Density matrix for a consistent non-extensive thermodynamics

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Abstract

Starting with the average particle distribution function for bosons and fermions for non-extensive thermodynamics, as proposed in [6], we obtain the corresponding density matrix operators and hamiltonians. In particular, for the bosonic case the corresponding operators satisfy a deformed bosonic algebra and the hamiltonian involves interacting terms in powers of $a_j^\dagger a_j$ standard creation and annihilation operators. For the unnormalized density matrix we obtain a nonlinear equation that leads to a two-parameter solution relevant to anomalous diffusion phenomena.

Keywords:
Non-extensive thermodynamics
Density matrix
Entropy functions
Anomalous diffusion.

1 Introduction

Since its formulation, non-extensive thermodynamics [1] has found applications to a vast number of fields [2]. Recently, some applications include proton-proton collisions [3] and neutron stars [4, 5]. These applications are based on the claim of thermodynamic consistency leading to a modified fermionic particle number distribution [6] which consists of the $q$-power of the original Tsallis distribution. In this manuscript, we obtain a factorized density matrix and partition function for the bosonic and fermionic cases. Then, we show that the unnormalized density matrix leads to a generalized nonlinear differential equation relevant to anomalous diffusion. In Section [2] we obtain the density

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matrices and partition functions in a factorized form for boson and fermion cases. In particular, for the boson case the adjoint operators satisfy a deformed algebra leading to an interacting hamiltonian. In Section 3 we find a thermodynamic expression for the bosonic and fermionic entropy functions, and in Section 4 we obtain and solve a two-parameter nonlinear differential equation relevant to anomalous diffusion. Section 5 contains our concluding remarks.

2 Density Matrix

In this Section we obtain the density operator for boson and fermions according to the particle distribution function defined in [4] and the corresponding partition functions. Let us define the function

\[ \rho_k = (1 + (q - 1)\beta\epsilon'_k)^{\frac{1}{q - 1}}, \]  

where \( \epsilon'_k = \epsilon_k - \mu \). We want to obtain, by using the operator formalism, the density operator \( \hat{\rho} \) that will give the number distributions:

\[ < N_k > = \frac{1}{(\rho_k \pm 1)^q}, \]  

where the upper (lower) sign are for fermions (bosons), and as it is well known these functions become the fermion and boson number distribution in the \( q \to 1 \) limit. From the definition

\[ < N_k > = Tr\hat{\rho}\phi_k^\dagger\phi_k, \]  

where \( \phi \) and its adjoint \( \phi^\dagger \) denote either boson or fermion operators and with use of the usual commutation and anticommutation relations we find that

\[ < N_k > = \mp Tr\phi_k^\dagger\hat{\rho}\phi_k \pm 1, \]  

Requiring that the density matrix \( \hat{\rho} \) satisfy the relations with the operator \( \phi_k^\dagger \)

\[ \phi_k^\dagger\hat{\rho} = \mp\hat{\rho}\phi_k^\dagger + (\rho_k \pm 1)^q\hat{\rho}\phi_k^\dagger, \]  

leads to

\[ < N_k > = \pm 1 + < N_k > \mp (\rho_k \pm 1)^q < N_k >, \]  

and

\[ 0 = \pm 1 \mp (\rho_k \pm 1)^q < N_k >, \]  

and then to Eq. (2).

2.1 Boson case

For the boson case, Eq. (5) reads

\[ a_k^\dagger\hat{\rho} = (1 + (\rho_k - 1)^q)\hat{\rho}a_k^\dagger, \]  

2
such that considering the scaling operator $\Lambda^{\tilde{n}_k} = \Lambda^{-1}a_k\Lambda^{n_k}$, where $n_k = a^\dagger a$ is the usual boson number operator, we see that Eq. (5) is satisfied by the following operator

$$\hat{\rho} = \frac{1}{Z} \prod_{k=0} \left(1 + (\rho_k - 1)^q\right)^{-\tilde{n}_k},$$

(9)

where $Z$ is the partition function

$$Z = \sum_{n_1=0} \ldots \sum_{n_\infty=0} \prod_{k=0} \left(1 + (\rho_k - 1)^q\right)^{-\tilde{n}_k},$$

(10)

leading to the product

$$Z = \prod_{k=0} \frac{1}{1 - (1 + (\rho_k - 1)^q)^{-1}}.$$  

(11)

From Eq. (9) we can find the corresponding hamiltonian $\hat{H}_k$ by equating

$$\left(1 + \beta(q - 1)\hat{H}_k\right)^{-\tilde{n}_k} = \left(1 + (\rho_k - 1)^q\right)^{-\tilde{n}_k},$$

(12)

where the left hand side becomes an exponential of the energy as $q \to 1$, giving after a simple manipulation

$$\hat{H}_k = \frac{(1 + (\rho_k - 1)^q)^{(1-q)\tilde{n}_k} - 1}{\beta(q - 1)},$$

(13)

which as a power series the hamiltonian becomes

$$\hat{H}_k = \sum_{l=1} \frac{(a^\dagger a)^l}{l\beta(q - 1)^{l-1}} \log(1 + (\rho_k - 1)^q)$$

(14)

indicating that this model contains interaction terms involving an even number of operators. A simple check shows that, as expected, $\hat{H}_k \to \tilde{n}_k\epsilon'_k$ as $q \to 1$.

We can rewrite Eq. (14) for the full hamiltonian in a standard form in terms of two adjoint operators

$$\hat{H} = \sum_k \epsilon'_k \Phi_k \Phi_k,$$

(15)

if we define

$$\Phi_k = a^\dagger_k, \quad \Phi = a^{-1}_{\epsilon_k} Q_{\tilde{n}_k}^{-1} - 1,$$

(16)

where $Q_k = (1 + (\rho_k - 1)^q)^{q-1}$, leading to the deformed bosonic algebra

$$\Phi_j \Phi_k - Q_k^{-1} \Phi_k \Phi_j = \delta_{j,k} Q_k^{-1} - 1.$$

(17)

The deformation of this boson algebra, in contrast to the usual $q$-boson algebras \[7\], depends on the value of the energy. In particular, for $\rho_k = 1$ and $q \neq 1$ the operators commute.
2.2 Fermion case

In this case, Eq. (5) is satisfied by the density operator
\[
\hat{\rho} = \frac{1}{Z} \prod_k ((\rho_k + 1)^q - 1)^{-\hat{n}_k},
\]
leading to
\[
\hat{\rho} = \frac{1}{Z} \prod_k (1 + \hat{n}_k (\Gamma_k^q - 1)^{-1} - 1),
\]
where \( \Gamma_k = (1 + \rho_k) \), \( \hat{n}_k = b_k^\dagger b_k \) is the usual fermion number operator and the partition function
\[
Z = \sum_{n_0=0}^1 \ldots \sum_{n_m=0}^1 \prod_k (1 + \hat{n}_k [ (\Gamma_k^q - 1)^{-1} - 1 ]),
\]
becomes
\[
Z = \prod_{k=0}^1 \frac{1}{1 - (1 + \rho_k)^{-q}}
\]
In this case equating the left hand side of Eq. (12) with the corresponding factor of the product in Eq. (18), we find that the hamiltonian is given by
\[
\hat{H}_k = \frac{(\Gamma_k^q - 1)(q-1)\hat{n}_k - 1}{\beta(q-1)}
\]
which reduces to the simple expression
\[
\hat{H}_k = \frac{\hat{n}_k ((\Gamma_k^q - 1)^{q-1} - 1)}{\beta(q-1)},
\]
implying that defining "new" fermionic operators will not lead to a different algebra than the usual fermionic one. Certainly, for \( q = 1 \) we get \( \hat{H}_k = \hat{n}_k \epsilon'_k \).

3 Entropy

The corresponding entropies were defined in [4] and the fermion case was previously discussed in [6] where the number distributions in Eq. (2) were obtained with use of the maximum entropy principle. Here we just want to find the thermodynamic expression for the entropy in terms of the average internal energy \( \langle U \rangle \) and the occupation number \( \langle N \rangle \). We define
\[
S = \sum_k \Theta_k + \beta \langle U \rangle - \beta \mu \langle N \rangle,
\]
where the functions \( \Theta_k \) are to be determined. A simple calculation gives
\[
\beta \langle U \rangle - \beta \mu \langle N \rangle = \sum_k \frac{1}{q-1} < N_k >^{1/q} \left((1+<N_k>^{1/q})^{(q-1)} - <N_k>^{q-1}\right),
\]
where the upper sign applies to the fermionic case. The entropy functions obtained in [4] and [6] are reproduced if we define the \( \Theta_k \) functions as
\[
\Theta_k = \mp \log_q \left( 1 \mp < n_k >^{1/q} \right),
\]
where \( \log_q x = \frac{1-x^{q-1}}{1-q} \). In addition, starting with the differential equation
\[
\frac{d < N_k >}{d \beta \epsilon_k'} = - \frac{q}{q} < N_k >^{(2q-1)/q} \left( 1 \mp < N_k >^{1/q} \right)^{2-q},
\]
and use of the Inverse Maximum Entropy Principle, [8], the second derivative of the entropy with respect to \( < N_k > \)
\[
S'' = \frac{c}{\Psi},
\]
leads to the entropy functions
\[
S = \mp \left( 1 \mp < N_k >^{1/q} \right) \log_q \left( 1 \mp < N_k >^{1/q} \right) - < N_k >^{1/q} \log_q < N_k >^{1/q}.
\]

4 Diffusion differential equations

It is well known that one can obtain differential equations from the unnormalized density matrix [9]. For the standard, \( q = 1 \), density matrix the corresponding simplest differential equation is
\[
- \frac{\partial \rho_U}{\partial \beta} = H \rho_U,
\]
where \( \rho_U = e^{-\beta H} \) is the unnormalized density matrix. Letting \( H = - \frac{\partial^2}{\partial x^2} \) will certainly leads to the standard diffusion equation. In our case, from Eq. (12) we obtain that the corresponding operator is given by
\[
\rho_U = (1 + \beta(q - 1)H_k)^{\frac{-\beta}{q}},
\]
leading to the nonlinear differential equation
\[
- \frac{\partial \rho_U}{\partial \beta} = H \rho_U^q.
\]
The simplest case is to consider \( H = - \frac{\partial^2}{\partial x^2} \) giving the differential equation
\[
\frac{\partial \rho_U}{\partial \beta} = \frac{\partial^2}{\partial x^2} \rho_U^q.
\]
whose solution
\[ \rho_U(x, t) \propto \frac{1}{\beta^{1/(1+q)}} \left( 1 - (q - 1) \frac{x^2}{\beta^{2/(1+q)}} \right)^{1/(q-1)}. \] (34)

was studied, among other applications, in the context of non-extensive Statistical Mechanics [10], anomalous diffusion in the presence of external forces [11], anomalous diffusion on fractals [12] [13], and \( \kappa \)-generalized Statistical Mechanics [14].

A more general differential equation can be obtained if we use the differential operator
\[ H = -\frac{\partial}{\partial x} \left( \frac{\partial f}{\partial x} \right)^\mu, \] (35)
where in our case the function \( f = \rho^q_U \) and \( \mu \) is a parameter. This differential operator \( \frac{\partial}{\partial x} \left( \frac{\partial}{\partial x} \right)^\mu \) was obtained, [15], from the Fisher-like measure that results when one expands the relative entropy
\[ H_\mu(p(x)||p(x + \Delta)) = \int p(x) \left( -\ln \frac{p(x + \Delta)}{p(x)} \right)^\mu dx, \] (36)
up to second order with respect to a small shift \( \Delta \). The origin of this relative entropy, [10], is the entropic function
\[ S_\mu(p) = \sum_i p_i (-\ln p_i)^\mu, \] (37)
obtained by applying the Weyl fractional derivative to the function \( \sum_i p_i^{-t} \) and then taking the limit \( t \to -1 \). As it is well known, the use of an ordinary derivative will lead to the Shannon entropy, and the use [17] of the Jackson \( q \)-derivative [18] will reproduce the Tsallis entropy [1]. In addition, similar operators to the one in Eq. (35) have been studied in Refs. [19]-[22] as an application to nonlinear diffusion in the context of disturbances in a non-Newtonian fluid, non-linear heat conduction and fractal diffusion. Equations (32) and (35) give the nonlinear differential equation
\[ \frac{\partial \rho_U}{\partial \beta} = \frac{\partial}{\partial x} \left( \frac{\partial}{\partial x} \rho^q_U \right)^\mu. \] (38)

It is natural to consider the ansatz
\[ \rho_U = \frac{A}{\beta^\lambda} \Phi^\mu(x, \beta), \]
\[ \Phi(x, \beta) = \left( 1 + \frac{(1 - q\mu) x^\gamma}{C \beta^\alpha} \right), \] (39)
where the constants \( \lambda, \gamma \) and \( \alpha \) in the \( q \to 1 \) limit become: \( \lambda = 1/2, \gamma = 2 \) and \( \alpha = 1 \). After performing the elementary derivatives and comparing powers in
\( \Phi(x, t), x \) and \( \beta \) and the constants in both sides of Eq. (38) we find

\[
\begin{align*}
\omega &= \frac{1}{\mu q - 1}, \\
\gamma &= \frac{1 + \mu}{\mu}, \\
\alpha &= \frac{1 + \mu}{\mu^2(1 + q)}, \\
\lambda &= \frac{1}{\mu(1 + q)}, \\
A^{1-q\mu} &= \left( \frac{q(1 + \mu)}{C\mu} \right)^\mu (1 + q),
\end{align*}
\]

where the requirement that the constant \( A \) has to be positive will restrict the values \( \mu = \frac{n}{m} \), where \( n \) and \( m \) are odd numbers. The general solution is given by

\[
\Phi(x, t) = \frac{A}{\beta^{\mu(1+q)}} \left( 1 + (1 - \mu q) \frac{x^{1+\mu}}{\beta^{x^{1+\mu}}} \right)^{-\frac{1}{1-\mu}},
\]

leading for \( q = 1 \) to the particular solution

\[
\Phi(x, t) \sim \frac{1}{\beta^{1/2\mu}} \left( 1 + (1 - \mu) \frac{x^{1+\mu}}{C\beta^{1+\mu}/2\mu^2} \right)^{-\frac{1}{1-\mu}},
\]

already obtained in [15] as a simple model for anomalous diffusion. An additional relation between the constants \( A \) and \( C \) can be obtained from the normalization of the function in Eq. (39)

\[
\frac{A}{\beta^{\mu}} \int_{-\infty}^{\infty} \Phi^\omega(x, \beta) dx = 1,
\]

which due to the fact that \( \Phi(-x, \beta) = -\Phi(x, \beta) \) we can change the limits from \(( -\infty, \infty )\) to \(( 0, \infty )\) and with use of the integral representation of the \( \Gamma(x) \) function we obtain

\[
A = \frac{\gamma}{2C^{1/\gamma}} \frac{(1 - q\mu)^{1/\gamma} \Gamma(-\omega)}{\Gamma(1/\gamma) \Gamma(-\omega - 1/\gamma)}.
\]

In the particular case of \( q\mu = 1 \) there is an infinite number of solutions involving the stretched exponential function

\[
\Psi(x, \beta) = \frac{A}{\beta^{1/(\mu+1)}} \exp \left( -\frac{x^{(1+\mu)/\mu}}{C\beta^{1/\mu}} \right),
\]

where from Eqs. (41) and (48) the constants

\[
A(q\mu = 1) = \frac{1}{2\Gamma(\mu/\mu)(\mu+1))\mu(1-\mu)/(\mu+1)}.
\]
and
\[ C(q\mu = 1) = \frac{1}{\mu^2}(\mu + 1)^{(\mu+1)/\mu}, \]
giving for the standard case \((q = 1 = \mu)\) the expected values \(A = \frac{1}{\sqrt{4\pi}}\) and \(C = 4\).

5 Conclusions

In this manuscript we obtained for non-extensive statistical mechanics, according to the particle number distributions discussed in Refs. [3]-[6], the corresponding density matrix and factorized partition function for the bosonic and fermionic cases and a thermodynamic expression for the entropy functions. In addition, we showed that the unnormalized density matrix leads to a nonlinear equation whose solution is a two-parameter function relevant to anomalous diffusion. The use of the nonlinear differential operator in Eq. (38) gives an alternative approach to study the diverse phenomena involving anomalous diffusion like for example Levy flights, turbulent diffusion and two-dimensional rotating flow, other than the cases of the nonlinear Fokker-Planck equation [23], linear [24][25] and nonlinear [26] fractional Fokker-Planck equations. A continuation of the work done in this manuscript could include two different directions. One, would involve a calculation of the thermodynamic curvature, as done [27] for the case of the dilute gas approximation [28] of non-extensive thermodynamics to learn about the stability and possible anyonic behavior of the system, and as a matter of comparison with other approaches to anomalous diffusion phenomena, to extend the applications of Eq. (38) including a time dependent source term and external forces.

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