A class of energy-based ensembles in Tsallis statistics

R Chandrashekar\(^1\) and S S Naina Mohammed\(^2,3\)

\(^1\) Department of Theoretical Physics, University of Madras, Guindy Campus, Chennai 600 025, India
\(^2\) Department of Education in Science and Mathematics, Regional Institute of Education, Mysore 570 006, India
E-mail: chandrashekar10@yahoo.co.in and ss_nmphysics@yahoo.co.in

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Abstract. A comprehensive investigation is carried out on the class of energy-based ensembles. The eight ensembles are divided into two main classes. In the isothermal class of ensembles the individual members are at the same temperature. A unified framework is evolved to describe the four isothermal ensembles using the currently accepted third constraint formalism. The isothermal–isobaric, grand canonical and generalized ensembles are illustrated through a study of the classical nonrelativistic and extreme relativistic ideal gas models. An exact calculation is possible only in the case of the isothermal–isobaric ensemble. The study of the ideal gas models in the grand canonical and the generalized ensembles has been carried out using a perturbative procedure with the nonextensivity parameter \((1 - q)\) as the expansion parameter. Though all the thermodynamic quantities have been computed up to a particular order in \((1 - q)\) the procedure can be extended up to any arbitrary order in the expansion parameter. In the adiabatic class of ensembles the individual members of the ensemble have the same value of the heat function and a unified formulation to described all four ensembles is given. The nonrelativistic and the extreme relativistic ideal gases are studied in the isoenthalpic–isobaric ensemble, the adiabatic ensemble with number fluctuations and the adiabatic ensemble with number and particle fluctuations.

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\(^3\) Present address: Department of Physics, Government Arts College (Men), Krishnagiri 635001, India.
A class of energy-based ensembles in Tsallis statistics

Contents

1. Introduction 2
2. Isothermal ensemble 5
3. Isothermal–Isobaric ensemble 7
   3.1. Nonrelativistic ideal gas ................................ 7
   3.2. Extreme relativistic ideal gas .......................... 10
4. Grand canonical ensemble 12
   4.1. Nonrelativistic classical ideal gas ....................... 12
   4.2. Extreme relativistic classical ideal gas ..................... 17
5. Generalized ensemble 18
   5.1. Nonrelativistic ideal gas ................................ 18
   5.2. Extreme relativistic ideal gas .......................... 22
6. Adiabatic ensemble 23
7. Isoenthalpic–isobaric ensemble 25
   7.1. Nonrelativistic ideal gas in \((N, P, H)\) ensemble ........ 25
   7.2. Extreme relativistic ideal gas in \((N, P, H)\) ensemble ....... 27
8. Adiabatic ensemble with number fluctuations 29
   8.1. Nonrelativistic ideal gas ................................ 29
   8.2. Extreme relativistic Ideal gas ............................ 30
9. Adiabatic ensemble with volume and number fluctuations 30
   9.1. Nonrelativistic ideal gas ................................ 30
   9.2. Extreme relativistic Ideal gas ............................ 31
10. Remarks 31
    Acknowledgments 33
    References 33

1. Introduction

Boltzmann–Gibbs extensive statistical mechanics was generalized by Tsallis through the use of a deformed logarithm function in the entropic expression [1]. The functional form of the entropy defined in terms of the deformed logarithm is

\[ S_q = -k \sum_i p_i^q \ln_q p_i, \]  

(1.1)

where \(k\) is the generalization of the Boltzmann constant and \(p_i\) is the probability associated with the \(i\)th microstate. Recently it has been proved [2, 3] that the \(q\)-entropy (1.1) is not Lesche stable when the \(L_1\)-norm (\(|P - P'|\)) is computed between the escort probabilities \(P_i = (p_i^q) / (\sum_i p_i^q)\). But the thermodynamic averages have been proved [3] to be stable under the same conditions. The \(q\)-deformed logarithm made use of in (1.1) and its

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A class of energy-based ensembles in Tsallis statistics

inverse, the \( q \) exponential, are defined below:

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

(1.2)

where we have used the notation \( [x]_+ = \max\{0, x\} \). In the \( q \to 1 \) limit, (1.1) reduces to the extensive Boltzmann–Gibbs entropy. A detailed account on the properties of the \( q \)-entropy and its applications may be found in [4].

To describe a system in thermodynamic equilibrium with its surroundings, we need three macroscopic variables corresponding to thermal, mechanical and chemical equilibrium. A system with fixed values of these parameters can exist in different microstates. A collection of systems existing in all the possible microstates corresponding to the same value of the macroscopic variables is called an ensemble. Each of these macroscopic parameters can be chosen between an extensive and an intensive variable. Thus we have eight different ways of choosing the three variables and consequently eight different ensembles. The eight different descriptions in thermodynamics and statistical mechanics in the Boltzmann–Gibbs extensive formulation have been studied in [5]. The eight ensembles can be divided into two different classes, namely the isothermal class and the adiabatic class. In the isothermal class of ensembles, the thermal equilibrium variable is the temperature and the individual members of the ensemble are at the same temperature. The canonical, isothermal–isobaric [6]–[8], grand canonical and generalized ensembles [6,7] belong to the isothermal class. Each one of these isothermal ensembles is characterized by a heat function and a free energy. A general expression for the heat function and the generalized free energy is given below:

\[
\mathcal{S}_\ell = U + \sum_{\{\ell\}} x_{\ell} X_{\ell}
\]

(1.3)

\[
\mathcal{F}_\ell = U - TS + \sum_{\{\ell\}} x_{\ell} X_{\ell}
\]

(1.4)

where \( X \) is an extensive thermodynamic quantity whose intensive conjugate is \( x \). The index \( \ell \) can take three different values of either 0, 1 or 2. In the \( \ell = 0 \) case the internal energy and the Helmholtz free energy are the heat function and the free energy, respectively. The ensemble pertaining to this situation is the canonical ensemble \((N, V, T)\). Both the isothermal–isobaric \((N, P, T)\) and the grand canonical \((\mu, V, T)\) ensembles relate to the \( \ell = 1 \) case in (1.3) and (1.4). The enthalpy \( H = U + PV \) and the Gibbs free energy \( G = U - TS + PV \) are the heat function and the free energy corresponding to the isothermal–isobaric ensemble. For the grand canonical ensemble the Hill energy \( L = U - \mu N \) and the \( \Phi = U - TS - \mu N \) are the heat function and the free energy, respectively. The \( \ell = 2 \) case describes the completely open system \((\mu, P, T)\) and the ensemble is usually referred to as the generalized ensemble. The \( R \) function (Ray energy) \( R = U + PV - \mu N \) and \( E = U + PV - TS - \mu N \) are the heat function and the free energy of the generalized ensemble. The adiabatic class of ensembles arises when the thermal equilibrium happens with respect to the heat function which is an extensive quantity. Based on the four different heat functions, namely \( U, H, L \) and \( R \), we have four different ensembles: the well known microcanonical \((N, V, U)\) ensemble; the isenthalpic–isobaric \((N, P, H)\) ensemble introduced in [9] and later extensively studied in [10,11]; more
recently the adiabatic ensemble with number fluctuations \((\mu, V, L)\) and the adiabatic ensemble with number and volume fluctuations \((\mu, P, R)\) were introduced through [12] and [13], respectively. All four adiabatic ensembles were treated in a unified way in [14]. Of the eight ensembles, the microcanonical, canonical and grand canonical ensembles have been extensively studied and are well known in statistical mechanics. But the other five ensembles are also of fundamental importance in studying physical problems whose experimental conditions emulate the conditions of these ensembles. For example, the isothermal–isobaric and the isenthalpic–isobaric ensembles are used to study fluids which are confined at constant pressure. A molecular dynamic simulation for these ensembles was evolved in [15]. The generalized ensemble has been studied in [16]. Applications of the generalized ensemble include lattice gas models and a system of polymer molecules of \(N\) monomers held together by weak forces such that the number \(N\) fluctuates [16].

An investigation of the ensemble formulation of nonextensive statistical mechanics based on \(q\)-entropy (1.1) was initiated in [1] through the study of a two-level system in the microcanonical and canonical ensembles. A further detailed study of the canonical ensemble was carried out in [17]–[19] wherein the various methods of optimization of the entropy were discussed. At present the third constraint formalism [18] which employs the normalized escort probabilities is the accepted version, and in our work we follow this formalism consistently. The definition of the \(q\) expectation in the third constraint formalism is

\[
\langle O \rangle_q = \frac{\sum_j (p_j(\beta))^q O_j}{c(\beta)}, \quad c(\beta) = \sum_j (p_j(\beta))^q. \tag{1.5}
\]

The various applications of the canonical formulation may be found in [20, 21]. The grand canonical ensemble has also been investigated in [22, 23]. A detailed investigation of the microcanonical ensemble based on the \(q\)-entropy (1.1) was carried out in [24] and the classical ideal gas was discussed as an application. Thus in the nonextensive statistical mechanics, based on \(q\)-entropy, only three ensembles, the canonical [1, 17, 18], microcanonical [1, 24] and grand canonical [22, 23], have been investigated so far.

In the current work we present two unified frameworks, one for the isothermal class of ensembles and the other for the adiabatic class of ensembles. The unified framework pertaining to the isothermal class of ensembles is based on the third constraint formalism which is the currently accepted formulation. An exact solution of the specific heats at constant pressure and at constant volume corresponding to both the classical nonrelativistic ideal gas and the extreme relativistic ideal gas has been obtained in the isothermal–isobaric ensemble. In contrast, obtaining an exact solution to these ideal gas models in the grand canonical and the generalized ensemble appears to be difficult. We make use of the technique of disentangling of the \(q\) exponential into a series of ordinary exponentials [25] to construct a perturbative approach to the problem. Such an approach has already been used in the context of the canonical ensembles [21, 26]. In the case of the grand canonical ensemble, the perturbative terms up to second order in the expansion parameter \((1−q)\) has been retained. The perturbative terms have been displayed up to first order in the expansion parameter \((1−q)\) in the case of the generalized ensemble. The limitations imposed on the order of \((1−q)\) is only for the sake of calculational simplicity and in practice the method could be extended to any arbitrary order in the perturbative parameter. A unified framework to describe all four adiabatic ensembles in the nonextensive \(q\) statistics has been put forward. A \(q\) generalization of the equipartition theorem and the virial theorem have also
been discussed. The specific heat at constant pressure and at constant volume corresponding to the nonrelativistic and extreme relativistic models of an ideal gas have been exactly computed. Since a summation over the number of particles could not be evaluated in the \((\mu, V, L)\) and \((\mu, P, R)\) adiabatic ensembles, the phase space volume and the equation of state are expressed as formal sums. In this paper the Lagrange multiplier \(\beta\) corresponding to the internal energy is associated \([18]\) with the inverse temperature, \(\beta \equiv (kT)^{-1}\), in contrast to the ‘physical temperature’ defined through the zeroth law of thermodynamics with an assumption that the entire system can be divided into independent subsystems \([27]\). Introducing the notion of the quasireversibility condition which requires the system to return to a microstate only in the neighborhood of the original state, and the first law of thermodynamics, it has been observed \([28]\) that the Tsallis entropy becomes identical to the thermodynamic Clausius entropy provided the Lagrange multiplier \(\beta\) is held proportional to the inverse temperature. It has also been observed \([29]\) that, in the context of nonextensive systems, the thermodynamic limit and the long-time limit do not commute. Based on this viewpoint we regard the temperature as the reciprocal of the Lagrange multiplier for the constraint on the internal energy. To settle the issue of temperature it is important to explore possibilities where alternative definitions of temperature leads to distinct experimental results.

The plan of this paper is as follows. The unified framework for the isothermal ensembles is presented in section 2, wherein the second and third constraint formulations are described in separate subsections. Using the classical nonrelativistic and extreme relativistic ideal gases the isothermal–isobaric ensemble, grand canonical ensemble and generalized ensemble are illustrated in sections 3, 4 and 5. A generalized formulation of the adiabatic ensembles is given in section 6. The ideal gas model in the isoenthalpic–isobaric ensemble have been worked out in section 7. In sections 8 and 9 the \((\mu, V, L)\) and \((\mu, P, R)\) ensembles are discussed. We present our concluding remarks in section 10.

2. Isothermal ensemble

The isothermal class of ensembles is used to study systems in which the thermal equilibration is with respect to the temperature. A unified framework to study the isothermal class of ensembles in the third constraint is introduced in this section. The definition of the internal energy, an arbitrary extensive variable and the heat function are

\[
U_q(\mathbf{x}_1, \mathbf{x}_2, \beta) = \frac{1}{c(\mathbf{x}_1, \mathbf{x}_2, \beta)} \sum_{i,X_{\{\ell\}}} (p_{i;X_{\{\ell\}}}(\mathbf{x}_1, \mathbf{x}_2, \beta))^q \epsilon_i, \tag{2.1}
\]

\[
H_q(\mathbf{x}_1, \mathbf{x}_2, \beta) = \frac{1}{c(\mathbf{x}_1, \mathbf{x}_2, \beta)} \sum_{i,X_{\{\ell\}}} (p_{i;X_{\{\ell\}}}(\mathbf{x}_1, \mathbf{x}_2, \beta))^q \epsilon_i, \tag{2.2}
\]

\[
H_q(\mathbf{x}_1, \mathbf{x}_2, \beta) = \frac{1}{c(\mathbf{x}_1, \mathbf{x}_2, \beta)} \sum_{i,X_{\{\ell\}}} (p_{i;X_{\{\ell\}}}(\mathbf{x}_1, \mathbf{x}_2, \beta))^q \left( \epsilon_i + \sum_{\{\ell\}} x_\ell X_{\ell} \right), \tag{2.3}
\]
where \( p_{i:X(\ell)} \) is the probability of finding the particle in a particular microstate and \( X \) is an extensive thermodynamic quantity whose intensive counterpart is \( x \). The chemical and the mechanical equilibrium variables are denoted by \( X_1 \) and \( X_2 \). A brief introduction of the variable \( \ell \) and the method to deduce the various ensembles corresponding to its different values is given in section 1. The factor \( c \) is the sum of \( q \) weights in the third constraint and is defined as

\[
c(\ell, X_1, X_2, \beta) = \sum_{i,X(\ell)} (p_{i,X(\ell)}(X_1, X_2, \beta))^q.
\]  

(2.4)

Along with the normalization condition, the definitions corresponding to the internal energy (2.1) and the arbitrary extensive variable (2.2) are used in the optimization of the entropy (1.1). The probability distribution obtained through this procedure is

\[
p_{i:X(\ell)}(X_1, X_2, \beta) = \frac{1}{\bar{Z}_q(X_1, X_2, \beta)} \exp\left( -\frac{\beta}{c(X_1, X_2, \beta)} \left( \epsilon_i + \sum_{\ell} x_\ell X_\ell - \bar{\mathcal{H}}_q \right) \right),
\]

(2.5)

where \( \bar{\mathcal{H}}_q \) is the heat function in the third constraint and \( \beta = 1/kT \). The generalized partition function \( \bar{Z}_q \) in (2.5) is as defined below:

\[
\bar{Z}_q(\beta, X_1, X_2) = \sum_{i,X(\ell)} \exp\left( -\frac{\beta}{c(\beta, X_1, X_2)} \left( \epsilon_i + \sum_{\ell} x_\ell X_\ell - \bar{\mathcal{H}}_q \right) \right).
\]

(2.6)

The generalized partition function and the sum of the \( q \) weights are related via the expression

\[
(\bar{Z}_q(\beta, X_1, X_2))^{1-q} = c(\beta, X_1, X_2),
\]

(2.7)

which holds for all isothermal ensembles and plays a crucial role in solving the implicit equations in the third constraint.

The heat function in the third constraint satisfies the differential equation

\[
\beta \frac{\partial}{\partial \beta} \bar{\mathcal{H}}_q(\beta, X_1, X_2) = \frac{\partial}{\partial \ln \bar{Z}_q} \ln \bar{Z}_q(\beta, X_1, X_2).
\]

(2.8)

From the knowledge of the heat function \( \bar{\mathcal{H}}_q \) and the generalized partition function \( \bar{Z}_q \) the expectation value of the extensive thermodynamic variable is found using

\[
X_{\ell q}(\beta, X_1, X_2) = \frac{\partial}{\partial x_\ell} \left( \bar{\mathcal{H}}_q(\beta, X_1, X_2) - \frac{1}{\beta} \ln \bar{Z}_q(\beta, X_1, X_2) \right).
\]

(2.9)

The internal energy can be obtained from the heat function and the extensive thermodynamic quantities using the Legendre transformation. Making use of the property (2.7), the nonextensive entropy (1.1) expressed in terms of the generalized partition function (2.6) is

\[
S_q = k \ln \bar{Z}_q(\beta, X_1, X_2).
\]

(2.10)

Substituting the entropy (2.10) in (1.4) we arrive at the free energy in the third constraint as

\[
\mathcal{F}_q = U_q - \frac{1}{\beta} \ln \bar{Z}_q(\beta, X_1, X_2) + \sum_{\ell} x_\ell X_{\ell q}.
\]

(2.11)
In terms of the generalized free energy defined in (2.11) the heat function and the $q$-expectation value of the extensive thermodynamic variable are

$$S_q = \frac{\partial}{\partial \beta} (\beta F_q), \quad X_{\ell q} = \frac{\partial F_q}{\partial x_{\ell}}.$$  \hspace{1cm} (2.12)

The heat capacities under different experimental conditions in the third constraint are

$$C_q^{\left| V \right.} = \frac{\partial U_q}{\partial T},$$  \hspace{1cm} (2.13)

$$C_q^{\left| x_{(\ell)} \right.} = \frac{\partial S_q}{\partial T} = T \frac{\partial S_q}{\partial T} = -T \frac{\partial^2 F_q}{\partial T^2}. \hspace{1cm} (2.14)$$

The thermodynamic relations for the canonical ensemble can be obtained from the unified framework by observing that the internal energy and the Helmholtz free energy are the heat function and the free energy, respectively. An elaborate exposition on the canonical ensemble may be found in [17,18] and, since this ensemble has been investigated in detail, we do not intend to discuss it anymore.

3. Isothermal–Isobaric ensemble

The isothermal–isobaric ensemble is used to study systems which attain equilibrium by exchanging both internal energy and volume with the heat bath. The enthalpy and the Gibbs free energy play the role of heat function and free energy, respectively. Using the unified framework described in section 2 the nonrelativistic and the extreme relativistic ideal gases are investigated.

3.1. Nonrelativistic ideal gas

The Hamiltonian of a classical ideal gas in the nonrelativistic regime with particles possessing momenta $p_i$ ($i = 1, \ldots, N$) in $D$ dimensions is

$$H_{nr}(p) = \sum_i \frac{p_i^2}{2m}, \quad p_i = |p_i|. \hspace{1cm} (3.1)$$

The generalized partition function corresponding to the third constraint in the $(N,P,T)$ ensemble is

$$\bar{Y}_q(\beta, P) = \frac{1}{N! h^{DN}} \int_V \text{d}V \int_{r_i} \prod_{i=1}^N \text{d}^D r_i \text{d}^D p_i \exp_q \left( -\frac{\beta}{c} \left( \sum_i \frac{p_i^2}{2m} - U_q + PV - PV_q \right) \right). \hspace{1cm} (3.2)$$

Carrying out the phase space integration in (3.2), we arrive at

$$\bar{Y}_q(\beta, P) = \frac{M^N}{N!} \frac{\Gamma((2-q)/(1-q))}{\Gamma((2-q)/(1-q)+(DN/2))} \int_V V^N \left( \exp_q \left( \frac{\beta}{c} (U_q - PV + PV_q) \right) \right)^{\Lambda} \text{d}V, \hspace{1cm} (3.3)$$

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where \( \mathcal{M} = (2\pi m/h^2)^{D/2} \) and \( \Lambda = 1 + (1 - q)DN/2 \). In order to express the thermodynamic variables in a simplified manner, we define the following quantities:

\[
\Lambda_\kappa = 1 + (1 - q)D_\kappa, \quad \mathcal{L}_\kappa = (1 - (1 - q)D_\kappa)^{-1}, \quad \mu_\kappa = \Lambda_\kappa\mathcal{L}_\kappa, \quad (3.4)
\]

where \( \kappa = 1 \) (2) for a nonrelativistic (extreme relativistic) case and \( D_1 = DN/2 + N(D_2 = DN + N) \). Integrating over volume in (3.3) we arrive at the generalized partition function:

\[
\bar{Y}_q(\beta, P) = \frac{\mathcal{M}^N \Gamma((2 - q)/(1 - q))}{\Gamma((2 - q)/(1 - q) + D_1 + 1)} \left( \frac{1}{1 - q} \right)^{D_1 + 1} \left( \exp_q \left( \frac{\beta}{c}(U_q + PV_q) \right) \right)^{\Lambda_1 - (1 - q)} \times \left( \frac{1}{P} \right)^{N + 1}.
\]

It is interesting to note that (3.5) has the dimensions of volume. This is due to the overcounting of volume eigenstates in systems in which the volume is a continuous variable. To overcome this we use the shell particle method of counting volume states \([30,31]\). In the shell particle method of counting we take into account only the minimum volume needed to confine a particular configuration. When there are many equivalent ways of choosing a minimum volume we treat all of them as the same volume eigenstate. The minimum volume is fixed by enforcing a condition where we require that at least one particle lies on the boundary of the system. Carrying out the volume integral of the generalized partition function using the shell particle counting technique to reject the redundant volume states we arrive at

\[
\bar{Y}_q(\beta, P) = \mathcal{M}^N G_1 \left( \exp_q \left( \frac{\beta}{c}(U_q + PV_q) \right) \right)^{\Lambda_1} \left( \frac{c}{\beta} \right)^{D_1} \left( \frac{1}{P} \right)^{N + 1}.
\]

The above expression of the generalized partition function (3.6), in contrast to (3.5), is dimensionless, making it consistent with the basic principles of statistical mechanics. The ratio of gamma functions \( G_1 \) made use of in (3.6) is

\[
G_1 = \frac{\Gamma((2 - q)/(1 - q))}{(1 - q)^{D_1} \Gamma((2 - q)/(1 - q) + D_1)}.
\]

The heat function of the isothermal–isobaric ensemble given by the basic relation (2.3) is computed and the result is

\[
H_q = D_1 \frac{\mathcal{M}^N }{\bar{Y}_q} G_1 \left( \exp_q \left( \frac{\beta}{c}H_q \right) \right)^{\Lambda_1} \left( \frac{1}{P} \right)^{N + 1}.
\]

The ratio between (3.6) and (3.8) is computed:

\[
H_q = D_1 \frac{c}{\beta}.
\]

Using (3.9) in conjunction with (2.7), in (3.6) the explicit form of the generalized partition function is

\[
\bar{Y}_q = (\mathcal{M}^N G_1)^{\mathcal{L}_1} \left( \exp_q(D_1) \right)^{\mu_1} \left( \frac{1}{\beta} \right)^{D_1\mathcal{L}_1} \left( \frac{1}{P} \right)^{N\mathcal{L}_1}.
\]

From the generalized partition function the range of the nonextensivity parameter has been obtained for some systems like the ideal gas \([20,21]\) and the rigid rotators \([26]\). We
notice from (3.10) that the generalized partition function has simple poles for the values of the nonextensive parameter $q = 1 + 1/n$, $n = 1, \ldots, D_1$. The generalized partition function is well defined in the interval $0 < q < 1 + (1/D_1)$. As the number $N$ increases there is an accumulation of poles in the neighborhood of $q = 1$ and so in the thermodynamic limit the above-mentioned interval reduces to $0 < q \leq 1$. The explicit expression of the enthalpy computed through the use of (3.8), (3.10) and (2.7) is

$$H_q = \frac{D_1}{\beta} \Xi_{nr} \left( \frac{1}{\beta} \right)^{(1-q)D_1 \xi_1} \left( \frac{1}{P} \right)^{(1-q)N \xi_1},$$  

(3.11)

where the constant factor $\Xi_{nr}$ used in (3.11) is

$$\Xi_{nr} = (\mathcal{M}^N \mathcal{G}_1)^{(1-q)\xi_1} \Lambda^m_1.$$  

(3.12)

The entropy of the system in the third constraint written down from the generalized partition function using the relation (2.10) is

$$S_q = \frac{k}{1-q} \left( \Xi_{nr} \left( \frac{1}{\beta} \right)^{(1-q)D_1 \xi_1} \left( \frac{1}{P} \right)^{(1-q)N \xi_1} - 1 \right).$$  

(3.13)

Making use of the thermodynamic Legendre structure (2.11) the Gibbs free energy of the classical ideal gas is obtained:

$$G_q = \frac{1}{(1-q)\beta} \left( (1-q)D_1 - 1 \right) \Xi_{nr} \left( \frac{1}{\beta} \right)^{(1-q)D_1 \xi_1} \left( \frac{1}{P} \right)^{(1-q)N \xi_1} - 1 \right).$$  

(3.14)

The average volume of the classical nonrelativistic ideal gas in the third constraint can be found via the expression (2.9) using the explicit expression of the generalized partition function (3.10) and the enthalpy (3.11). The calculated expression of the average volume is

$$V_q = \frac{N}{\beta P} \Xi_{nr} \left( \frac{1}{\beta} \right)^{(1-q)D_1 \xi_1} \left( \frac{1}{P} \right)^{(1-q)N \xi_1}.$$  

(3.15)

The average volume which was computed using enthalpy can also be calculated through two other different methods. The first method is based on a specific form of (2.12) applicable to the isothermal–isobaric ensemble in which the average volume is related to the Gibbs free energy. The second method makes use of the defining relation of the average volume (2.2) to obtain an implicit expression. Using the implicit expression in conjunction with (3.11), (3.10) and (2.7) we can obtain the final explicit form. The results obtained through both these methods are in agreement with those obtained in (3.15). Rewriting the expression for the average volume (3.15) we arrive at the nonextensive form of the equation of state corresponding to the isothermal–isobaric ensemble:

$$PV_q = \frac{N}{\beta} \Xi_{nr} \left( \frac{1}{\beta} \right)^{(1-q)D_1 \xi_1} \left( \frac{1}{P} \right)^{(1-q)N \xi_1}.$$  

(3.16)

From the knowledge of the enthalpy and the average volume, the internal energy evaluated using the Legendre structure is

$$U_q = \frac{D N}{2\beta} \Xi_{nr} \left( \frac{1}{\beta} \right)^{(1-q)D_1 \xi_1} \left( \frac{1}{P} \right)^{(1-q)N \xi_1}.$$  

(3.17)
The defining relation of the internal energy (2.1) has been used to verify (3.17) in a manner analogous to the calculation of the average volume.

The specific heat at constant pressure can be found from either the enthalpy (3.11) or entropy (3.13) or the Gibbs free energy (3.14) using (2.14):

\[ C_q |_P = \left( \frac{DN}{2} + N \right) k \xi_1 \Xi_{nr} \left( \frac{1}{\beta} \right)^{(1-q)\xi_1} \left( \frac{1}{P} \right)^{(1-q)N\xi_1}. \]  

(3.18)

From the internal energy (3.17) the specific heat at constant volume is evaluated through the use of (2.13):

\[ C_q |_V = \frac{DN}{2} k \Xi_{nr} \xi_1 \left( \frac{1}{\beta} \right)^{(1-q)\xi_1} \left( \frac{1}{P} \right)^{(1-q)N\xi_1}. \]  

(3.19)

The difference between the specific heat at constant pressure (3.18) and the specific heat at constant volume (3.19) is

\[ C_q |_P - C_q |_V = Nk \xi_1 \Xi_{nr} \left( \frac{1}{\beta} \right)^{(1-q)\xi_1} \left( \frac{1}{P} \right)^{(1-q)N\xi_1}, \]  

(3.20)

which is the generalized form of Meyer’s relation and in the extensive limit the lhs goes as \( Nk \). It is interesting to note that the factor \( \gamma \) expressing the ratio between the two specific heats:

\[ \gamma = \frac{C_q |_P}{C_q |_V} = 1 + \frac{2}{D}, \]  

(3.21)

is independent of the nonextensive parameter \( q \) and the number of particles \( N \), though the specific heats (3.18) and (3.19) depend on these parameters explicitly.

3.2. Extreme relativistic ideal gas

The Hamiltonian of the extreme relativistic classical ideal gas in \( D \) dimensions is

\[ \mathcal{H}_{er}(p) = c \sum p_i, \quad p_i = |p_i|, \]  

(3.22)

where the factor \( c \) is the velocity of light. The nonextensive study of the Hamiltonian (3.22) is carried out in the isothermal–isobaric ensemble. Since the calculational procedure is identical to the nonrelativistic case we present only the core steps leading to the calculation of the specific heats. The generalized partition function calculated using the basic definition is

\[ \bar{Y}_q = \Delta^N \mathcal{G}_2 \left( \frac{1}{P} \right)^N \left( \frac{\xi}{\beta} \right)^{DN+N}. \]  

(3.23)

The notations made use of in (3.23) are

\[ \Delta = \frac{2\pi^{D/2}\Gamma(D)}{(ch)^D\Gamma(D/2)}, \quad \mathcal{G}_2 = \frac{\Gamma((2-q)/(1-q))}{(1-q)^{D_2}\Gamma((2-q)/(1-q)+D_2)}. \]  

(3.24)

Equation (3.23) is an implicit equation since it is a function of the sum of \( q \) weights which is related to the generalized partition function through the relation (2.7). The nonextensive enthalpy of the extreme relativistic ideal gas is

\[ H_q = \mathcal{D}_2 \frac{\Delta^N}{\bar{Y}_q} \mathcal{G}_2 \left( \exp_q \left( \frac{\beta}{\xi} H_q \right) \right)^{\Lambda_2} \left( \frac{1}{P} \right)^N \left( \frac{\xi}{\beta} \right)^{D_2+1}. \]  

(3.25)
where the factors $\Lambda_2$, $\mathcal{L}_2$ and $\mu_2$ used in this section are described in (3.4) and the discussions following it. The ratio between (3.23) and (3.25) is

$$H_q = \mathcal{D}_2 \frac{c}{\beta}. \tag{3.26}$$

Using (3.26) in (3.23) we obtain the explicit expression corresponding to the generalized partition function:

$$\bar{Y}_q = (\Delta N \mathcal{G}_2)^{\mathcal{L}_2} \left( \exp_q(\mathcal{D}_2) \right)^{\mu_2} \left( \frac{1}{P} \right)^{N \mathcal{L}_2} \left( \frac{1}{\beta} \right)^{\mathcal{D}_2 \mathcal{L}_2}. \tag{3.27}$$

Similarly the calculated value of the explicit form of the enthalpy is

$$H_q = \mathcal{D}_2 \frac{\Xi_{er}}{\beta} \left( \frac{1}{P} \right)^{(1-q)N \mathcal{L}_2} \left( \frac{1}{\beta} \right)^{(1-q)\mathcal{D}_2 \mathcal{L}_2}, \tag{3.28}$$

where the factor $\Xi_{er}$ is defined as

$$\Xi_{er} = (\Delta N \mathcal{G}_2)^{(1-q)\mathcal{L}_2} \Lambda_2^{\mu_2}. \tag{3.29}$$

The average volume of the extreme relativistic ideal gas is evaluated through the use of (6.7). The equation of state obtained by rewriting the expression for the average volume is

$$PV_q = \frac{N}{\beta} \Xi_{er} \left( \frac{1}{P} \right)^{(1-q)\mathcal{D}_2 \mathcal{L}_2} \left( \frac{1}{\beta} \right)^{(1-q)N \mathcal{L}_2}. \tag{3.30}$$

To find the internal energy we use the Legendre transform (1.3) and the expressions for the enthalpy and the average volume. The computed expression of the internal energy is

$$U_q = \frac{DN}{\beta} \Xi_{er} \left( \frac{1}{P} \right)^{(1-q)\mathcal{D}_2 \mathcal{L}_2} \left( \frac{1}{\beta} \right)^{(1-q)N \mathcal{L}_2}. \tag{3.31}$$

The specific heat capacity of the extreme relativistic ideal gas at constant volume and at constant pressure can be established from the final explicit expressions of the internal energy and the enthalpy, respectively. We exhibit the results below:

$$C_q|_V = DN k \Xi_{er} \mathcal{L}_2 \left( \frac{1}{\beta} \right)^{(1-q)\mathcal{D}_2 \mathcal{L}_2} \left( \frac{1}{P} \right)^{(1-q)N \mathcal{L}_2}, \tag{3.32}$$

$$C_q|_P = (DN + N) k \Xi_{er} \mathcal{L}_2 \left( \frac{1}{\beta} \right)^{(1-q)\mathcal{D}_2 \mathcal{L}_2} \left( \frac{1}{P} \right)^{(1-q)N \mathcal{L}_2}. \tag{3.33}$$

The ratio between the heat capacity at constant pressure and at constant volume:

$$\frac{C_q|_P}{C_q|_V} = 1 + \frac{1}{D}, \tag{3.34}$$

is found to be independent of both the nonextensive parameter $q$ and the number of particles $N$. All the results in this section have been calculated directly in the third constraint where the generalized partition function, sum of $q$ weights and the enthalpy are computed. Since these quantities are implicit in nature, they are systematically solved to obtain the explicit forms. The proper counting of volume states advocated in [30,31].

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A class of energy-based ensembles in Tsallis statistics

has been used in both methods. In the extensive \( q \to 1 \) limit, the standard physical quantities corresponding to the classical Boltzmann–Gibbs statistics are recovered.

Another interesting model is the Tonks gas [32] which is a one-dimensional model of a hard rod gas. The Hamiltonian describing the dynamics of a Tonks gas is

\[
\mathcal{H}_{\text{tg}}(p) = \sum_i \frac{p_i^2}{2m} + V(r), \quad p_i = |p_i|,
\]

where the potential \( V(r) \) is

\[
V(r) = \begin{cases} 
0 & x \geq \sigma \\
\infty & x < \sigma.
\end{cases}
\]

An exact solution of the Tonks gas in the free length ensemble can be seen from the results of the nonrelativistic ideal gas. In this discussion the term ‘free length’ refers to the actual volume available for a particle \( L_{f,q} = L - (N - 1)\sigma \). The equation of state of the Tonks gas in the free length ensemble can be read from the expression corresponding to the classical nonrelativistic ideal gas by observing that the number of dimensions is 1 and replacing the volume by the free length. The equation of state of the Tonks gas in the free length ensemble is

\[
PL_{f,q} = \frac{N}{\beta} \left( M_1^N \mathcal{G}_{1:1} \right)^{(1-q)\Sigma_{1:1}} \left( \Lambda_{1:1} \right)^{\mu_{1:1}} \left( \frac{1}{\beta} \right)^{(3N/2)\Sigma_{1:1}} \left( \frac{1}{P} \right)^{N\Sigma_{1:1}},
\]

where the functions \( \mathcal{G}_{1:1} \) and \( \Lambda_{1:1} \) are special cases of (3.7), obtained by substituting \( D = 1 \), and \( M_1 \) is the one-dimensional analog of \( M \). A direct computation of the Tonks gas has been used to verify the expression for the equation of state. The correct counting of volume states has been applied and the Boltzmann–Gibbs results are recovered in the \( q \to 1 \) limit.

4. Grand canonical ensemble

A system which exchanges both the internal energy and the number of particles with its surroundings is described using the grand canonical ensemble. The Hill energy \( L = U - \mu N \) is the heat function and the free energy is \( \Phi = U - TS - \mu N \). In this section we extend the perturbative formulation developed in [21] and [26] to study the nonrelativistic and extreme relativistic ideal gas in the grand canonical ensemble.

4.1. Nonrelativistic classical ideal gas

A perturbative study of the nonrelativistic classical ideal gas described by the Hamiltonian (3.1) is carried out in the grand canonical ensemble. The generalized partition function in the third constraint is

\[
\tilde{Z}_q(\mu, V, \beta) = \sum_{N=0}^{\infty} \frac{1}{N!} \int d^D r \int d^D p \exp_q \left( -\tilde{\beta} \left( \sum_i \frac{p_i^2}{2m} - \mu N - L_q^{(3)} \right) \right),
\]

where \( \tilde{\beta} = \beta/c \) and \( c \) is the sum of \( q \) weights corresponding to the grand canonical ensemble in the third constraint. The Hill function \( L_q = U_q - \mu N_q \) is the heat function corresponding
to the grand canonical ensemble where $U_q$ and $N_q$ are the internal energy and the average number of particles, respectively, in the third constraint and $\mu$ is the chemical potential of the system.

The observation in [25], that the $q$ exponential can be written as an infinite multiplicative series of ordinary exponentials:

$$\exp_q(x) = \prod_{k=1}^{\infty} \exp \left( -1^{k-1} \frac{(1-q)^k x^k}{k} \right), \quad \text{(4.2)}$$

which in turn can be expanded up to any order in $(1-q)$, is used to construct a perturbative procedure for the generalized partition function. Assuming the generalized partition function (4.1) to be well defined in the region $q = 1$, we replace the $q$ exponential by the ordinary exponential. The resultant expression for the generalized partition function is

$$\tilde{Z}_q(\mu, V, \beta) = \tilde{D}_1(d_\beta) \exp(\mathcal{L}) \sum_{N=0}^{\infty} \frac{1}{N! h^{DN}} \int d^{DN} r \; d^{DN} p \exp \left( -\tilde{\beta} \left( \sum_i \frac{p_i^2}{2m} - \mu N \right) \right). \quad \text{(4.3)}$$

where $\mathcal{L} = \tilde{\beta} L_q$ and the operator-valued series $\tilde{D}_1(d_\beta)$ in (4.3) is

$$\tilde{D}_1(d_\beta) = 1 - \frac{(1-q)}{2} d_\beta^2 + \frac{(1-q)^2}{3} \left( d_\beta^3 + \frac{3}{8} d_\beta^4 \right) + \cdots, \quad d_\beta^n = \beta^n \frac{\partial^n}{\partial \beta^n}. \quad \text{(4.4)}$$

In the expression (4.3), we assume that the summation over the number of particles is convergent, at least in the region where the nonextensive parameter is close to one. Carrying out the phase space integration and the summation over the number of particles in (4.3), the generalized partition function in the third constraint can be expressed as

$$\tilde{Z}_q(\mu, V, \beta) = \tilde{D}_1(d_\beta) \exp(\mathcal{L}) \; Z_{BG}(\tilde{\beta}), \quad \text{(4.5)}$$

where $Z_{BG}(\beta) = \exp(\exp(\beta \mu) V \mathcal{M} \beta^{-D/2})$ is the Boltzmann–Gibbs partition function. The perturbative series of the generalized partition function (4.5) calculated up to second order in the expansion parameter $(1-q)$ is

$$\tilde{Z}_q = \exp(\mathcal{L}) \; Z_{BG}(\tilde{\beta}) \left( 1 + (1-q) \; Z_1 + (1-q)^2 \; Z_2 + \cdots \right), \quad \text{(4.6)}$$

where the coefficients of the perturbative series (4.6) are listed below:

\[
\begin{align*}
Z_1 &= \frac{1}{4} (2L^2 + 2N_{BG}(\tilde{\beta}) (\alpha(\tilde{\beta}))^2 + (N_{BG}(\tilde{\beta}))^2 (2 (\alpha(\tilde{\beta}))^2 + 4 \alpha(\tilde{\beta}) \; \mathcal{L} + D)), \\
Z_2 &= \frac{1}{8} L^4 + \frac{1}{6} L^3 + \frac{1}{8} (N_{BG}(\tilde{\beta}))^4 (\alpha(\tilde{\beta}))^4 + \frac{1}{96} (N_{BG}(\tilde{\beta}))^3 (72 (\alpha(\tilde{\beta}))^4 + 12 L (\alpha(\tilde{\beta}))^3 \\
&\quad+ 4 (8 (\tilde{\beta} \mu)^3 - 3D^2) \alpha(\tilde{\beta}) + D (4 (\tilde{\beta} \mu)^3 - D^2)) + \frac{1}{32} (N_{BG}(\tilde{\beta}))^2 (48 L (\alpha(\tilde{\beta}))^2 \\
&\quad+ 8 (3 \mathcal{L} + 2) (\alpha(\tilde{\beta}))^2 - 12 D (\tilde{\beta} \mu \alpha(\tilde{\beta}) + 8 (4 - 7D) (\tilde{\beta} \mu)^3 + 42 D^2 (\tilde{\beta} \mu)^2 \\
&\quad- 2D^3 (9 + 7D) \beta + D^2 (3 + 5D + 7D^2)) + \frac{1}{16} N_{BG}(\tilde{\beta}) (12 (\alpha(\tilde{\beta}))^4 \\
&\quad+ 48 L (\alpha(\tilde{\beta}))^3 + (72 L - 48) \mathcal{L} (\alpha(\tilde{\beta}))^2 + (48 L^3 + 72 \mathcal{L}^2 - 12 D^2) \alpha(\tilde{\beta}) \\
&\quad+ 64 (\tilde{\beta} \mu)^3 - 12D (\tilde{\beta} \mu)^3 + 24D \tilde{\beta} \mu \mathcal{L} - D (4 + 9D - D^2)).
\end{align*}
\]

The factor $\alpha(\tilde{\beta}) = \tilde{\beta} - D/2$ and the average number in the standard Boltzmann–Gibbs statistics $N_{BG}(\beta) = \exp(\beta \mu) V \mathcal{M} \beta^{-D/2}$ are used in (4.7). We notice that the generalized
A class of energy-based ensembles in Tsallis statistics

The integral form of the sum of $q$ weights written down from the defining relation (2.4) is

$$c(\mu, V, \beta) = \frac{1}{(Z_q(\mu, V, \beta))^q} \times \sum_{N=0}^{\infty} \frac{1}{N! h^{DN}} \int d^{DN}r \, d^{DN}p \left( \exp \left( -\tilde{\beta} \left( \sum_i \frac{p_i^2}{2m} - \mu N - L_q \right) \right) \right)^q.$$  

(4.8)

A perturbative computation of the sum of $q$ weights is evolved in the following manner.

First the $q$ exponential is expressed in terms of the ordinary exponential:

$$c(\mu, V, \beta) = \frac{1}{(Z_q(\mu, V, \beta))^q} \mathcal{D}_2(d_\beta) \exp(\mathcal{L}) \times \sum_{N=0}^{\infty} \frac{1}{N! h^{DN}} \int d^{DN}r \, d^{DN}p \exp \left( -\tilde{\beta} \left( \sum_i \frac{p_i^2}{2m} - \mu N \right) \right),$$  

(4.9)

where the operator series $\mathcal{D}_2(d_\beta)$ appearing in (4.9) is

$$\mathcal{D}_2(d_\beta) = 1 - (1 - q) \left( d^{(1)}_\beta + \frac{1}{2} d^{(2)}_\beta \right) + (1 - q)^2 \left( d^{(2)}_\beta + \frac{5}{8} d^{(3)}_\beta + \frac{3}{8} d^{(4)}_\beta \right) + \cdots.$$  

(4.10)

In the second step the phase space integral and the summation over the number of particles $N$ is carried out in (4.9) and the resultant expression is

$$c(\mu, V, \beta) = \frac{1}{(Z_q(\mu, V, \beta))^q} \mathcal{D}_2(d_\beta) \exp(\mathcal{L}) \, Z_{BG}(\tilde{\beta}).$$  

(4.11)

In the final step, the rhs in (4.11) is computed and the series corresponding to the generalized partition function (4.6) is substituted to obtain the perturbative series corresponding to the sum of $q$ weights:

$$c = 1 + (1 - q) \mathfrak{P}_1 + (1 - q)^2 \mathfrak{P}_2 + \cdots,$$  

(4.12)

where the perturbative coefficients $\mathfrak{P}_1$ and $\mathfrak{P}_2$ are

$$\mathfrak{P}_1 = -N_{BG}(\tilde{\beta}) (\alpha(\tilde{\beta}) - 1)$$  

$$\mathfrak{P}_2 = -\frac{1}{2} \mathcal{L} (\mathcal{L} - 1) + \frac{1}{4} (N_{BG}(\tilde{\beta}))^2 \left( 2 (\alpha(\tilde{\beta}))^3 + (\alpha(\tilde{\beta}))^2 + (2 - D) \alpha(\tilde{\beta}) \right)$$  

$$+ \frac{1}{4} N_{BG}(\tilde{\beta})(2 (\alpha(\tilde{\beta}))^3 + 2 (2 \mathcal{L} + 1) (\alpha(\tilde{\beta}))^2 + 6D \alpha(\tilde{\beta})$$  

$$- (2 \mathcal{L} - 1) (4 - D) + 4 \mathcal{L}).$$  

(4.13)
The integral form of the grand canonical heat function, the Hill energy \( L_q^{(3)} \) in the third constraint picture is

\[
L_q(\mu, V, \beta) = \frac{1}{(Z_q(\mu, V, \beta))^q} \sum_{N=0}^{\infty} \frac{1}{N!} h^{DN} \int d^{DN}r \, d^{DN}p \left( \sum_i \frac{p_i^2}{2m} - \mu N \right) \times \left( \exp \left( -\tilde{\beta} \left( \sum_i \frac{p_i^2}{2m} - \mu N - L_q \right) \right) \right)^q.
\]

(4.14)

Using a perturbative procedure akin to the one employed in the sum of \( q \) weights, the Hill energy in terms of the derivative series (4.10) is

\[
L_q^{(3)}(\mu, V, \beta) = \frac{1}{(Z_q^{(3)}(\mu, V, \beta))^q} \tilde{D}_2(d_\beta) \left( \frac{D}{2\beta} - \mu \right) \exp(\mathcal{L}) \, N_{BG}(\tilde{\beta}) \, Z_{BG}(\tilde{\beta}).
\]

(4.15)

Calculating the derivatives in the above expression and substituting the Boltzmann–Gibbs partition function, the perturbative series of the Hill energy up to \((1 - q)^2\) order is

\[
L_q = L_{BG}(\tilde{\beta})(1 + (1 - q) \, L_1 + (1 - q)^2 \, L_2 + \cdots).
\]

(4.16)

where \( L_{BG}(\beta) = (D/2\beta - \mu)N_{BG}(\beta) \) and the coefficients of perturbation are listed below:

\[
L_1 = \alpha(\tilde{\beta}) + 2 \mathcal{L} + (1 + \alpha(\tilde{\beta})) \, N_{BG}(\tilde{\beta}),
\]

\[
L_2 = -\frac{1}{8} \left( 4(\alpha(\tilde{\beta}))^3 - 4 \left( 2 + D - 4 \left( (1 - D/2\beta) \beta \right) - 4(\tilde{\beta}\mu)^2 \right) \mathcal{L} + 4 \left( 3 + 4\tilde{\beta}\mu \right) \mathcal{L}^2 + 8 \right.
\]

\[
+ 2D \beta\mu - 8 \tilde{\beta}^2 \right) - \frac{1}{2} \, N_{BG}(\tilde{\beta}) \left( 2 - D + 4 D^2 \beta \mu - 8 (\tilde{\beta}\mu)^2 - 6 (\alpha(\tilde{\beta}))^3 \right)
\]

\[
+ (3D - 2D^2 + 8(1 - D) \tilde{\beta}\mu - 8(\tilde{\beta}\mu)^2) \mathcal{L} - \frac{1}{8} \left( N_{BG}(\tilde{\beta}) \right)^2 \left( 3D^2 - 16 D \tilde{\beta} \right.
\]

\[
+ 20\tilde{\beta}^2 - 16 (\alpha(\tilde{\beta}))^3 \right).
\]

(4.17)

From the perturbative solutions we notice that the generalized ensemble (4.6), the sum of \( q \) weights (4.12) and the Hill energy (4.16) are coupled equations. The explicit expression corresponding to these quantities are obtained by employing a recursive procedure to solve these equations. The important characteristic feature that all these equations are uncoupled at \( q = 1 \) enables us to obtain a solution. Through the use of the recursive procedure, an explicit form of the generalized partition function is obtained up to second order in \((1 - q)\) and is

\[
Z_q(\beta) = Z_{BG}(\beta)(1 + (1 - q) \, Z_1(\beta) + (1 - q)^2 \, Z_2(\beta) + \cdots).
\]

(4.18)

where the coefficients of perturbation are

\[
Z_1(\beta) = -\frac{1}{16}(4D + 4D^2 + D^3 - (4D - 2D^2)\beta\mu + (8 - 4D)(\beta\mu)^2 + 8(\beta\mu)^3) \, N_{BG}(\beta)
\]

\[
+ \frac{1}{8}(4D + 4D^2 + D^3 - (8D + 4D^2)\beta\mu + 8(1 + D)(\beta\mu)^2 - 8(\beta\mu)^3) \, (N_{BG}(\beta))^2,
\]

\[
Z_2(\beta) = +\frac{1}{16}(32D^2 + 88D^2 + 28D^3 + 2D^4 + 3D^5 - (32D + 16D^2 + 40D^3)
\]

\[
- 18D^4) \beta\mu + (96D + 96D^2 - 24D^3) (\beta\mu)^2 - (512 - 416D + 240D^3) (\beta\mu)^3
\]

\[
- (544 - 432D) (\beta\mu)^4 - 96 (\beta\mu)^5) N_{BG}(\beta) + \frac{1}{512}(176D^2 - 32D^4 + 8D^5 + D^6)
\]

\[
- (160D^2 - 432D^3 - 8D^4 - 4D^5) \beta\mu + (576D - 656D^2 - 160D^3)
\]

\[
+ 12D^4) (\beta\mu)^2 - (1024 + 640D - 704D^2 + 32D^3) (\beta\mu)^3 - (704 + 1024D)
\]

\[
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\]

15
A class of energy-based ensembles in Tsallis statistics

\[ -48D^2 (\beta \mu)^4 + (384 - 64D) (\beta \mu)^5 + 64 (\beta \mu)^6 (N_{BG}(\beta))^2 - \frac{1}{128} (32D + 48D^2 + 16D^3 + 2D^5 + D^6 - (32D - 32D^2 - 96D^3 - 24D^4 + 6D^5) \beta \mu + (192 - 64D - 208D^2 - 152D^3 - 20D^4)(\beta \mu)^2 - (320 - 128D - 368D^2 + 48D^3) (\beta \mu)^3 - (128 + 480D - 80D^2) (\beta \mu)^4 + (192 - 96D) (\beta \mu)^5 - 64 (\beta \mu)^6) (N_{BG}(\beta))^3 + \frac{1}{128} (16D^2 + 32D^3 + 24D^4 + 8D^5 + D^6 - (64D^2 + 96D^3 + 48D^4 + 8D^5) \beta \mu + (64D + 192D^2 + 144D^3 + 32D^4) (\beta \mu)^2 - (192D + 256D^2 + 80D^3)(\beta \mu)^3 + (64 + 256D + 128D^2) (\beta \mu)^4 - 128(1 + D) (\beta \mu)^5 + 64 (\beta \mu)^6) (N_{BG}(\beta))^4 \].

A similar application of the recursive procedure enables us to calculate the explicit expression of the Hill energy up to second order in \((1 - q)\). The perturbative series corresponding to the Hill energy is

\[ L_q(\beta) = L_{BG}(\beta) (1 + (1 - q) L_1(\beta) + (1 - q)^2 L_2(\beta) + \cdots), \]

and the coefficients of perturbation are listed below:

\[ \begin{align*}
L_1(\beta) &= -\left(\frac{1}{10} (D^3 + 2D^2 + 12D \beta \mu + 4D \beta \mu \alpha(\beta) + 16 (\beta \mu)^2 + 8(\beta \mu)^3) + \frac{1}{2} (4D + 2D^2 + D^3 + 8D \beta \mu \alpha(\beta) + 8(\alpha(\beta))^2 - 8(\beta \mu)^3) N_{BG}(\beta))^2 U_{BG}(\beta),
L_2(\beta) &= \frac{1}{768} (16D^2 - 12D^3 - 4D^4 + 3D^5 - (32D + 72D^2 - 8D^3 - 18D^4) \beta \mu + (192D - 48D^2 - 24D^3) (\beta \mu)^2 - (768 - 608D - 240D^2) (\beta \mu)^3 - (640 - 432D) (\beta \mu)^4 + 96 (\beta \mu)^5) + \frac{1}{16} (4D^2 - 2D^3 - (8D + 10D^2 - 13D^3) \beta \mu + (32D - 18D^2 - 5D^3) (\beta \mu)^2 + 28D (\beta \mu)^4 + 8 (\beta \mu)^5) N_{BG}(\beta) + \frac{1}{64} (8D^2 + 20D^3 + 14D^4 + 3D^5 - (16D + 56D^2 + 76D^3 + 26D^4) \beta \mu - (64 - 80D - 128D^2 - 100D^3) (\beta \mu)^2 + (96 - 80D - 208D^2) (\beta \mu)^3 + (64 + 224D) (\beta \mu)^4 - 96(\beta \mu)^5) (N_{BG}(\beta))^2 U_{BG}(\beta).
\end{align*} \]

The knowledge of the explicit form of the generalized partition function \((4.18)\) and the Hill energy \((4.20)\) enables us to compute the average number of particles and the internal energy. First the entropy of the system is calculated from the generalized partition function \((4.18)\) through the use of \((2.10)\). In the next step the explicit form of the Hill energy \((4.20)\) is used in conjunction with the entropic expression in the relation \(\Phi_q = L_q - TS\) to obtain the free energy. From the free energy the average number of particles can be found through the use of a specific form of \((2.12)\), i.e. \(N_q = -(\partial \Phi_q) / (\partial \mu)\).

The explicit expression corresponding to the average number of particles in the third constraint \(N_q\) is

\[ N_q = N_{BG}(\beta) + (1 - q) M_1(\beta) + (1 - q)^2 M_2(\beta) + \cdots, \]

where the terms \(M_1\) and \(M_2\) are

\[ \begin{align*}
M_1(\beta) &= -\frac{1}{2} N_{BG}(\beta) ((2 (\alpha(\beta))^2 + 4 \alpha(\beta) - D) - 4 N_{BG}(\beta) ((\alpha(\beta))^2 - \alpha(\beta)))
M_2(\beta) &= \frac{1}{96} N_{BG}(\beta) (12 ((\alpha(\beta))^4 + 80 (\alpha(\beta))^3 + 12(8 - 7D)(\beta \mu) + 6D^2(2 - D)^2) \beta \mu + D(1 - D)(4 + D)) - \frac{1}{8} (N_{BG}(\beta))^2 (4 (\alpha(\beta))^4 + 8 (\alpha(\beta))^3 + 8D(\alpha(\beta))^2 - 16 \beta \mu \alpha(\beta) - D(4 + D)) + \frac{1}{8} (N_{BG}(\beta))^3 (24(\alpha(\beta))^4 - 16 \beta \mu (1 + \beta \mu) \alpha(\beta) - 8(1 - 8D)(\beta \mu)^2 + 8(2 - 3D^2) \beta \mu - D(4 - 2D - 5D^2)).
\end{align*} \]
The calculated results corresponding to the Hill energy (4.20) and the average number of particles (4.22) is used in the relation $L_q^{(3)} = U_q^{(3)} - \mu N_q^{(3)}$ to find the internal energy. The perturbative series corresponding to the internal energy is

$$U_q(\beta) = U_{BG}(\beta) + (1 - q) U_1 + (1 - q)^2 U_2 + \cdots,$$  \hfill (4.24)

where the perturbative terms are listed below:

\begin{align*}
U_1(\beta) &= -\frac{1}{2} ((\beta \mu)^2 - 2 \beta \mu + D(2 + D)) + 2 (D \alpha(\beta) + 2 \beta \mu \\
U_2(\beta) &= \frac{1}{96} (12 (\alpha(\beta))^4 + 48 (\beta \mu)^4 - 16 (\beta \mu)^3 + 36 D(1 - D) (\beta \mu)^2 + 12 D(2 - D^2) \beta \mu \\
&\quad + D(4 - 3D - D^2)) - 4 N_{BG}(\beta) (24 (\beta \mu)^3 + 42 D (\beta \mu)^2 - 88 D^2 \beta \mu \\
&\quad - 6 D(1 - D)(2 + D) - \alpha(\beta) (36 (\beta \mu)^3 + 12 D (\beta \mu)^2 + 3(16 + D^2) \beta \mu) \\
&\quad + 3(N_{BG}(\beta))^2 (32 (\alpha(\beta))^4 + 4(8 + D^2) \alpha(\beta)\beta \mu + 16(\beta \mu)^3 + 32(5 + 2D)(\beta \mu)^2 \\
&\quad - (32 + 32D - 56D^2 - 2D^3) \beta \mu + D(8 + 20 D + 14D^2 + D^3)) U_{BG}(\beta). \\
\end{align*}

\hfill (4.25)

The average number and the internal energy can also be calculated in a different manner wherein the basic definition of these quantities in (2.1) and (2.2) is used to find the implicit expressions. The implicit expressions are then solved to arrive at the final explicit forms. The results obtained through this method agree precisely with those obtained in (4.22) and (4.24). This is a nontrivial consistency check on the results obtained for the physical quantities.

The entire calculation has been carried out directly in the third constraint picture and consistently up to second order in the expansion parameter $(1 - q)$. However, the process is not limited only to the second order and it can be extended to any arbitrary order in the expansion parameter.

### 4.2. Extreme relativistic classical ideal gas

The perturbative study carried out for the nonrelativistic classical ideal gas can also be extended to the system of an extreme relativistic classical ideal gas. Since the calculational procedure is the same as in the nonrelativistic case detailed in section 4.1, we present only the final expressions corresponding to the internal energy and the average number of particles. The average number of particles is

$$N_q(\beta) = N_{BG}(\beta) + (1 - q) N_1(\beta) + (1 - q)^2 N_2(\beta) + \cdots,$$  \hfill (4.26)

where the term $N_{BG} = \exp(\beta \mu) V \Delta \beta^{-D}$ and the coefficients of perturbation are

\begin{align*}
N_1(\beta) &= -\frac{1}{2} N_{BG}(\beta) ((\beta \mu)^2 + 2(1 + D) \beta \mu - D(1 - D)) + (N_{BG}(\beta))^2 ((\beta \mu)^2 \\
&\quad - (2 + D) \beta \mu + 3D - 1), \\
N_2(\beta) &= -\frac{1}{24} N_{BG}(\beta) (3 (\beta \mu)^4 + (20 - 12D) (\beta \mu)^3 + (24 - 42D)(\beta \mu)^2 \\
&\quad - 12D(1 - 2D - D^2) \beta \mu + 2D - 3D^2 - 2D^3 + 3D^4) - \frac{1}{2} (N_{BG}(\beta))^2 ((\beta \mu)^4 \\
&\quad - 2D (\beta \mu)^3 - (8 - 10D) (\beta \mu)^2 - (6 - 12D + 16D^2 - 2D^3) \beta \mu \\
&\quad - D^2(1 - 6D + D^2)) + \frac{1}{2} (N_{BG}(\beta))^3 (3 (\beta \mu)^4 - (9 - 6D) (\beta \mu)^3 \\
&\quad - (2 - 28D - 3D^2)(\beta \mu)^2 + (22 - 20D - 19D^2)\beta \mu + 2 - 11D + 20D^2 + D^3). \\
\end{align*}

\hfill (4.27)

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The final expression for the internal energy is
\[ U_q(\beta) = U_{BG}(\beta) + (1 - q) U_1(\beta) + (1 - q)^2 U_2(\beta) + \cdots, \] (4.28)
and the coefficients of perturbation are listed below:
\[
\begin{align*}
U_1(\beta) &= -((\beta \mu)^2 - 2D \beta \mu + D(1 + D))U_{BG}(\beta) + N_{BG}(\beta)((\beta \mu)^2 - (3 + D)\beta \mu \\
&\quad + (1 + 3D))U_{BG}(\beta), \\
U_2(\beta) &= \left(\frac{1}{2}\right)(3(\beta \mu)^4 + (8 - 12D)(\beta \mu)^3 - 6D(1 + 3D)(\beta \mu)^2 - 12D^2(D + 1)\beta \mu \\
&\quad + 2D + 6D^2 + 10D^3 + 3D^4) - \frac{1}{2}N_{BG}(\beta)((\beta \mu)^4 - 2(1 + D)(\beta \mu)^3 \\
&\quad - (4 - 2D)(\beta \mu)^2 - (4D + 14D^2 - 2D^3)\beta \mu + 2D + 7D^2 - 4D^3 + 2D^4) \\
&\quad + \frac{1}{2}(N_{BG}(\beta))^2(3(\beta \mu)^4 + (13 - 6D)(\beta \mu)^3 + (13 - 32D + 3D^2)(\beta \mu)^2 \\
&\quad - (1 + 40D + 19D^2)\beta \mu + 1 + 9D + 21D^2 + D^3)U_{BG}(\beta). \tag{4.29}
\end{align*}
\]
and the Boltzmann–Gibbs factor is \( U_{BG} = (D/\beta) N_{BG} \). The Boltzmann–Gibbs values for both quantities are recovered in the \( q \to 1 \) limit.

The thermodynamic results corresponding to a one-dimensional model of an interacting gas known as a Tonks gas described by the Hamiltonian (3.35) can be read from the results of the classical nonrelativistic ideal gas. For this purpose we employ a special kind of grand canonical ensemble where the free length or the total length available to the molecules is used instead of the volume. Also the number of dimensions is set to be 1 and the factor \( M_1 \), the one-dimensional analog of \( M \), is used.

5. Generalized ensemble

The generalized ensemble describes a completely open system which can exchange the internal energy, the volume and the number of particles. The heat function is the \( R \) function described by \( R = U + PV - \mu N \) and the generalized free energy is the function \( E = U - TS + PV - \mu N \).

5.1. Nonrelativistic ideal gas

The classical nonrelativistic ideal gas is analyzed in the generalized ensemble picture. A perturbative process based on the idea of the disentangling of \( q \) exponentials [25] is used. Though the thermodynamic quantities are evaluated uniformly up to \((1 - q)^2\) order, the results are presented only up to the first order in \((1 - q)\) since some of the quantities are too cumbersome to be displayed up to second order. The generalized partition function in the third constraint picture is
\[
\tilde{\Gamma}_q(\mu, V, \beta) = \sum_{N=0}^{\infty} \frac{1}{N! h^{DN}} \int d^{DN} r d^{DN} p \exp \left( -\hat{\beta} \left( \sum_i \frac{p_i^2}{2m} + P V - \mu N - R_q \right) \right), \tag{5.1}
\]
where the factor \( \hat{\beta} = \beta/\epsilon \) and \( \epsilon \) is the third constraint sum of \( q \) weights in the generalized ensemble. The heat function \( R_q = U_q + PV_q - TS - \mu N_q \), where \( U_q, V_q, \) and \( N_q \) are the internal energy, average volume and average number of particles, respectively, in the third constraint. The quantities \( P \) and \( \mu \) denote the pressure and the chemical potential of the system.

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In (5.1) the phase space integrals can be carried out after the due substitution of the perturbative expansion of the $q$ exponential in terms of the ordinary exponential. Since the volume states are very close to each other, we approximate the volume summation by an integral. Employing the correct counting of volume states advocated in [30,31], we carry out the volume integral. Finally we assume that the summation over the number of particles is convergent at least, in the neighborhood of $q = 1$, and thus arrives at the final perturbative series of the generalized partition function:

$$\bar{\Upsilon}_q(\mu, P, \beta) = \hat{D}_1(d_\beta) \exp(\mathcal{R}) \Upsilon_{BG}(\hat{\beta}),$$  \hspace{1cm} (5.2)$$

where $\mathcal{R} = \hat{\beta} R_q^{(3)}$ and $\hat{D}_1(d_\beta)$ is the derivative series defined in (4.4). The partition function and the average number of particles in the Boltzmann–Gibbs framework are

$$\Upsilon_{BG}(\beta) = \frac{1}{1 - \omega(\beta)}, \hspace{0.5cm} N_{BG}(\beta) = \frac{\omega(\beta)}{1 - \omega(\beta)}, \hspace{0.5cm} \omega(\beta) = \exp(\beta \mu) M \left( \frac{1}{P} \right)^{\frac{D}{2} + 1}, \hspace{1cm} (5.3)$$

where the factor $\omega(\beta)$ is considered to be less than one so as to maintain the positivity of the partition function. From (5.2) the perturbative series corresponding to the third constraint generalized partition function up to $(1 - q)$ order is computed:

$$\bar{\Upsilon}_q(\mu, P, \beta) = \exp(\mathcal{R}) \Upsilon_{BG}(\hat{\beta}) (1 + (1 - q) \frac{1}{4} ((2 (\alpha(\hat{\beta}))^2 + 4 R \hat{\beta} \alpha(\hat{\beta}) - 4 (R + \mu) \hat{\beta} + (4 + 3D)) N_{BG}(\hat{\beta}) + (2 (\alpha(\hat{\beta}))^2 - 4 \alpha(\hat{\beta}) + 2)(N_{BG}(\hat{\beta}))^2) + \cdots). \hspace{1cm} (5.4)$$

Applying a similar perturbative technique, the sum of $q$ weights in the generalized ensemble picture is

$$c(\mu, P, \beta) = \frac{1}{(\bar{\Upsilon}_q(\mu, P, \beta))^q} \hat{D}_2(d_\beta) \exp(\mathcal{R}) \Upsilon_{BG}(\hat{\beta}), \hspace{1cm} (5.5)$$

where the derivative series $\hat{D}_2(d_\beta)$ is defined in (4.10). Employing the derivative series, the perturbative expression of the sum of $q$ weights up to first order in $(1 - q)$ is

$$c(\hat{\beta}) = 1 + (1 - q) \left( ((\alpha(\hat{\beta}) + 1) - \Upsilon_{BG}(\hat{\beta})) \omega(\hat{\beta}) - \Upsilon_{BG}(\hat{\beta}) \right) \ln \Upsilon_{BG}(\hat{\beta}) + \cdots. \hspace{1cm} (5.6)$$

Adopting a procedure identical to the one used for the generalized partition function and the sum of $q$ weights, the $R_q$ heat function can be written as

$$R_q(\mu, P, \beta) = \frac{1}{(\bar{\Upsilon}_q(\mu, P, \beta))^q} \hat{D}_2(d_\beta) \left( \left( \frac{D}{2} + 1 \right) \frac{1}{\hat{\beta}} - \mu \right) \exp(\mathcal{R}) N_{BG}(\hat{\beta}) \Upsilon_{BG}(\hat{\beta}). \hspace{1cm} (5.7)$$

The perturbative series of the $R_q$ up to $(1 - q)$ order found from (5.7) is

$$R_q(\mu, P, \beta) = \left( \left( \frac{D}{2} + 1 \right) \frac{1}{\hat{\beta}} - \mu \right) N_{BG}(\hat{\beta}) + (1 - q) (R_1 + R_2 + R_3) + \cdots. \hspace{1cm} (5.8)$$
The perturbative coefficients of \((1 - q)\) term in (5.8) is

\[
R_1 = (R^2 \beta^2 (1 - \alpha(\beta)) + \frac{1}{16} ((4(D + 2)(D + 4) P^{-1} \beta^{-2} - (D + 2)(D + 4)(D + 6) + 8(R + 2\mu)P^{-1})\beta^{-1} + (R + \mu)\mu P^{-1} + 3\mu - 4((D + 2)(R + 4\mu)R - (2R^2 - 6\mu - 3D\mu)\mu) + 6D(D + 6)\mu + 8(R + \mu)(\beta \mu)^2) + \omega(\beta)(2(D^3 + 40D^2 + 32D + 32 + 2(D + 2)R^2 + 4(D + 2)(R + 2\mu))P^{-1}\beta^{-1} - 4(D + 2)(D + 4) P^{-1} \beta^{-2} - 4((D + 2)(D + 4)R + (D + 2)(3D + 10))\mu + 4(R + \mu)\mu P^{-1}) + 8((2D + 4) R + 3D\mu)\beta \mu - ((R + 2\mu)^2 - 2(\beta \mu)^2)) (N_{BG}(\beta))^2, 
\]

\[
R_2 = \frac{1}{8} ((D + 2)^3 \beta^{-1} + (D + 2)(D + 4)(3D + 8) + 12\mu^2 - 2(12\mu^3 P + 4\mu^3 P^{-1} + 4(9D^2 + 34D + 32)\mu P^2 + 2(D + 2)^2RP^2) \beta^2 + 4((9D + 14)\mu^2 + (D + 2)\beta P)^2 - 12(D + 2)^2 \mu - ((3D^3 + 20D^2 + 44D + 32)p^2 \beta - 2((D + 2)2\mu + 2(D + 2)^2 R)\beta P^2 - 4(4(D + 2)R + (D + 14)\mu)P^2\beta^3 + (2R + 3\mu)\beta^5 P^2)\beta(\beta) (N_{BG}(\beta))^2, 
\]

\[
R_3 = \frac{1}{8} (3\omega(\beta)((D + 2)^3 \beta^{-2} - 6(D + 2)^2 \mu P^3 \beta^3 + 12(D + 2)\mu^2 P^3 \beta^3 - 8\mu^3 \beta^5 P^3) - 3((D + 2)^3 \beta^2 P^3 - 6(D + 2)^2 \mu^2 P^3 \beta^3 + 12(D + 2)\beta^4 P^3 - 8\beta^5 \mu^3 P^3) \beta(\beta) (N_{BG}(\beta))^3, 
\]

The generalized partition function (5.4), the sum of \(q\) weights (5.6) and the \(R_q\) heat function (5.8) form a set of coupled implicit perturbative expansions. The fact that these equations are uncoupled at the lowest perturbative order allows us to obtain an explicit form of these quantities through the use of a recursive procedure. The final explicit form of the generalized partition function computed up to first order in the expansion parameter \((1 - q)\) is

\[
\Upsilon_q(\beta) = \Upsilon_{BG}(\beta) \exp(\beta R) (1 + (1 - q)(\Upsilon_1(\beta) + \Upsilon_2(\beta) + \Upsilon_3(\beta) + \Upsilon_4(\beta)) + \cdots), 
\]

and the coefficients of perturbation are listed below:

\[
\Upsilon_1(\beta) = -\frac{1}{16} (4(2(\alpha(\beta))^2 - 4\alpha(\beta) + D) - ((2 + D)\frac{1}{\beta P}((2 + D)(4 + D - \beta\mu) - 4(\beta \mu)^2) - 4(4 + 6D + D^2 + 2(2 + D)\beta \mu) \ln \Upsilon_{BG}(\beta) - (\beta \mu)^2) + (\beta \mu)^2) \ln \Upsilon_{BG}(\beta) \Upsilon_{BG}(\beta) ((\Upsilon_{BG}(\beta))^2 + 16(1 + (1 + \alpha(\beta))(\Upsilon_{BG}(\beta))^3) (N_{BG}(\beta)), 
\]

\[
\Upsilon_2(\beta) = -\frac{1}{8} (6 + 3D - (8 + D)\beta \mu - (\beta \mu)^2 - 2(1 + D - \beta \mu) \ln \Upsilon_{BG}(\beta) + (16 + 8D - 2D^2 - 16\beta P - (8 - 10D + D^2 + 8\beta P - 4\beta P) \beta \mu - (8 + 4D + 8\beta P) (\beta \mu)^2 + 12(\beta \mu)^3 + 4(6 + 3D - 2(\beta P)^{-1} - (4 - D) \beta \mu + (\beta \mu)^2) \ln \Upsilon_{BG}(\beta) \Upsilon_{BG}(\beta) - 2((\beta P)^{-2} - 4(\beta P)^{-1} \alpha(\beta) - (\alpha(\beta))^2) (\Upsilon_{BG}(\beta))^2 (N_{BG}(\beta))^2, 
\]
\[ \Upsilon_3(\beta) = -\frac{(\Upsilon_{BG}(\beta))^3}{\beta P} \ln \Upsilon_{BG}(\beta) - \frac{1}{4} (8 + 6 D + D^2 - (16 + 4 D + 4 \beta P) \beta \mu \\
+ 12 (\beta \mu)^2 + 4 (1 - \alpha(\beta)) \ln \Upsilon_{BG}(\beta) + 4(\alpha(\beta))^2 + (\beta P)^{-1} \alpha(\beta) \langle N_{BG}(\beta) \rangle^3, \]
\[ \Upsilon_4(\beta) = -\frac{1}{12} (\alpha(\beta))^2 \langle N_{BG}(\beta) \rangle^4. \] (5.11)

Proceeding similarly, the final explicit form of the heat function \( R_q \) is obtained up to (1 – q) order:
\[ R_q = \left( \left( \frac{D}{2} + 1 \right) \frac{1}{\beta} - \mu \right) + (1 - q) (R_1 + R_2 + R_3) + \cdots, \] (5.12)
where the perturbative coefficients may be listed as
\[ R_1 = \frac{1}{4} ((D + 2)(D + 4)\beta^{-1} - (D + 2)\mu - \beta \mu^2) (\Upsilon_{BG}(\beta))^2 \ln \Upsilon_{BG}(\beta) \langle N_{BG}(\beta) \rangle, \]
\[ R_2 = -\frac{1}{16} (((D + 2)(3 D + 10)P - (D + 2)(3 \mu - (D^2 - 10 D - 40) P) \beta \\
+ 2 (24 \mu - (D + 2)(3 D - 16) P) \mu P \beta^3 + 4(3 D - 20) \mu^2 P \beta^3 - 8 \mu^3 P \beta^4 \\
+ 2 (8 \mu - 3(D + 2)(D + 4) P) \beta \mu + 12(D + 2) P(\beta \mu)^2 - 8 P(\beta \mu)^3 \\
- (D + 2)(16 \mu + (D + 4)(D + 6) P)) \Upsilon_{BG}(\beta) - 2((D + 2)^2(D + 4)\beta^{-1} \\
- 2(D + 2)(3 D + 8) \mu^2 + 12(D + 2) \beta \mu^2 - 8 \beta^2 \mu^3 + 2 ((D + 2)^2 \beta^{-1} \\
- 4(D + 2) \mu + 4 \beta \mu^2) \ln \Upsilon_{BG}(\beta) (\Upsilon_{BG}(\beta))^2 (\langle N_{BG}(\beta) \rangle)^2, \]
\[ R_3 = \frac{1}{8} ((2(D + 2)((9 D + 10)\mu + 2(D^2 + 3 D + 1) P) P^2 \beta^2 - D(D + 2)(3 D + 8) P^2 \beta \\
- 4((9 D + 14)\mu + (D + 2)(3 D + 4) P^2) \mu \beta^2 + 8 (3 \mu + 2(3 D + 5) P) \mu^2 P \beta^2 \\
- 2 P^3 \mu^3 \beta^5) (\langle N_{BG}(\beta) \rangle)^3. \] (5.13)

To compute the other thermodynamic quantities like the internal energy, average volume and the average number of particles we need to calculate the free energy via the expression
\[ \mathcal{E}_q = U_q + PV_q - TS - \mu N_q = R_q - TS. \] The entropy, which can be read from the generalized partition function (5.10) using the relation (2.10), and the perturbative expansion of the heat function \( R_q \) are used in this process. From the free energy, the average volume can be found through the use of the thermodynamic relation \( V_q = (\partial \mathcal{E}_q)/(\partial P) \). The perturbative expansion of the average volume up to (1 – q) order is
\[ V_q = V_{BG}(\beta) + (1 - q) \frac{1}{2} (2 (\alpha(\beta))^2 - 2 \alpha(\beta) + 4 + D + 3(2 (\alpha(\beta))^2 - 4 \alpha(\beta) \\
+ 8 + D) \Upsilon_{BG}(\beta) + 4 ((\omega(\beta))^2 + (\alpha(\beta) - 3) \omega(\beta) - (\alpha(\beta) - 2)) \ln \Upsilon_{BG}(\beta) \\
+ \omega(\beta) (1 + \omega(\beta)) ((\alpha(\beta))^2 - \alpha(\beta) + 2)) \Upsilon_{BG}(\beta) + \cdots, \] (5.14)
where \( V_{BG}(\beta) \) is the average volume in the Boltzmann–Gibbs formalism. Similarly the average number of particles can be arrived at through the use of the relation \( N_q = (\partial \mathcal{E}_q)/(\partial \mu) \). The final expression of the average number as a perturbative series up to first order in (1 – q) is
\[ N_q = N_{BG}(\beta) + (1 - q) \frac{1}{6} ((4 (\beta \mu)^2 + 8 \beta P \alpha(\beta) - D(2 + D) + 8 (\alpha(\beta) \\
+ 1) \ln \Upsilon_{BG}(\beta)) N_{BG}(\beta) - (12 (\beta \mu)^2 - 4 D \beta \mu - 8 \beta P(\alpha(\beta) + 1) - D(2+D) \\
+ 8 (\alpha(\beta) - 1) \ln \Upsilon_{BG}(\beta)) (\langle N_{BG}(\beta) \rangle)^2 + 4(2 \beta \mu - \beta P - 1)(\langle N_{BG}(\beta) \rangle)^3 + \cdots. \] (5.15)

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Using the perturbative expansions of the heat function (5.12), the average volume (5.14) and the average number of particles (5.15), the internal energy can be computed via the Legendre transformation $R_q = U_q + PV_q - \mu N_q$. The computed perturbative series of the internal energy up to $(1 - q)$ order is

$$U_q = U_{BG}(\beta) - (1 - q) \frac{1}{8} \mathcal{Y}_{BG}(\beta)((8 \ln \mathcal{Y}_{BG}(\beta) + \alpha(\beta) - 1) \omega(\beta) + 8 (\alpha(\beta) - 2) \ln \mathcal{Y}_{BG}(\beta) + 4 (\beta \mu - 2) \alpha(\beta) + 2 D \beta \mu - (D + 1)^2) U_{BG}(\beta) + \cdots. \tag{5.16}$$

The quantities evaluated above can also be arrived at using the basic definition of the internal energy, the average volume and the average number of particles. For this purpose we employ the basic definition of these quantities to find the corresponding implicit equations which are then solved recursively to obtain the final explicit expressions. The results obtained through this method perfectly agree with the results displayed above. All the quantities recover the corresponding Boltzmann–Gibbs results in the $q \to 1$ limit.

### 5.2. Extreme relativistic ideal gas

The extreme relativistic ideal gas has been studied using the perturbative formalism. The actual process of calculation is the same as in the nonrelativistic case and so we present the final results directly. The perturbative expansion corresponding to the average number of particles is

$$N_q = N_{BG} - \frac{(1 - q)}{2} \mathcal{Y}_{BG}(\beta)(D + D^2 - 2D \beta \mu + (\beta \mu)^2$$

$$- 2(1 + D - \beta \mu) \ln \mathcal{Y}_{BG}(\beta)) N_{BG}(\beta) + \cdots. \tag{5.17}$$

The factors $\mathcal{Y}_{BG}(\beta)$ and $N_{BG}(\beta)$ are the partition function and the average number in the Boltzmann–Gibbs statistics, respectively, and their expressions are given below:

$$\mathcal{Y}_{BG}(\beta) = \frac{1}{1 - \xi(\beta)}, \quad N_{BG} = \frac{\xi(\beta)}{1 - \xi(\beta)}, \quad \xi(\beta) = \exp(\beta \mu) \Delta \frac{1}{P} \left( \frac{1}{\beta} \right)^{D+1}, \tag{5.18}$$

where $\xi(\beta)$ is assumed to be less than one. The average volume in nonextensive statistical mechanics is

$$V_q = V_{BG} - \frac{(1 - q)}{2} \mathcal{Y}_{BG}(\beta)((2 + 3D + D^2 - 2(1 + D)\beta \mu - (\beta \mu)^2 - 2(2 + D - \beta \mu)$$

$$\times \ln \mathcal{Y}_{BG}(\beta)) V_{BG}(\beta) - 2(1 + D - \beta \mu - \ln \mathcal{Y}_{BG}) V_{BG}(\beta)) + \cdots. \tag{5.19}$$

where the Boltzmann–Gibbs value corresponding to it is $V_{BG} = (1/\beta P) N_{BG}(\beta)$. A similar perturbative series corresponding to the internal energy is

$$U_q = U_{BG} - \frac{(1 - q)}{2} \mathcal{Y}_{BG}(\beta)((2 + 3D + D^2 - (1 + D)\beta \mu - (\beta \mu)^2 - 2(2 + D - \beta \mu)$$

$$\times \ln \mathcal{Y}_{BG}(\beta)) U_{BG}(\beta) - 2(1 + D - \beta \mu - \ln \mathcal{Y}_{BG}) U_{BG}(\beta)) + \cdots. \tag{5.20}$$

The Boltzmann–Gibbs internal energy used in (5.20) is $U_{BG}(\beta) = (D/\beta) N_{BG}(\beta)$. From the results displayed above we can observe that in the $q \to 1$ limit we recover the standard Boltzmann–Gibbs values.

The Tonks gas described by the Hamiltonian (3.35) can also be studied through the generalized ensemble. The results corresponding to such a model of an interacting gas in the free-length generalized ensemble can be obtained by substituting $D = 1$ in the results obtained for the nonrelativistic classical ideal gas.

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6. Adiabatic ensemble

The adiabatic class of ensembles is used to describe a system of particles for which the thermal equilibration is with respect to the heat function. In the adiabatic class the individual members of the ensemble have the same value of the heat function though they can be at different temperatures. There are four different adiabatic ensembles, namely microcanonical ensemble ($N$, $V$, $U$), isoenthalpic–isobaric ensemble ($N$, $P$, $H$), the ensemble with number fluctuations ($\mu$, $V$, $L$) and the ensemble with both number and volume fluctuations ($\mu$, $P$, $R$). In the current section we present a unified framework to describe the adiabatic class of ensembles.

At any given instant in time the microstate of a system consisting of $N$ particles is represented by a point in the $6N$-dimensional phase space, which is comprised of $3N$ position coordinates and $3N$ momentum coordinates. Since the position and momentum coordinates evolve with time, the representative point moves in the phase space. The motion of the representative point traces a trajectory of constant heat function $H$ in the phase space. The points which lie on the surface of the constant heat function curve are the various microstates corresponding to the macrostate of the constant heat function. As the number of microstates is very high and lie very close to each other, the surface area of the constant heat function curve can be considered as a measure of the total number of microstates. The surface area of the constant heat function $\mathcal{H}$ curve in an adiabatic ensemble is

\[
\Omega(x_1, x_2, \mathcal{H}) = \sum_{X(\ell)} \frac{1}{N!} h^{DN} \int_{r_1} \int_{p_1} \delta \left( H + \sum_{\ell} x_{\ell} x_{\ell} - \mathcal{H} \right) \prod_{i=1}^{N} d^D r_i d^D p_i .
\]  

(6.1)

The computation of the area of the constant heat function is difficult, and so we usually calculate the volume enclosed by such a curve. The phase space volume enclosed by the constant heat function $\mathcal{H}$ curve is

\[
\Sigma(x_1, x_2, \mathcal{H}) = \sum_{X(\ell)} \frac{1}{N!} h^{DN} \int_{r_1} \int_{p_1} \Theta \left( H + \sum_{\ell} x_{\ell} x_{\ell} - \mathcal{H} \right) \prod_{i=1}^{N} d^D r_i d^D p_i .
\]  

(6.2)

The surface area of the heat function curve (6.1) and the volume (6.2) enclosed by it are related via the relation

\[
\Omega(x_1, x_2, \mathcal{H}) = \frac{\partial}{\partial \mathcal{H}} \Sigma(x_1, x_2, \mathcal{H}).
\]  

(6.3)

Based on this kind of adiabatic confinement there are four different definitions of the entropy. A unified definition of the entropy for an adiabatic nonextensive system is

\[
S_q(x_1, x_2, \mathcal{H}) = k \ln_q \Sigma(x_1, x_2, \mathcal{H}),
\]  

(6.4)

where $\Sigma(x_1, x_2, \mathcal{H})$ is the volume enclosed by the curve of the constant heat function and a measure of the number of microstates. The temperature of a general adiabatic ensemble is defined via the relation

\[
T = \left( \frac{\partial S_q}{\partial \mathcal{H}} \right)^{-1} = \frac{\left( \Sigma(x_1, x_2, \mathcal{H}) \right)^q}{k \Omega(x_1, x_2, \mathcal{H})}.
\]  

(6.5)
In the usual procedure of calculation the heat function can be computed through the use of (6.5) and the relations (6.1) and (6.2). Using the heat function the specific heat can be calculated through the expression

$$C_q|_{x(\ell)} = \frac{\partial S_q}{\partial T} \bigg|_{x(\ell)}.$$  \hspace{1cm} (6.6)

The extensive thermodynamic variable whose intensive counterparts are held fixed can be obtained from the relation

$$X_{\ell q}(x_1, x_2, \mathfrak{y}) = -\frac{1}{\beta} \frac{\partial}{\partial x_\ell} S_q(x_1, x_2, \mathfrak{y}).$$  \hspace{1cm} (6.7)

The volume and the average number of particles can be calculated in \((N, P, H)\) and \((\mu, V, L)\), respectively, through the use of (6.7). In the case of the \((\mu, P, R)\) ensemble, both the volume and the average number of particles can be calculated using (6.7). The expectation value of an observable \(O\) for any adiabatic ensemble can be defined in a unified way through the relation

$$\langle O \rangle = \frac{1}{\Omega(x_1, x_2, \mathfrak{y})} \sum_{x_{(\ell)}} \frac{1}{N! h^{DN}} \int_{r_i} \int_{p_i} O \delta \left( \mathcal{H} + \sum_{(\ell)} x_\ell X_{\ell} - \mathfrak{y} \right) \prod_{i=1}^{N} d^{D}r_i d^{D}p_i. \hspace{1cm} (6.8)$$

The internal energy is the natural heat function of the microcanonical ensemble and so it can be directly evaluated, whereas in the other three ensembles, equation (6.8) is used to calculate the internal energy. From the internal energy the specific heat at constant volume can be evaluated using

$$C_q|_{V} = \frac{\partial U_q}{\partial T} \bigg|_{V}. \hspace{1cm} (6.9)$$

A nontrivial way of checking the internal energy can be accomplished by using the Legendre transform (1.3) to find the internal energy.

A \(q\) generalization of the equipartition theorem is developed in the unified framework. Let \(y_i\) be a phase space variable which can denote either the position \(r_i\) or the momentum \(p_i\) \((i = 1, \ldots, 3N)\) coordinate. Calculating the expectation value of \(y_i(\partial \mathcal{H}/\partial y_j)\) we arrive at

$$\langle y_i \frac{\partial \mathcal{H}}{\partial y_j} \rangle = kT \left( \Sigma(x_1, x_2, \mathfrak{y}) \right)^{q-1} \delta_{ij}. \hspace{1cm} (6.10)$$

Equation (6.10) obtained above is the generalized form of the \(q\)-nonextensive equipartition theorem. It is interesting to note that the nonextensive generalization of the equipartition theorem depends on the factor \(\Sigma(x_1, x_2, \mathfrak{y})\) which is a measure of the number of microstates corresponding to a given macrostate. However, we notice that in the extensive \(q \rightarrow 1\) limit the dependence on the number of microstates vanishes. The form of (6.10) suggests that the expectation value described has a nonzero value only when \(i = j\). When the phase space variable \(y_i\) is set to be the coordinate \(r_i\) then we get a specific form of the equipartition theorem:

$$\langle r_i \frac{\partial \mathcal{H}}{\partial r_i} \rangle = -\langle r_i \dot{r}_i \rangle = \langle r_i F_i \rangle = kT \left( \Sigma(x_1, x_2, \mathfrak{y}) \right)^{q-1}, \hspace{1cm} (6.11)$$

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where we have used Hamilton’s equation of motion \( \frac{\partial H}{\partial r_i} = -\dot{p_i} \). Following an identical approach for the situation where the generalized variable is set to be the momentum variable \( y_i = p_i \) we arrive at

\[
\langle p_i \frac{\partial H}{\partial p_i} \rangle = (p_i \dot{q}_i) = kT \left( \Sigma(x_1, x_2, \mathcal{F}) \right)^{q-1}. \tag{6.12}
\]

We observe that (6.12) is nothing but twice the expectation value of the kinetic energy. From (6.11) and (6.12) it can be proved that systems whose Hamiltonians can be cast in the form \( H = \sum_i A_i P_i^2 + \sum_i B_i Q_i^2 \) through a canonical transformation the expectation value of the Hamiltonian is

\[
H = \frac{DN}{2} kT \left( \Sigma(x_1, x_2, \mathcal{F}) \right)^{q-1}. \tag{6.13}
\]

The virial theorem in the nonextensive framework obtained from (6.11) is

\[
\langle 3N \sum_i q_i \dot{p}_i \rangle = -3NkT \left( \Sigma(x_1, x_2, \mathcal{F}) \right)^{q-1}. \tag{6.14}
\]

Previously an extensive study of the equipartition and virial theorems has been carried out in the framework of the canonical ensemble [33]–[35] and microcanonical ensemble [24]. The results obtained above may be considered as a ensemble-independent generalization of the above-mentioned theorems.

The unified framework derived above is made use of in the following sections to demonstrate the isoenthalpic–isobaric ensemble \((N, P, H)\), the ensemble with number fluctuations \((\mu, V, L)\) and the ensemble with both number and volume fluctuations \((\mu, P, R)\). Though all the relations in the microcanonical ensemble \((N, V, U)\) can be read from the equations in the unified framework above, we do not discuss the \((N, V, U)\) ensemble, since a detailed study has already been carried out in [24].

7. Isoenthalpic–isobaric ensemble

The study of adiabatically confined systems with constant enthalpy is done using the isoenthalpic–isobaric ensemble. In the following discussion we study the classical nonrelativistic and extreme relativistic ideal gas.

7.1. Nonrelativistic ideal gas in \((N, P, H)\) ensemble

The nonrelativistic ideal gas is studied in the isoenthalpic–isobaric ensemble. The volume enclosed by the surface of constant enthalpy is calculated in the following manner. First the Hamiltonian corresponding to the nonrelativistic gas (3.1) is substituted in equation (6.2) and the resultant expression is

\[
\Sigma(N, P, H) = \sum_V \frac{1}{N!h^{DN}} \int_{r_i} \int_{p_i} \Theta \left( \sum_i \frac{p_i^2}{2m} + PV - H \right) \prod_{i=1}^N d^D r_i \, d^D p_i. \tag{7.1}
\]
The momentum integration in (7.1) is geometrically the volume of the $DN$-dimensional sphere of radius $\sqrt{2m(H - PV)}$ and is equal to

$$\int_{\sum_i^{DN}(p_i^2/2m) \leq H - PV} d^{DN}p_i = \frac{(2\pi m)^{DN/2}}{\Gamma((DN/2) + 1)} (H - PV)^{DN/2}. \tag{7.2}$$

Substituting the result of the momentum integration (7.2) in (7.1) the expression for the volume is

$$\Sigma(N, P, H) = \frac{M^N}{N!} \frac{1}{\Gamma((DN/2) + 1)} \sum_V (H - PV)^{DN/2} \int d^{DN}r_i. \tag{7.3}$$

In the next step the integral over the position coordinates is carried out in (7.3) and this yields

$$\Sigma(N, P, H) = \frac{M^N}{N!} \frac{1}{\Gamma((DN/2) + 1)} \sum_V V^N(H - PV)^{DN/2}. \tag{7.4}$$

Finally the summation over the volume eigenstates is considered. Since the volume states are very closely spaced the summation is approximated by an integral. But, as we have discussed earlier an integration leads to overcounting of volume states. To overcome this we employ the shell particle method of counting volume states proposed in [30, 31], wherein only the distinct minimum volume states needed to confine the particle are taken into account. The volume enclosed by the isoenthalpic curve in phase space is

$$\Sigma(N, P, H) = \frac{M^N}{N!} \frac{1}{\Gamma(D_1 + 1)} \sum_{\nu} (H - PV)^{D_1/2} \tag{7.5}$$

The surface area of the constant enthalpy curve in the phase space is

$$\Omega(N, P, H) = \frac{M^N}{N!} \frac{1}{\Gamma(D_1)} \tag{7.6}$$

From the volume of the isoenthalpic curve in the phase space the nonextensive entropy of the classical ideal gas in this ensemble is

$$S_q(N, P, H) = k \left( \frac{(M^N (1/P)^N (H^{D_1}/(\Gamma(D_1 + 1))))^{1-q} - 1}{1-q} \right). \tag{7.7}$$

Using the definition of temperature (6.5), the heat function corresponding to the ensemble, the enthalpy is found:

$$H_q = \mathcal{M}^{(1-q)N\xi_1} \left( \frac{(D_1)^q}{(\Gamma(D_1))^{1-q}} \right)^{\xi_1} \left( \frac{1}{P} \right)^{(1-q)N\xi_1} \left( \frac{1}{\beta} \right)^{\xi_1}. \tag{7.8}$$

The specific heat at constant pressure evaluated from (7.8) through the use of (6.6) is

$$C_q|_P = (D_1)^{q\xi_1} k \xi_1 \left( \frac{M^N}{\Gamma(D_1)} \left( \frac{1}{P} \right)^N \left( \frac{1}{\beta} \right)^{D_1} \right)^{(1-q)\xi_1}. \tag{7.9}$$
The average volume calculated using (6.7) can be rewritten to obtain the equation of state given below:

\[ PV_q = \frac{N}{\beta} \left( \mathcal{M}^N \left( \frac{\Omega_1}{\Gamma(\Omega_1)} \right)^\Omega_1 \left( \frac{1}{P} \right)^N \left( \frac{1}{\beta} \right) \right)^{1-q}\Omega_1. \]  

(7.10)

The internal energy evaluated through the definition of the expectation value of the observable (6.8) is

\[ U_q(\beta) = \frac{DN}{2\beta} \left( \frac{\mathcal{M}^N}{\Gamma(\Omega_1 + 1)} \left( \frac{1}{P} \right)^N \left( \frac{1}{\beta} \right) \right)^{1-q}\Omega_1. \]  

(7.11)

The calculated value of the internal energy has also been checked through a different procedure using the Legendre transformation

\[ H_q = U_q + PV_q. \]

From (7.11) the specific heat at constant volume found using (6.9) is

\[ C_q|_V = \frac{DN}{2} k \Omega_1 \left( \frac{\mathcal{M}^N}{\Gamma(\Omega_1 + 1)} \left( \frac{1}{P} \right)^N \left( \frac{1}{\beta} \right) \right)^{1-q}\Omega_1. \]  

(7.12)

Using the results corresponding to the specific heat at constant pressure (7.9) and the specific heat at constant volume (7.12) the q generalization of Mayer’s relation is obtained:

\[ C_q|_P - C_q|_V = Nk \Omega_1 \left( \frac{\mathcal{M}^N}{\Gamma(\Omega_1 + 1)} \left( \frac{1}{P} \right)^N \left( \frac{1}{\beta} \right) \right)^{1-q}\Omega_1. \]  

(7.13)

The ratio between the specific heat at constant pressure (7.9) and the specific heat at constant volume (7.12):

\[ \gamma = \frac{C_q|_P}{C_q|_V} = 1 + \frac{2}{D} \]  

(7.14)

is interestingly independent of q and N. We have observed the same result in the isothermal–isobaric ensemble (3.21). In the extensive q → 1 limit the standard Boltzmann–Gibbs results are recovered.

### 7.2. Extreme relativistic ideal gas in \( (N, P, H) \) ensemble

The extreme relativistic classical ideal gas described by the Hamiltonian (3.22) is studied in the \( (N, P, H) \) ensemble. The volume enclosed by the surface of constant enthalpy is given by

\[ \Sigma(N, P, H) = \sum_V \frac{1}{N! h^{DN}} \int_{r_i} \int_{p_i} \Theta \left( c \sum_i p_i + PV - H \right) \prod_{i=1}^N d^D r_i d^D p_i. \]  

(7.15)

In (7.15) the result of the momentum integration is

\[ er_{T_P} = \int e^{\sum_i p_i \leq H-PV} d^D p_i = \frac{1}{\Gamma(DN + 1)} \left( \frac{2\pi^{D/2} \Gamma(D)}{\Gamma(D/2)} \right)^N (H-PV)^{DN}. \]  

(7.16)
The expression (7.16) is substituted in (7.15) and the resulting expression is integrated over the position coordinates. Replacing the summation over the volume eigenstates by an integration to consider the continuum nature of volume and adopting the shell particle method of counting volume states the final expression for \( \Sigma(N, P, H) \) is

\[
\Sigma(N, P, H) = \Delta^N \left( \frac{1}{P} \right)^N \frac{H_{\Delta^2}}{\Gamma(\Delta^2 + 1)},
\]

which enables us to calculate the surface of the isoenthalpic curve via the relation (6.3):

\[
\Omega(N, P, H) = \Delta^N \left( \frac{1}{P} \right)^N \frac{H_{\Delta^2-1}}{\Gamma(\Delta^2)}.
\]

The nonextensive entropy (6.4) of the extreme relativistic ideal gas obtained from (7.17) is

\[
S_q(N, P, H) = k \left( \frac{\Delta^N \left( 1 - q \right)^N \frac{H_{\Delta^2}}{\Gamma(\Delta^2 + 1)} \left( \Delta^N \frac{H_{\Delta^2}}{\Gamma(\Delta^2 + 1)} \right)^{1-q} - 1}{1 - q} \right).
\]

Using the definition of temperature in the isoenthalpic–isobaric ensemble (6.5) in conjunction with the expression for the entropy (7.19) we find the enthalpy:

\[
H_q = \Delta^{(1-q)N\Delta^2} \left( \frac{(\Delta^2)^q}{\Gamma(\Delta^2)} \right)^{\Delta^2} \left( \frac{1}{P} \right)^N \left( \frac{1}{\beta} \right)^{\Delta^2}. \quad (7.20)
\]

The specific heat at constant pressure obtained from the enthalpy via (6.6) is

\[
C_q|_P = (\Delta^2)^q k \Delta^2 \left( \frac{\Delta^N \left( 1 - q \right)^N \frac{H_{\Delta^2}}{\Gamma(\Delta^2 + 1)} \left( \Delta^N \frac{H_{\Delta^2}}{\Gamma(\Delta^2 + 1)} \right)^{1-q} - 1}{1 - q} \right). \quad (7.21)
\]

The computed expression for the average volume using (6.7) is rewritten to give the equation of state:

\[
P V_q = \frac{N}{\beta} \left( \Delta^N \left( \frac{\Delta^2}{\Gamma(\Delta^2)} \right)^{\Delta^2} \left( \frac{1}{P} \right)^N \left( \frac{1}{\beta} \right)^{\Delta^2} \right)^{(1-q)\Delta^2}. \quad (7.22)
\]

Making use of the formula for the expectation value (6.8), the calculated form of the internal energy is

\[
U_q(\beta) = \frac{D N}{\beta} \left( \frac{\Delta^N \left( \frac{\Delta^2}{\Gamma(\Delta^2)} \right)^{\Delta^2} \left( \frac{1}{P} \right)^N \left( \frac{1}{\beta} \right)^{\Delta^2}}{\Gamma(\Delta^2 + 1)} \right)^{(1-q)\Delta^2}, \quad (7.23)
\]

and this perfectly agrees with the result found using the Legendre transformation \( H = U + PV \). From the internal energy the specific heat at constant volume can be found:

\[
C_q|_V = D N k \Delta^2 \left( \frac{\Delta^N \left( \frac{\Delta^2}{\Gamma(\Delta^2 + 1)} \right)^{\Delta^2} \left( \frac{1}{P} \right)^N \left( \frac{1}{\beta} \right)^{\Delta^2}}{(1-q)\Delta^2} \right). \quad (7.24)
\]
The ratio between the heat capacities at constant pressure and constant volume:
\[
\gamma = \frac{C_q|_P}{C_q|_V} = 1 + \frac{1}{D},
\]
(7.25)
is found to be independent of both the nonextensive parameter and the number of particles \(N\), similar to the result observed in (3.34). The enthalpy, internal energy and specific heats go to their respective Boltzmann–Gibbs values in the \(q \to 1\) limit.

The thermodynamic quantities corresponding to the Tonks gas (3.35) can also be computed through a procedure identical to the one employed in the case of the nonrelativistic and extreme relativistic classical ideal gas. The results can be easily read from the expressions corresponding to the nonrelativistic gas through the use of the free length \(L_{f q}\) in the place of the volume \(V\) and setting the dimension \(D = 1\). The equation of state of the Tonks gas thus obtained is
\[
PL_{f q} = N \frac{\gamma}{\beta} M(1+q)^{1/1} \left( \frac{3N/2}{\Gamma(3N/2)} - \frac{1}{P} \right) \left( \frac{1}{\beta} \right) \left( \frac{3N}{2} \right)^{-1/1} \left( \frac{1}{P} \right). 
\]
(7.26)

It can be seen that equation (7.26) recovers its standard Boltzmann–Gibbs result \(PL_{f q} = NkT\) in the \(q \to 1\) limit.

8. Adiabatic ensemble with number fluctuations

The adiabatic ensemble with number fluctuations was first discussed in detail in [12] in the context of Boltzmann–Gibbs ensemble. This ensemble is the adiabatic counterpart of the grand canonical ensemble and the Hill energy is the corresponding heat function. Though the integration with respect to the position and momentum coordinates can be carried out easily, it is not possible to carry out the sum over all possible values of \(N\). So in this section we give only a formal expression corresponding to the phase space volume, surface area, Hill energy and equation of state.

8.1. Nonrelativistic ideal gas

The volume of phase space enclosed by the curve of constant Hill energy \(L\) after carrying out the integrations over the position and the momentum coordinates is
\[
\Sigma(\mu, V, L) = \sum_{N=0}^{\infty} \frac{V^N}{N! \Gamma(DN/2 + 1)} M^N (L + \mu N)^{DN/2}.
\]
(8.1)
The surface area corresponding to the phase space curve of constant Hill energy can arrived at through the use of (6.3). The equation of state describing the classical ideal gas in this ensemble is
\[
PV_q = kT \sum_{N=0}^{\infty} \frac{V^N}{N! \Gamma(DN/2 + 1)} M^N (L + \mu N)^{DN/2}.
\]
(8.2)
The formal expression for the average number of particles arrived at through the use of (6.7) is
\[
N_q = kT \sum_{N=0}^{\infty} \frac{V^N}{N! \Gamma(DN/2)} M^N (L + \mu N)^{(DN/2)-1}.
\]
(8.3)

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8.2. Extreme relativistic Ideal gas

For an extreme relativistic classical ideal gas described by the Hamiltonian (3.22), the phase space volume calculated is

$$\Sigma(\mu, V, L) = \sum_{N=0}^{\infty} \frac{V^N}{N! \Gamma(DN + 1)} \Delta^N (L + \mu N)^{DN}. \quad (8.4)$$

The equation of state and the average number of particles of the extreme relativistic gas corresponding to this adiabatic ensemble are

$$PV_q = \frac{kT}{\Sigma^q} \sum_{N=0}^{\infty} N \frac{V^N}{N! \Gamma(DN)} \Delta^N (L + \mu N)^{DN}, \quad (8.5)$$

$$N_q = \frac{kT}{\Sigma^q} \sum_{N=0}^{\infty} N \frac{V^N}{N! \Gamma(DN - 1)} \Delta^N (L + \mu N)^{DN-1}. \quad (8.6)$$

In the $q \to 1$ the above quantities reduce to the standard Boltzmann–Gibbs equations. Substituting $D = 1$ and replacing the volume by the free length in the thermodynamic expression for the nonrelativistic ideal gas, we can arrive at relations corresponding to the Tonks gas.

9. Adiabatic ensemble with volume and number fluctuations

An adiabatically confined system which can exchange both volume and particles with the bath is described by this ensemble. In the classical Boltzmann–Gibbs case such an ensemble was first described and discussed in detail in [13]. The heat function of the system is the $R$ heat function and this is the adiabatic counterpart of the generalized ensemble. Similar to the previous ensemble, the $N$ summation is difficult to carry out and so we present the results as a formal sum.

9.1. Nonrelativistic ideal gas

In the ensemble with both volume and number fluctuations, the phase space volume of the classical nonrelativistic ideal gas enclosed by a curve of constant $R$ is

$$\Sigma(\mu, P, R) = \sum_{N=0}^{\infty} \frac{\mathcal{M}^N}{\Gamma(D_1 + 1)} \left( \frac{1}{P} \right)^N (R + \mu N)^{D_1}. \quad (9.1)$$

Using the expression for the phase space volume (9.1), the equation of state and the average number of particles is obtained:

$$PV_q = \frac{kT}{\Sigma^q} \sum_{N=0}^{\infty} N \frac{\mathcal{M}^N}{\Gamma(D_1 + 1)} (R + \mu N)^{D_1}, \quad (9.2)$$

$$N_q = \frac{kT}{\Sigma^q} \sum_{N=0}^{\infty} N \frac{\mathcal{M}^N}{\Gamma(D_1)} (R + \mu N)^{D_1-1}. \quad (9.3)$$
9.2. Extreme relativistic Ideal gas

In the case of an extreme relativistic ideal gas, the phase space volume enclosed by a curve of constant \( R \) is

\[
\Sigma(\mu, P, R) = \sum_{N=0}^{\infty} \frac{\Delta^N}{\Gamma(D_2 + 1)} \left( \frac{1}{P} \right)^N (R + \mu N)^{D_2},
\]

which leads to the equation of state and the average number of particles given below:

\[
P V_q = \frac{kT}{\Sigma^q} \sum_{N=0}^{\infty} N \frac{\Delta^N}{\Gamma(D_2)} \left( \frac{1}{P} \right)^N (R + \mu N)^{D_2},
\]

\[
N_q = \frac{kT}{\Sigma^q} \sum_{N=0}^{\infty} N \frac{\Delta^N}{\Gamma(D_2 - 1)} \left( \frac{1}{P} \right)^N (R + \mu N)^{D_2 - 1}.
\]

The \( q \to 1 \) limit is respected in all the above-mentioned cases. The thermodynamic expressions corresponding to the Tonks gas can be arrived at directly from the relations given for the nonrelativistic gas by substituting \( D = 1 \) and replacing the volume by the free length.

The summation over the number of particles could not be evaluated in both the ensemble with the number fluctuations and the ensemble with number and volume fluctuations. But the thermodynamic quantities in both these ensembles may be obtained through the use of a molecular dynamics simulation.

10. Remarks

A comprehensive investigation on the different kinds of ensembles has been carried out in the present work. There are two different classes of ensembles, namely the isothermal class and the adiabatic class.

The thermal equilibration in the isothermal class happens with respect to the temperature. The Isothermal class comprises the canonical ensemble, the isothermal–isobaric ensemble, the grand canonical ensemble and the generalized ensemble. The thermodynamic relations corresponding to these four ensembles has been presented through a unified framework in the currently accepted third constraint formalism of the nonextensive \( q \)-statistical mechanics. The unified formulation developed is applied to study the isothermal–isobaric, grand canonical and generalized ensembles through specific examples, viz the classical nonrelativistic and extreme relativistic ideal gas models. Since the canonical ensemble has already been studied in detail in \[17, 18\] it has not been considered in our present work. In the isothermal–isobaric ensemble, the implicit equations corresponding to the generalized partition function and the enthalpy are solved to obtain their corresponding explicit expressions. From these quantities the average volume, the internal energy, the specific heat at constant pressure and the specific heat at constant volume are obtained. All the above-mentioned thermodynamic quantities are obtained as exact results. The specific heats were dependent on the nonextensivity parameter \( q \) and the temperature in both the models. Interestingly we notice that the ratio between the specific heat at constant pressure and the specific heat at constant volume is independent of both \( q \) and \( N \). A similar exact computation of the gas models in the grand canonical and
A class of energy-based ensembles in Tsallis statistics

generalized ensembles was found to be difficult. So, we employed a perturbative procedure developed in [21, 26] based on the disentangling of the \( q \) exponential [25]. The perturbative series corresponding to the generalized partition function, the sum of \( q \) weights and the heat function are obtained up to a predetermined order in the third constraint formalism. The determined implicit quantities are then solved recursively to obtain the final explicit forms which are used to find the thermodynamic results. The fact that these quantities are uncoupled and exactly solvable in the \( q = 1 \) limit facilitates the recursive procedure. In the grand canonical ensemble, the final results are computed up to second order in the expansion variable \((1 - q)\) whereas in the generalized ensemble the results are displayed only up to the first order. The perturbation method developed may be continued to any arbitrary order in \((1 - q)\). Since our method is of perturbative origin, it is obvious that the results obtained here are valid in the regime \(|1 - q| \ll 1\).

The adiabatic class of ensembles contains the microcanonical ensemble, the isoenthalpic–isobaric ensemble, the adiabatic ensemble with number fluctuations and the adiabatic ensemble with both number and volume fluctuations. A generalized method of representing the thermodynamic relations corresponding to the adiabatic ensembles is discussed and a \( q \) generalization of the equipartition theorem and the virial theorem have also been obtained in a unified sense. The \((N, P, H)\) ensemble, the \((\mu, V, L)\) ensemble and the \((\mu, P, R)\) ensemble have been studied through the examples of a classical nonrelativistic ideal gas and an extreme relativistic ideal gas. The above-mentioned ideal gas models have been solved in the isoenthalpic–isobaric ensemble. The exact expression corresponding to the entropy, enthalpy, internal energy and heat capacities at both constant pressure and at constant volume were found. In the case of the \((\mu, V, L)\) and the \((\mu, P, R)\) ensembles an exact solution could not be arrived at and so the thermodynamic quantities have been expressed as formal sums. An interesting observation is made from the study of the ideal gas models in the various ensembles. The gas models were exactly solvable in the isothermal–isobaric and the isoenthalpic–isobaric ensembles. In both these ensembles we notice that the ratio of the specific heat at constant pressure and the specific heat at constant volume was found to be independent of the nonextensivity parameter \(q\), the number of particles \(N\) and the temperature. This is despite the fact that the individual heat capacities were dependent on these three factors. Meanwhile the difference between the heat capacities was found to be dependent on these three factors.

The experimental conditions are the key determining factors in choosing the ensemble appropriate to any given system. The microcanonical ensemble is used to study completely isolated systems, whereas the canonical ensemble is used to study closed systems which exchange energy with the surroundings. The grand canonical ensemble is used to study systems capable of exchanging particles with its surroundings. Depending on whether a fluid under constant pressure is isothermally or adiabatically confined, we can use the isothermal–isobaric or the isoenthalpic–isobaric ensemble. It has been argued [15,36] that the onset of a glass transition in atomic fluids can be more suitably studied in the isothermal–isobaric ensemble since the temperature and pressure of an atomic fluid can be manipulated easily. Similarly in molecular dynamic simulations of lipid bilayers the isothermal–isobaric ensemble is more appropriate since an exact determination of the volume of a lipid is not feasible [37]. The generalized ensemble has been used in the investigation of the critical behavior of ferromagnets using the mean-field cluster model [38]. In the above-mentioned model [38], clusters of unrestricted sizes are considered.
A class of energy-based ensembles in Tsallis statistics

and the properties of individual clusters are defined using the microcanonical ensemble. Meanwhile the interaction of the cluster with the ensemble of other clusters has been studied using the generalized ensemble. The magnetic susceptibility calculated through this model [38] agrees with the experimentally measured values at all temperature above the Curie temperature and thus provides a unified picture for both the critical-scaling and Curie–Weiss regimes.

The unification procedure developed in the current work for the nonextensive $q$ entropy (1.1) can be extended to other kinds of nonextensive entropies like $\kappa$ entropy [39] and the two parameter entropies [40,41]. Such an effort will help us to understand the change in the structure of thermostatistics due to nonextensivity. It has been noticed in [12] that there is an inherent pairing between the isothermal and the adiabatic ensembles, that is each isothermal ensemble has an adiabatic counterpart. These pairs can be identified through the fact that they have the same heat function. An interrelation between the isothermal and adiabatic ensembles can be established through a Laplace transformation. The canonical ensemble and the microcanonical ensemble have been interrelated in the nonextensive $q$ statistics through a $q$ generalization of the Laplace transform [42]. Currently we are working on developing a unified formulation of the $q$-Laplace transform to connect any of the isothermal ensemble to its adiabatic counterpart. The results will appear elsewhere.

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