^\tau_{(q^*)} \sum_n [1 + (1 - q^*) \tau_n] \frac{1}{1 - q^*} \frac{d\tau_n}{d\lambda} \right\} \frac{d\tau}{d\lambda}$$

$$- \frac{1}{\beta^*} \left\{ \sum_n [1 + (1 - q^*) \tau_n] \frac{1}{1 - q^*} \frac{d\tau_n}{d\lambda} D^\tau_{(q^*)} \tilde{Z} (\tau)^{-1} \right\} \frac{d\tau}{d\lambda}. \quad (37)$$

Evaluating (37) term-wise with the aid of (15), yields

$$\text{Term} - 1 = -\frac{1}{\beta^*} \left\{ \tilde{Z} (\tau)^{-1} D^\tau_{(q^*)} \sum_n [1 + (1 - q^*) \tau_n] \frac{1}{1 - q^*} \frac{d\tau_n}{d\lambda} \right\} \frac{d\tau}{d\lambda}$$

$$= -\frac{1}{\beta^*} \left\{ \tilde{Z} (\tau)^{-1} \sum_n [1 + (1 - q^*) \tau_n] \frac{1}{1 - q^*} \left( \frac{d\tau_n}{d\lambda} \right)^2 \right\}$$

$$+ \tilde{Z} (\tau)^{-1} \sum_n [1 + (1 - q^*) \tau_n] \frac{2q^*}{1 - q^*} \left( \frac{d\tau_n}{d\lambda} \right) \left( \frac{d^2\tau_n}{d\lambda^2} \right) \right\}$$

$$= -\frac{1}{\beta^*} \left\{ \tilde{Z} (\tau)^{-1} \sum_n [1 + (1 - q^*) \tau_n] \frac{1}{1 - q^*} \left( \frac{d\tau_n}{d\lambda} \right)^2 \right\}$$

$$+ \tilde{Z} (\tau)^{-1} \sum_n [1 + (1 - q^*) \tau_n] \frac{2q^*}{1 - q^*} \left( \frac{d\tau_n}{d\lambda} \right) \left( \frac{d^2\tau_n}{d\lambda^2} \right) \right\}$$

$$= -\frac{1}{\beta^*} \left\{ \tilde{Z} (\tau)^{-1} \sum_n [1 + (1 - q^*) \tau_n] \frac{1}{1 - q^*} \left( \frac{d\tau_n}{d\lambda} \right)^2 \right\}$$

$$+ \tilde{Z} (\tau)^{-1} \sum_n [1 + (1 - q^*) \tau_n] \frac{2q^*}{1 - q^*} \left( \frac{d\tau_n}{d\lambda} \right) \left( \frac{d^2\tau_n}{d\lambda^2} \right) \right\}, \quad (38)$$

and
Term 2 = \(-\frac{1}{\beta^*} \left\{ \sum_n [1 + (1 - q^*) \tau_n] \frac{1}{1-q^*} \frac{dE_n}{d\lambda} D_{q^*}^\tau (\tau^{-1}) \right\} \frac{d\tau}{d\lambda} \)
\[= \frac{1}{\beta^*} \left\{ \tilde{Z}(\tau)^{-1} \sum_n [1 + (1 - q^*) \tau_n] \frac{2}{1-q^*} \left( \frac{dE_n}{d\lambda} \right)^2 \right\}. \quad (39)\]

\[\mathfrak{A}_{q^*}^{(2)} = -\frac{1}{\beta^*} \left\{ \tilde{Z}(\tau)^{-1} \sum_n [1 + (1 - q^*) \beta^* E_n] \frac{1}{1-q^*} \left( \frac{dE_n}{d\lambda} \right)^2 \right\} \]
\[+ \tilde{Z}(\tau)^{-1} \sum_n [1 + (1 - q^*) \beta^* E_n] \frac{2}{1-q^*} \left( \frac{dE_n}{d\lambda} \right)^2 \right\}. \quad (40)\]

Setting \(\tau_n = -\beta^* E_n\), (40) yields
\[\mathfrak{A}_{q^*}^{(2)} = \beta^* \left\{ \tilde{Z}(\tau)^{-1} \sum_n [1 + (1 - q^*) \beta^* E_n] \frac{1}{1-q^*} \left( \frac{dE_n}{d\lambda} \right)^2 \right\} \]
\[+ \tilde{Z}(\tau)^{-1} \sum_n [1 + (1 - q^*) \beta^* E_n] \frac{2}{1-q^*} \left( \frac{dE_n}{d\lambda} \right)^2 \right\}. \quad (41)\]

With the aid of the Hellmann-Feynman theorem (4), the second-order perturbation term in (28) is
\[\mathfrak{A}_{q^*}^{(2)}|_{\lambda=0} = \beta^* \left\{ \langle H_1 \rangle_{q^*}^{(0)} - \sum_n p_n (E_n^{(0)}) (H_{1nn})^2 \right\} \]
\[+ \tilde{Z}(\tau)^{1-q^*} \sum_n p_n (E_n^{(0)}) \frac{\partial (n|H_1|n)}{\partial \lambda}\bigg|_{\lambda=0}. \quad (42)\]

Employing (23) \(\left. \frac{d(n|H_1|n)}{d\lambda} \right|_{\lambda=0} = |n(1)\rangle\) and (24), (42) acquires the compact form
\[\mathfrak{A}_{q^*}^{(2)}|_{\lambda=0} = \beta^* \left\{ \langle H_1 \rangle_{q^*}^{(0)} - \sum_n p_n (E_n^{(0)}) (H_{1nn})^2 \right\} \]
\[+ 2\tilde{Z}(\tau)^{1-q^*} \sum_n p_n (E_n^{(0)}) \sum_{m \neq n} \frac{|H_{1mn}|^2}{E_n^{(0)} - E_m^{(0)}}. \quad (43)\]

where: \(H_{1nn} = (0) \langle n|H_1|m(0)\rangle\). Note that (43) is the direct equivalent of Eq. (6) in Ref. [8] and Eq. (24) in Ref. [10]. In the classical limit, the last term in (43) vanishes, since the Hamiltonians \(H_0\) and \(H_1\) commute. In keeping with the gist of previously cited works on GVPA’s [8,10], this paper employs the classical harmonic oscillator to examine the properties and efficacy of the \(q\)-deformed GVPA principle introduced herein. Thus, the second-order perturbation term becomes
\[\mathfrak{A}_{q^*}^{(2)}|_{\lambda=0} = \beta^* \left\{ \langle H_1 \rangle_{q^*}^{(0)} - \sum_n p_n (E_n^{(0)}) (H_{1nn})^2 \right\}. \quad (44)\]
Thus, for commuting Hamiltonians $H_0$ and $H_1$, the perturbation expansion of the GFE is

$$
\Im_{q^*} (\lambda) = -\frac{1}{\beta} \frac{\partial^2 \langle q^* \rangle}{\partial \beta^* \partial \beta^*} + \lambda \langle H_1 \rangle_{q^*}^{(0)} + \frac{\lambda^2}{2!} \beta^* \left\{ \left( \langle H_1 \rangle_{q^*}^{(0)} \right)^2 - \sum_n p_n \left( E_n^{(0)} \right) (H_{1nn})^2 \right\} + \theta (\lambda^3) + ... 
$$

The above analysis and (17) make tacit assumptions concerning the commutation between the Newtonian derivative $\frac{d}{d\lambda}$ and the summation sign. To analyze the contribution of the cut-off in the $q$-deformed GVPA model for $\beta^* > 0$ and $E_n \geq 0$, parallels are drawn with the analysis in Ref. [8]. First, the summation sign $\sum$ is replaced by the integral $\int d\Gamma$, where: $\Gamma = \prod_s dx_s dp_s h$, $p_s$ is the canonical momentum, and $h$ is Planck’s constant. The integration is performed over the phase-space region defined by: $[1 - (1 - q^*) \beta^* H] \geq 0$. Defining: $f = [1 - (1 - q^*) \beta^* H]^{\frac{1}{1-q^*}} = [1 + (1 - q^*) \tau]^{\frac{1}{1-q^*}} = f(\tau)$, the following identity is employed by invoking (9) and Theorem 1

$$
\frac{d}{d\lambda} \int d\Gamma D_{q^*} \tau f(\tau) = \int d\Gamma D_{q^*} \tau f(\tau) \frac{df}{d\lambda} + \int d\Gamma \sum_u dS_u \left( D_{q^*} \tau f(\tau) \frac{df}{d\lambda} \right). 
$$

Note that the distinction of (46) vis-à-vis Eq. (10) in Ref. [8] is due to replacing: $\frac{df(\tau)}{d\lambda}$ by: $\delta(\tau)f(\tau)$ (see (9)), in the $q$-deformed GVPA model. Here, $f(\tau)$ is a function of the phase-space variables $y_u$, and, $\partial V$ is the hypersurface defined by: $[1 - (1 - q^*) \beta^* H] = [1 + (1 - q^*) \tau] = 0$. The $n^{th}$-order perturbation $\Im_{q^*}^{(n)}$ contains a term proportional to: $[1 + (1 - q^*) \tau]^{\frac{n}{1-q^*}}$. For example, $\Im_{q^*}^{(2)}$ in (40), contains a term: $\sum_n [1 + (1 - q^*) \tau]^{\frac{n}{1-q^*}}$ corresponding to $n = 2$. In order that $\Im_{q^*}^{(n)}$ not contribute to the second term in (46), the condition: $n - (n - 1) q^* > 0 \Rightarrow q^* < 1 + \frac{1}{n-1}$ is to be observed so that: $D_{q^*} \tau f(\tau) = 0 \Rightarrow f(\tau) = 0$ on $\partial V$.

4 The generalized Bogoliubov inequality

Within the context of the $q$-deformed GVPA, the generalized Bogoliubov inequality truncated to first-order terms is

$$
\Im_{q^*} \leq \Im_{q^*}^{(0)} + \langle H_1 \rangle_{q^*}^{(0)}. 
$$

For a 1-D classical harmonic oscillator of mass $M$ and angular frequency $\omega$,
the Hamiltonian is: \( H = \frac{p^2}{2M} + \frac{M\omega^2 x^2}{2} \). Here, \( x \) is the coordinate and \( p \) is the canonical momentum. Following a procedure analogous to that in Ref. [10], from (6), the canonical partition function is expressed in continuous form as

\[
\tilde{Z} (\beta^*) = \int_0^N \left[ 1 - (1 - q^*) \beta^* n \delta_0 \right] \frac{1}{1 - q^*} dn = \frac{1}{(2 - q^*) \beta^* \delta_0}; \beta^* > 0.
\] (48)

Here, \( 0 < q^* < 2 \), \( N \to \infty \) for \( q^* > 1 \), and \( N = \frac{1}{(1-q^*) \beta^* \delta_0} \) for \( q^* < 1 \). Akin to [10], \( \delta_0 = h\omega_0 \), is a positive constant with units of energy. Also, \( h = h/2\pi \), where \( h \) is Planck’s constant. Thus, (26) is re-written as

\[
\Im(q^*) = -\frac{1}{(q^*-1)^2} \left[ \frac{1}{(2-q^*) \beta^* \delta_0} \right]^{q^*-1} - 1 \right].
\] (49)

The unperturbed Hamiltonian for a particle of mass \( M \) in a 1-D box is: \( H_0 = \frac{p^2}{2M} + V_0 \), where \( V_0 = 0 \) for \( |x| < L/2 \) and \( V_0 \to \infty \) for \( |x| \geq L/2 \). In accordance with [10], the continuous energy spectrum of the particle is: \( E_n^{(0)} = \frac{\delta_0^2 n^2}{2ML^2} \), where \( \delta_0 = h\pi \) is a constant with the dimension of action. Thus, (29) is described in terms of the Euler \( \Gamma \) function as

\[
\tilde{Z}(q^*,0) (\beta^*) = \int_0^N \left[ 1 - (1 - q^*) \beta^* n \delta_0 \right]^{\frac{1}{1-q^*}} dn = \left\{ \begin{array}{ll}
\frac{L}{\delta_0} \sqrt{\frac{M\pi}{2(1-q^*) \beta^* \Gamma(\frac{q^*}{q^*-1})}}; & q^* < 1, \\
\frac{L}{\delta_0} \sqrt{\frac{M\pi}{2(1-q^*) \beta^* \Gamma(\frac{q^*}{q^*-1})}}; & 3 > q^* > 1
\end{array} \right.
\] (50)

where \( N \to \infty \) for \( q^* > 1 \) and \( N = \frac{L}{\delta_0} \sqrt{\frac{2M}{(1-q^*) \beta^*}} \) for \( q^* < 1 \). Note that (50) is identical to Eq. (11) in [8], with \( q^* \) replacing \( q \).

Following the procedure employed in [10], the matrix elements of \( H_{1nm} \) in (33) and (43) are (Eq. (33) in [10])

\[
H_{1nm} = \delta_{nm} 2 \int_{-L/2}^{L/2} \frac{M\omega^2 x^2}{2} \frac{dx}{2L} = \delta_{nm} \frac{M\omega^2 L^2}{24}.
\] (51)

Here, \( \delta_{nm} \) is the Kronecker delta. Employing (50), the first-order perturbation

\footnote{Symbolic integration was performed using \textsc{Mathematica®}.}
term (33) becomes

$$\lim_{\lambda \to 0} = \langle H_1 \rangle_{q^*}^{(0)} = \sum_n p_n \langle E_n^{(0)} \rangle H_{1n}$$

$$= \frac{M^2 L^2}{4} \frac{1}{Z_{\langle q^* \rangle \beta(\beta^*)}} \prod_{n=0}^{N} \left[ 1 - \left( 1 - q^* \right) \beta^* \frac{n^2 \beta^2}{2M L^2} \right]^{1/\eta} \, dn = \frac{M^2 L^2}{24}.$$  \hspace{1cm} (52)

From (25), (26), (29), (48)-(50), and (52), the generalized Bogoliubov inequality truncated at first-order terms in Refs. [8,10] is

$$\Delta_q \leq \Delta_q^{(0)} + \langle H_1 \rangle_{q^*}^{(0)}$$

\[ \Rightarrow - \frac{1}{(q^*-1)\beta} \left[ Z(\beta^*)(q^*-1) - 1 \right] = - \frac{1}{(q^*-1)\beta} \left[ \left( \frac{2\pi}{(2-q^*)\beta^* n\omega} \right)^{(q^*-1)} - 1 \right] \]

\[ \leq - \frac{1}{(q^*-1)\beta} \left[ Z(q^*), 0(\beta^*)(q^*-1) - 1 \right] + \frac{M^2 L^2}{24}, \]

where

\[ Z(q^*, 0)(\beta^*) = \frac{L}{h} \sqrt{\frac{2\pi}{(1-q^*)\beta^* \Gamma(\frac{1}{2} + \frac{1}{q^*})}} \left( q^* < 1 \right) \]

\[ \frac{L}{h} \sqrt{\frac{2\pi}{(q^*-1)\beta^* \Gamma(\frac{1}{q^*-1})}} \left( 3 > q^* > 1 \right) \]

and

\[ \beta = \beta^* \bar{Z} = \beta^* (\beta^*) (q^*-1) = \beta^* \left( \frac{2\pi}{(2-q^*)\beta^* n\omega} \right) \frac{1}{q^*-1}. \]

The value of $L$ is obtained by minimizing the right hand side of (53), yielding

$$- \frac{L(q^*-1)}{\beta} C_{q^*} (\beta^*) + \frac{M^2}{12} = 0 \Rightarrow L = \left[ \frac{\beta M^2}{12 C_{q^*}(\beta^*)} \right]^{1/\eta-3/2},$$

where

\[ C_{q^*} (\beta^*) = \left[ \frac{\Gamma\left( \frac{2-q^*}{1-q^*} \right)}{h^2 (1-q^*)^{\beta^*} \Gamma\left( \frac{1}{2} + \frac{1}{q^*} \right)} \right]^{q^*-1} ; \left\{ \begin{array}{l} q^* < 1 \\ 3 > q^* > 1 \end{array} \right\} \]

(54)

Here, (54) demonstrates that $L$ accounts for both sub-additivity ($q^* > 1$) and super-additivity ($q^* < 1$). This feature is absent in formulations of the generalized Bogoliubov inequality truncated at first-order terms in Refs. [8,10]. Specifically, Eq. (13) in Ref. [8] and Eq. (40) in Ref. [10] make no allowance for sub-additivity and super-additivity in the expression for $L$.

Note that sub-additivity and super-additivity are defined in terms of $q^*$ because (53) and (54) are parameterized by $q^*$. 

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5 Numerical studies

The \textit{q-deformed} GVPA model is numerically studied by evaluating the generalized Bogoliubov inequality (53) for values of $\beta^* \in [0.01, 3.5]$, akin to the parametric perspective described in [18] for various values of $q^*$. Here, $M = \omega = h = 1$. Representative examples for the generalized Bogoliubov inequality (47) and (53) are demonstrated in Figure 1, for $q^* = 0.5$ and $q^* = 0.95$. Numerical examples for the generalized Bogoliubov inequality for $q^* = 1.3$ and $q^* = 1.75$ are depicted in Figure 2.

From Figure 1 and Figure 2, it is readily observed that the generalized Bogoliubov inequality in (47) and (53) tends to an equality with decreasing values of $q^*$. Specifically, the difference between the exact solution ($\Im_{q^*}$) and the perturbation solution ($\Im_{q^*} + < H_1 >_{q^*}$) decreases with decreasing $q^*$. Note that the exact solution of the GVE (the LHS of the inequality in (47) and (53)) almost exactly coincides with the perturbation solution, for $q^* = 0.5$. The relations between $\tilde{\beta}$ and $\beta^*$ are displayed in Figure 3 for both $q^* < 1$ and $q^* > 1$.

The expression for $L$ (54) is the most explicit manifestation of sub-additivity and super-additivity possessed by the \textit{q-deformed} GVPA, for $k^{th}$-order perturbation expansions of the $q^*-deformed$ GFE (26), $k \geq 1$. Figure 4 displays the dependence of $L$ on $\beta^*$. For $0 < q^* < 1$, $L$ increases with increasing values of $q^*$. In contrast, for $1 < q^* < 3$, $L$ decreases with increasing values of $q^*$.

6 Summary and conclusions

The theoretical framework for a \textit{q-deformed} GVPA model which generalizes previous works on GVPA models [8-10], has been formulated. The underlying theory for the variational procedure of the \textit{q-deformed} GVPA model employs \textit{q-deformed} calculus [21]. The significant feature of the \textit{q-deformed} GVPA is that expectation values may be self-consistently formulated in the form of normal averages, instead of the Curado-Tsallis form [8-10]. This feature acquires special significance owing to recent results that establish that expectations in the normal averages form, in contrast to the vastly more utilized $q$-averages form, are physical and consistent with both the generalized H-theorem and the generalized Stosszahlansatz (molecular chaos hypothesis) [19, 20].

It is qualitatively and quantitatively demonstrated that the \textit{q-deformed} GVPA model exhibits both sub-additivity and super-additivity in terms of the non-additivity parameter $q^*$ for the generalized Bogoliubov inequality, truncated at first-order terms. This property is not possessed by previous GVPA models [8, 10]. Specifically, it may be construed that the \textit{q-deformed} GVPA presented
in this paper exhibits authentic characteristics of a VPA even for the generalized Bogoliubov inequality truncated at first-order terms. In contrast, previous cited analyses [8, 10] do not exhibit any equivalent property, rendering them purely variational principles when the generalized Bogoliubov inequality is truncated at first-order terms. Numerical simulations that demonstrate the results and the efficacy of the \textit{q-deformed} GVPA are presented.

Future works that will be presented elsewhere accomplish a three-fold objective: (i) a comparative study taking into account higher-order terms between the \textit{q-deformed} GVPA model presented in this paper, its counterpart based on the \textit{dual Tsallis entropy}: \( S_{q^*} = s_{2-q} \) (see Ref. [3] and the references therein), and the results of previous cited studies [8-10], (ii) a \textit{q-deformed} GVPA model for the homogeneous Arimoto entropy [23] with normal averages constraints, defined in terms of the \textit{escort probability} [24]. The homogeneous nonadditive Arimoto entropy is defined in terms of the \textit{escort probability} as:

\[
S_{q}^{H}(P) = -\left( \frac{\sum P_{i}^{\frac{1}{q}}}{} \right)^{q-1},
\]

and, (iii) use of the \textit{q-deformed} GVPA to analyze critical point behavior in deterministic annealing [25], within the framework of generalized statistics, and, the deformed statistics information bottleneck method [4] in machine learning.

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FIGURE CAPTIONS

Fig. 1: Generalized Bogoliubov inequality for the \( q - deformed \) GVPA model for \( q^* = 0.5 \) and \( q^* = 0.95 \). Here, \( \Im_{q^*} \) is the LHS of (53) (the exact solution) and \( \Im_{q^*}^{(0)} + < H_1 >_{q^*}^{(0)} \) is the RHS of (53) (the perturbation solution). The generalized Bogoliubov inequality increases with increasing \( q^* \). Note the near overlap of the exact solution and the perturbation solution for \( q^* = 0.5 \).

Fig. 2: Generalized Bogoliubov inequality for the \( q - deformed \) GVPA model for \( q^* = 1.3 \) and \( q^* = 1.75 \). Here, \( \Im_{q^*} \) is the LHS of (53) (the exact solution) and \( \Im_{q^*}^{(0)} + < H_1 >_{q^*}^{(0)} \) is the RHS of (53) (the perturbation solution). Note the increase in the generalized Bogoliubov inequality with increasing \( q^* \).

Fig. 3: Relation between the scaled ”inverse thermodynamic temperature“ \( (\beta/q = \tilde{\beta}) \) and the ”physical inverse temperature“ \( (\beta^*) \) for \( q^* =0.5, 0.95, 1.3, \) and, \( 1.75 \).

Fig. 4: Dependence of \( L \) on \( \beta^* \). Note the increase in the value of \( L \) for increasing \( q^* < 1 \), and the decrease in the value of \( L \) for increasing \( q^* > 1 \).
\[ \Im \theta(q, \beta) = \Im \theta(q^*, \beta^*) \]

The graph shows the behavior of \( \Im \theta(q, \beta) \) for different values of \( q^* \) and \( \beta^* \). The curves represent different scenarios:

- \( \Im \theta(q^*, \beta^*) \) with \( q^* = 0.5 \) and \( \beta^* \)
- \( \Im \theta(q^*, \beta^*) \) with \( q^* = 0.95 \) and \( \beta^* \)

The graph is labeled with the corresponding \( q^* \) values for each scenario.
\[
\Im q^*(\beta^*) = \Im q^*(0) + \Im q^* \langle \beta^* \rangle q^* = 1.3
\]
\[
\Im q^*(\beta^*) = \Im q^*(0) + \Im q^* \langle \beta^* \rangle q^* = 1.75
\]
\[ \tilde{q} = 0.5, q = 0.95, q' = 1.3, q' = 1.75 \]
Appendix A: Derivation of expression for $q^*$-deformed Generalized Free Energy

The canonical probability that maximizes the Tsallis entropy using constraints defined in terms of normal averages is (Eq. (23) in Ref. [18])

$$p_n = \left[ \mathcal{N}_q + \frac{(q-1)}{q} \beta U_q - \frac{(q-1)}{q} \beta E_n \right]^{1 \over q - 1} = \left[ 1 - \frac{(q-1)}{\mathcal{N}_q + (q-1) \beta U_q} \beta E_n \right]^{1 \over q - 1};$$

where

$$U_q = \sum_n p_n E_n, \bar{\beta} = \frac{\beta}{q}, \mathcal{N}_q = \sum_n p_q^n, \text{and, } \bar{Z} (\bar{\beta}) = \left( \mathcal{N}_q + (q-1) \beta U_q \right)^{1 \over 1-q}.$$ (A.1)

From the definition of the partition function in (A.1), the following thermodynamic relation is obtained

$$\ln_q \bar{Z} (\bar{\beta}) = \frac{\mathcal{N}_q + (q-1) \beta U_q - 1}{1-q} \Rightarrow \frac{d \ln_q \bar{Z} (\bar{\beta})}{d \bar{\beta}} = -U_q. \quad (A.2)$$

The Tsallis entropy is

$$S_q = \frac{\mathcal{N}_q - 1}{1-q}. \quad (A.3)$$

Using the definition of $\bar{Z}(\bar{\beta})$ in (A.1), (A.3) yields the thermodynamic relation

$$S_q = \frac{\bar{Z} (\bar{\beta})^{1-q} + (1-q) \beta U_q - 1}{1-q} \Rightarrow \frac{dS_q}{dU_q} = \bar{\beta}. \quad (A.4)$$

From (A.4), the GFE is thus defined as

$$F_q = U_q - \frac{1}{\bar{\beta}} S_q = U_q - \frac{1}{\bar{\beta}} \left( \frac{\bar{Z} (\bar{\beta})^{1-q} + (1-q) \beta U_q - 1}{1-q} \right) = -\frac{1}{\bar{\beta}} \ln_q \bar{Z} (\bar{\beta}). \quad (A.5)$$

From (A.1) and (A.5)

$$F_q = -\frac{1}{\beta} \ln_q \sum_n \left[ 1 - (q-1) \frac{\beta}{\bar{Z} (\bar{\beta})^{1-q}} E_n \right]^{1 \over q - 1} = -\frac{1}{\beta} \ln_q \sum_n [1 - (q-1) \beta^* E_n]^{1 \over q - 1} = -\frac{1}{\beta} \ln_q \bar{Z} (\beta^*), \quad (A.6)$$
where: $\beta^* = \frac{\tilde{\beta}}{Z(\beta)}$. Here, $\tilde{Z}(\beta^*) = \sum_n \left[ 1 - (q - 1) \beta^* E_n \right]^{\frac{1}{q^* - 1}}$.

Invoking the additive duality: $q^* = 2 - q$ (see Ref. [1] and the references therein) resulting in: $\tilde{Z}(\beta^*) = \sum_n \left[ 1 - (1 - q^*) \beta^* E_n \right]^{\frac{1}{1 - q^*}}$, setting: $\tau_n = -\beta^* E_n$ and employing Eq. (25) of this paper, the $q^*$-deformed GFE (Eq. (26) of this paper) is expressed as

$$F_{q\rightarrow q^* = 2-q} = \mathcal{S}_{q^*} = -\frac{1}{\beta} \frac{\tilde{Z}(\beta^*)q^{*-1} - 1}{q^* - 1} = -\frac{1}{\beta} \frac{\tilde{Z}(\tau)q^{*-1} - 1}{q^* - 1}.$$  \hspace{1cm} (A.7)