Ideal gas in nonextensive optimal Lagrange multipliers formalism

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Based on the prescription termed the optimal Lagrange multipliers formalism for extremizing the Tsallis entropy indexed by q, it is shown that key aspects of the treatment of the ideal gas problem are identical in both the nonextensive q ≠ 1 and extensive q = 1 cases.

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I. INTRODUCTION

The purpose of this work is to discuss the classical ideal gas problem in Tsallis thermostatistics within the framework of the method of optimal Lagrange multipliers (OLM) recently proposed in Ref. [1].

The ideal gas problem in the normalized Tsallis thermostatistics has recently been exhaustively discussed in Ref. [2]. Correlations induced by Tsallis’ nonextensivity were analyzed in Ref. [3]. An interesting relation, analogous to that yielding the mean energy of the (ordinary) ideal gas was thereby found. However, the ensuing results still depend upon Tsallis’ nonextensivity index q, even if one deals with a purely classical system. Here, we show that more insights can be gained into the problem if i) one takes advantage of a degree of freedom implicit in Tsallis’ formalism, i.e., choice of the entropy constant kT, playing the role of Boltzmann’s constant kB, and ii) uses the OLM technique in Ref. [1].

Tsallis’ thermostatistics [4-18] is by now known to offer a nonextensive generalization of traditional Boltzmann-Gibbs statistical mechanics. A key ingredient in this formalism is the introduction of a particular definition of expectation value termed the normalized q-expectation value [1]. Actually, during the last ten years before the work in Ref. [1], several proposals have been made regarding definition of expectation value [3]. No matter what definition one chooses, ordinary Boltzmann-Gibbs results are always reproduced in the extensive limit q → 1.

Tsallis thermostatistics involves extremization of Tsallis’ entropy

\[ \frac{S_q}{kT} = 1 - \int dx \frac{f^q(x)}{q - 1}, \]  

by recourse to Lagrange’s constrained variational technique. Here, x is a phase space element (N particles in a D-dimensional space), q ∈ ℝ is Tsallis’ nonextensivity index, f stands for any normalized probability density, and kT is the entropy constant that is akin to the celebrated Boltzmann constant appearing in traditional statistical mechanics.

The formalism of Ref. [1] gives rise to a non-diagonal form of the Hessian associated with examining the extremum structure of the entropy and free energy through the Legendre transform procedure. In Ref. [1], a new approach has been advanced, in which the Hessian is diagonal. This approach was shown to enormously facilitate ascertaining what kind of extrema the Lagrange technique yields.

A quite interesting fact is to be emphasized concerning the entropy constant kT, which is usually identified simply with Boltzmann’s kB in the literature: the only certified fact one can be sure of is “kB → kB for q → 1” [1], which entails that there is room to choose kT = k(q) in a suitable way. It is seen [1] that if one chooses (with Zq the generalized partition function)

\[ k_T = k_B Z_q^{q-1}, \]  

in conjunction with the OLM formalism [1], the classical harmonic oscillator determines a specific heat Cq = kB, so that the ordinary Boltzmann-Gibbs result arises without invoking the limit q → 1. In addition, the OLM treatment is able to reproduce the zero-th law of thermodynamics, a goal that had previously eluded Tsallis-thermostatistics practitioners [1]. One is then tempted to conjecture that many other ordinary results can be reproduced by Tsallis thermostatistics without invoking the limit q → 1. In this paper, we revisit the ideal gas problem in Tsallis thermostatistics with such a goal in mind. More precisely, we perform an OLM treatment of the problem following the canonical ensemble structure. We will show that the ordinary expression for the mean value of the energy is reproduced by Tsallis thermostatistics without the need of going to the limit q → 1, in contrast to the previous treatment of this problem.

It is worth noting here that, as shown in Ref. [20], the usual thermodynamic limit N → ∞ implies the limit q → 1. There, the Tsallis probability distribution is deduced in a way that mimics Gibbs’ celebrated derivation of the canonical distribution for a system in contact with a heat bath [20]. It was shown that Tsallis’ distribu-
tion naturally arises for finite heat baths, the nonextensivity index $q$ being related to the particle number $N$ that characterizes the bath. Gibbs’ canonical distribution, instead, results for infinite heat baths [2]. This leads one to conclude that $q$ goes over to unity in the limit $N \to \infty$. This result was found employing the unnormalized expectation values of Curado and Tsallis (see Ref. [2]). Analogously, if one uses the normalized expectation values of Ref. [4], a similar argument leads to

$$q = \frac{DN - 4}{DN - 2} \quad (3)$$

for the ideal gas in $D$ dimensions. Since the limit $N \to \infty$ corresponds to $q \to 1$, the same ordinary result is obtained from the nonextensive formalisms with various definitions of generalized expectation value (both normalized and unnormalized) in such a limit.

### II. BRIEF REVIEW OLM FORMALISM

A general classical treatment requires consideration of the probability density $f(x)$ that maximizes Tsallis’ entropy, subject to the foreknowledge of the generalized expectation values of certain physical quantities.

Tsallis’ probability distribution [4] is obtained by following the well known MaxEnt principle [21]. The Tsallis-Mendes-Plastino variational treatment [4] involves a set of Lagrange multipliers $\lambda_j$. The OLM technique developed in Ref. [4] pursues an alternative path that involves a different set of Lagrange multipliers $\lambda_j$: one maximizes Tsallis entropy $S_q$ in Eq. (4) [13,14,18], subject to the modified constraints (“centered” generalized expectation values) [13,14,18]:

$$\int dx \, f(x) - 1 = 0, \quad (4)$$

$$\int dx \, f(x)^q \left( O_j(x) - \langle O_j \rangle_q \right) = 0, \quad (5)$$

where $O_j(x) (j = 1, 2, \ldots, M)$ denote the $M$ relevant dynamical quantity (the observation level [22]). In the above, $\langle O_j \rangle_q$ are defined by [4]

$$\langle O_j \rangle_q = \frac{\int dx \, f^q(x) O_j(x)}{\int dx \, f^q(x)}, \quad (6)$$

which are assumed to be a priori known. (The procedure given in Ref. [4] employs non-centered expectation values.) The resulting probability distribution reads [6]

$$f(x) = Z_q^{-1} \left[ 1 - (1 - q) \sum_j \lambda_j' \left( O_j(x) - \langle O_j \rangle_q \right) \right]^{-\frac{1}{q-1}}, \quad (7)$$

where $Z_q$ stands for the generalized partition function

$$Z_q = \int dx \left[ 1 - (1 - q) \sum_j \lambda_j' \left( O_j(x) - \langle O_j \rangle_q \right) \right]^{-\frac{1}{q-1},} \quad (8)$$

Although the procedure originally devised in Ref. [4] overcomes some problems posed by the old, unnormalized way of evaluating Tsallis’ generalized expectation values [13,14,18], it yields probability distributions that are self-referential. The resulting distribution includes the integral of the $q$th power of the distribution itself. This fact entails difficulties in numerical model calculations, for example. The complementary OLM treatment of Ref. [1] surmounts such difficulties. The above-mentioned self-reference problem does not arise in Eq. (8).

It is shown in Ref. [4] that the Lagrange multipliers $\lambda_j$ of the Tsallis-Mendes-Plastino procedure [4] and the corresponding $\lambda_j'$ in OLM are connected to each other as follows:

$$\lambda_j' = \frac{\lambda_j}{\int dx \, f^q(x)}, \quad (9)$$

However, the genuine Lagrange multipliers are $\lambda_j'$ in OLM.

The probability density appearing in Eq. (9) is the one that maximizes the entropy $S_q$ which can be expressed in the alternative form [6]

$$S_q = k_T \frac{\ln_q Z_q^{q-1} - 1}{q-1} \int dx \, f^q(x). \quad (10)$$

Also, the identical relation

$$\int dx \, f^q(x) = Z_q^{1-q} \quad (11)$$

holds, from which it follows [6] that

$$S_q = k_T \ln_q Z_q, \quad (12)$$

where $\ln_q x = (1 - x^{1-1/q})/(q - 1)$.

Eq. (12) allows us to rewrite Eq. (8) as

$$\lambda_j' = \frac{\lambda_j}{Z_q^{1-q}}, \quad (13)$$

However, we again stress that the basic variables in OLM are $\lambda_j'$.

Now, following Ref. [6], we define

$$\ln_q Z_q' = \ln_q Z_q - \sum_j \lambda_j' \langle O_j \rangle_q, \quad (14)$$

Introducing

$$k' = k_T Z_q^{q-1} \quad (15)$$

as in Ref. [6], we straightforwardly obtain
$$\frac{\partial S}{\partial \langle Q_j \rangle} = k' \lambda_j', \quad (16)$$

$$\frac{\partial}{\partial \lambda_j'} \ln_q Z_j' = - \langle Q_j \rangle_q. \quad (17)$$

Eqs. (16) and (17) constitute the basic information-theoretic relations, on which statistical mechanics can be built à la Jaynes [21]. Here, one should remind the well known fact that in reconstructing statistical mechanics based on information theory, Jaynes could remove the concept of ensemble [21]. In this sense, it is appropriate to emphasize that both the OLM [1] and Tsallis-Mendes-Plastino [4] formalisms employ identical a priori information, so that they are physically equivalent.

Notice that $k'$, as defined by Eq. (15), obeys the condition $k' \to k_B$ as $q \to 1$. It is a condition that this constant must necessarily fulfill. (See Ref. [13]). Notice that if one makes use of the possibility of choosing $k_T$ as in (2), one obtains, on account of (13),

$$k' = k_B, \quad (18)$$

i.e., the classical results are obtained without going to the limit $q \to 1$, as stated in the introduction.

Moreover, another interesting result obtained from OLM is [1]

$$k' \lambda_j' = k_T \lambda_j, \quad (19)$$

which entails that the intensive variables are the same in both the OLM and Tsallis-Mendes-Plastino formalisms.

As a special instance of Eqs. (16), (17) and (14), let us discuss the canonical ensemble. In this case, only a single constraint regarding the system Hamiltonian is considered. Writing the associated Lagrange multiplier as $\beta'$ and the generalized internal energy as $U_q$,

$$\frac{\partial S}{\partial U_q} = k' \beta' = k_T \beta = \frac{1}{T}, \quad (20)$$

$$\frac{\partial}{\partial \beta'} \ln_q Z_j' = -U_q, \quad (21)$$

where

$$\ln_q Z_j' = \ln_q Z_q - \beta' U_q. \quad (22)$$

The temperature $T$ in Eq. (20) is the same as that in the Tsallis-Mendes-Plastino formalism.

**III. IDEAL GAS IN TSALLIS-MENDES-PLASTINO FORMALISM**

The classical ideal gas in $D$-dimensional space in the Tsallis-Mendes-Plastino formalism has been considered in Refs. [2,3]. For comparison, we recapitulate here some of its main results in the case $0 < q < 1$. The Hamiltonian reads

$$H(P) = \sum_{i=1}^{N} \frac{p_i^2}{2m}, \quad (23)$$

where $m$ is the particle mass, $N$ the particle number and $p_i$ the momentum of the $i$th particle. We are writing the $N$-particle momenta collectively as $P = (p_1, p_2, \ldots, p_N)$. One extremizes the entropy in Eq. (1), subject to the constraints [4]

$$\int d\Omega f(P) = 1, \quad (24)$$

$$\frac{1}{c} \int d\Omega f(P)^q H(P) = U_q, \quad (25)$$

where $d\Omega = (1/(N!h^{DN})) \prod_{i=1}^{N} dq_i dp_i$, with $h$ the linear dimension (i.e. the size) of the elementary cell in phase space, and $\int \prod_{i=1}^{N} dq_i = V^N$ with the spatial volume $V$. We have also introduced the quantity $c$

$$c = \int d\Omega f(P)^q. \quad (26)$$

The equilibrium probability density is found to be

$$f(P) = \frac{1}{Z_q} [1 - (1 - q)(\beta/c)(H(P) - U_q)]^{1/q}, \quad (27)$$

where the generalized partition function is

$$Z_q = \int d\Omega [1 - (1 - q)(\beta/c)(H(P) - U_q)]^{1/q}, \quad (28)$$

and we have

$$c = [\tilde{Z}_q]^{1-q}. \quad (29)$$

In the above, $\beta$ is the Lagrange multiplier associated with the constraint in Eq. (25). Notice that Eq. (23) is indeed a self-referential expression through $c$. In the present circumstances, however, this problem can be overcome, since a straightforward mathematical manipulation yields

$$\frac{\beta U_q}{c} = \frac{DN}{2}, \quad (30)$$

with $c$ given by

$$c = \left\{ \frac{\Gamma\left(\frac{1}{1-q}\right) V^N}{\Gamma\left(\frac{1}{1-q} + \frac{DN}{2}\right) N! h^{DN} \left[ 2\pi m \right]^{DN}} \right\}^{\frac{2DN}{2}} \frac{\left[ 1 + (1 - q) \frac{DN/2}{2(1-q)h^{DN}} \right]^{2(1-q)h^{DN}}}{\left[ 1 + (1 - q) \frac{DN/2}{2(1-q)h^{DN}} \right]^{2(DN/2)}}. \quad (31)$$

To discuss the statistical properties of the particle energies, the $i$th and $j$th single-particle Hamiltonians may be considered, namely, $H_i = p_i^2/2m$ and $H_j = p_j^2/2m$, etc.
respectively. Their generalized variance, covariance and correlation coefficient are defined by [3]

\[(\Delta_q H_i)^2 = \langle \langle H_i^2 \rangle \rangle_q - \langle \langle H_i \rangle \rangle_q^2,\]

\[C_q(H_i, H_j) = \langle \langle H_i H_j \rangle \rangle_q - \langle \langle H_i \rangle \rangle_q \langle \langle H_j \rangle \rangle_q,\]

\[\rho(H_i, H_j) = \frac{C_q(H_i, H_j)}{\sqrt{(\Delta_q H_i)^2(\Delta_q H_j)^2}},\]

respectively. A straightforward calculation shows that these quantities are given by

\[(\Delta_q H_i)^2 = \frac{c^2}{2\beta^2} \frac{2D + (1 - q)D^2(N - 1)}{4 - 2q - (1 - q)DN},\]

\[C_q(H_i, H_j) = -\frac{c^2}{2\beta^2} \frac{(1 - q)D^2}{4 - 2q + (1 - q)DN},\]

\[\rho(H_i, H_j) = -\frac{(1 - q)D}{2 + (1 - q)D(N - 1)}.\]

In the limit \( q \rightarrow 1 \), one gets

\[(\Delta_q H_i)^2 \rightarrow \frac{D}{2} \left( \frac{h^2}{2\pi m} \right)^2 e^{-(2+4/D)} \left( \frac{N}{V} \right)^{4/D},\]

\[C_q(H_i, H_j) \rightarrow 0,\]

\[\rho(H_i, H_j) \rightarrow 0.\]

**IV. IDEAL GAS IN OLM FORMALISM**

We revisit here the classical ideal gas problem considered in the previous section within the OLM framework. We extremize Eq. (1), subject now to the constraints

\[\int d\Omega f(\mathbf{p}) - 1 = 0\]

\[\int d\Omega f(\mathbf{p})^\beta(H(\mathbf{p}) - U_q) = 0,\]

with \( H \) given in Eq. (23).

The probability distribution \( f(\mathbf{p}) \) reads

\[f(\mathbf{p}) = \frac{1}{Z_q} [1 - (1 - q)\beta'(H(\mathbf{p}) - U_q)]^{\frac{1}{\beta'}},\]

where

\[Z_q = \int d\Omega [1 - (1 - q)\beta'(H(\mathbf{p}) - U_q)]^{\frac{1}{\beta'}}.\]

In these equations, \( \beta' \) is the Lagrange multiplier associated with the constraint in Eq. (23).

We now follow the steps indicated in Ref. [4], and summarized in Section II. Our interest lies in the interval \( 0 < q < 1 \) again. First, define

\[R_1 = \frac{\Gamma\left(\frac{2-q}{2}\right)}{\Gamma\left(\frac{2-q}{2} + \frac{DN}{2}\right)},\]

and

\[R_2 = \left[ \frac{2\pi mc}{(1-q)\beta'} \right]^{\frac{DN}{2}} \left[ 1 + (1 - q)\frac{\beta'U_q}{c} \right]^{\frac{1}{\beta'}} \cdot \frac{DN}{2}.\]

The associated generalized partition function is given by

\[\bar{Z}_q(\beta') = R_1 \frac{V^N}{N! \hbar DN} R_2,\]

while, introducing

\[G_1 = \frac{DN}{2\beta' Z_q(\beta')},\]

the generalized internal energy turns out to be

\[U_q = G_1 R_1 \frac{V^N}{N! \hbar DN} R_2.\]

After replacing \( \bar{Z}_q(\beta') \) by Eq. (3), one finds

\[U_q = \frac{DN}{2\beta'}.\]

Now, taking advantage of the fact that (Cf. Eq. (20))

\[\beta' = \frac{1}{k_BT},\]

one is immediately led to

\[U_q = \frac{D}{2} Nk_BT,\]

i.e., to the ordinary result. Note that this result is obtained here without going to the limit \( q \rightarrow 1 \). By following the methodology advanced in Ref. [4], we see that, with the identification of Eq. (2), Tsallis thermostatistics is able to reproduce ordinary results independently of the specific choice of the value of \( q \).

Now, let us discuss statistical properties of the single-particle energies. Following again Section II, we focus our attention on the single particle Hamiltonians pertaining to the \( i \)th and the \( j \)th particles, \( H_i = \mathbf{p}_i^2/2m \) and \( H_j = \mathbf{p}_j^2/2m \), respectively. Their generalized variance, covariance and correlation coefficient are defined collectively in Eq. (yields

\[(\Delta_q H_i)^2 = \frac{1}{2(\beta')^2} \frac{2D + (1 - q)D^2(N - 1)}{4 - 2q - (1 - q)DN},\]

\[C_q(H_i, H_j) = -\frac{1}{2(\beta')^2} \frac{(1 - q)D^2}{4 - 2q + (1 - q)DN},\]

\[\rho(H_i, H_j) = -\frac{(1 - q)D}{2 + (1 - q)D(N - 1)},\]

respectively. In the limit \( q \rightarrow 1 \), one has
\[(\Delta_q H_i)^2 \to \frac{D}{2(\beta')}^2,\]
\[C_q(H_i, H_j) \to 0,\]
\[\rho(H_i, H_j) \to 0.\]

We see that the limit \(q \to 1\), \(C_q\) and \(\rho\) behave as in the Tsallis-Mendes-Plastino formalism in Ref. [3]. However, for \((\Delta_q H_i)^2\), we find something new: the result becomes independent of the density. It depends only on the temperature, as it does in the ordinary Boltzmann-Gibbs treatment.

V. CONCLUSIONS

In this work, we have addressed the ideal gas problem within the framework of Tsallis thermostatistics reformulated by the optimal Lagrange multipliers (OLM) method advanced in Ref. [1]. Three interesting observations have been presented:

- The internal energy was found to be given by
  \[U_q = \frac{D}{2} N k_B T,\]
  which is the same as the ordinary result obtained by Boltzmann-Gibbs theory. We derived this result without going to the limit \(q \to 1\). That is, it is valid for all \(q\).

- The correlation coefficient for the particle energies become density-independent in OLM, in contrast to that in the Tsallis-Mendes-Plastino formalism in Ref. [4].

- The constant \(k_T\) in the definition of the Tsallis entropy may depend on \(q\) and, therefore, on the number of particles. In the Boltzmann-Gibbs canonical ensemble theory, the limit particle number \(N\) going to infinity is always in mind, both explicitly and implicitly. This indicates that \(k_T \to k_B\) and \(q \to 1\) may correspond to \(N \to \infty \approx\) Avogadro’s number.

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