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Radial distribution function within the framework of the Tsallis statistical mechanics

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HIGHLIGHTS

- A new equation is derived for the RDF in the Tsallis statistics.
- The momentum and the coordinates are independent in this equation.
- The correlation increases with an increase in the values of q.
- Increase of the non-extensivity parameter and that of ε has similar effects.

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ABSTRACT

This study is conducted to obtain the radial distribution function (RDF) within the Tsallis statistical mechanics. To this end, probability distribution functions are applied in the first and fourth versions of the Tsallis statistics. Moreover, a closed formula is proposed for RDF. The power nature of the probability distribution in the Tsallis statistics makes it difficult to separate kinetic energy and configurational potential parts. By using the Taylor expansion around $q = 1$ of the power distribution, it is possible to show the independency of momenta and coordinates through integrating over the phase space variables. In addition, at low densities, numerical calculations have been performed for the RDF. Our results show that the correlation increases as q values increase.

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1. Introduction

The Boltzmann–Gibbs (BG) statistical mechanics is considered as a powerful theory for interpretation of the thermodynamic behavior of physical systems. Despite its relative success, the BG statistics is only suitable to describe extensive systems with short-range interactions, Markovian stochastic processes and, indeed, the systems whose phase space is ergodic [1–4]. However, among the phenomena in nature, one encounters cases in which this statistics is not able to predict and describe their behavior. Thus, another statistical mechanics is needed to interpret these phenomena. The basis of the difference in various statistics emanates from the definition of entropy and how it relates to probability functions. Nowadays, many phenomena have been known whose thermodynamic behavior, due to non-extensive effects, is not explicable by the common BG statistical mechanics. For instance, one can mention the systems involving long-range interactions that have a microscopic long-range memory and the systems containing a multi-fractal structure [2,3]. Also, such entities as self-gravitating systems [5,6], inflationary cosmology [7,8], complex networks [9,10], the study of stochastic systems [11,12],

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dark energy models [13], electron trapping in a degenerate plasma [14], the nonlinear statistical coupling [15], negative heat capacity [16,17], anomalous diffusive behavior (e.g. Brownian motion with a random diffusion coefficient) [18], and high-energy proton–proton collisions [19–21], indicate that the correction of the Boltzmann entropy seems to be essential. In this regard, various extensions of BG entropy have been reported [22–26]. Among them, the Tsallis entropy is known as an efficient extension. The Tsallis statistical mechanics was introduced in 1988 to discuss multifractal systems [22]. In addition to the phenomena listed above, there are other usual phenomena to which the Tsallis statistics has successfully been applied. A few of these phenomena are ideal gas [27–30], harmonic oscillators [28,31,32], linear response theory [33,34], blackbody radiation [35,36], specific heat of ^{4}He [37], Bose–Einstein condensation [38,39], Ising model [40], and plasma two-dimensional turbulence [41].

The expression of the generalized entropy proposed by Tsallis is as follows [42]:

$$S_q = k\frac{1-\sum_{i=1}^{W} p_i^q}{q-1}\left(\sum_{i=1}^{W} p_i = 1, q \in R\right), \tag{1}$$

where k is a positive constant, W implies the total number of possible microscopic configurations of the system, p_i stands for the probability in the ith microstate, and q is an entropic index which demonstrates the degree of non-extensivity in the system. It should be emphasized that the entropy S_q is reduced to the well-known Boltzmann–Gibbs–Shannon formula [43] within the limit $q \to 1$. By extremizing the entropy S_q, using $\sum_{i=1}^{W} p_i\varepsilon_i = U_q$, and $\sum_{i=1}^{W} p_i = 1$ as two constraints, a probability distribution [22] can be obtained

$$p_i = \frac{\left[1-(q-1)\,\beta\varepsilon_i\right]^{\frac{1}{q-1}}}{Z_q}, \tag{2}$$

with

$$Z_q = \sum_{i=1}^{\infty}\left[1-(q-1)\,\beta\varepsilon_i\right]^{\frac{1}{q-1}}, \tag{3}$$

where U_q is referred to as the internal energy, $\beta = \frac{1}{kT}$ is the Lagrange parameter, ε_i is related to the eigenvalue of the Hamiltonian system, and Z_q is the partition function. The formula of entropy, Eq. (1), can be adapted to fit the physical characteristics of the non-extensive systems, whereas it retains the essential property of entropy in the Second Law of thermodynamics [44].

Many modern theories proposed in the fields of liquids and fluids have greatly drawn upon the concept of radial distribution function (RDF). The RDF is a helpful function in the liquid-state theory where the thermodynamic properties of a fluid (e.g., internal energy, pressure, and chemical potential) can be calculated by using the pair-wise additive approximation and RDF [45–47]. For a system consisting of N particles at the temperature T and in the volume V, the equilibrium N-particle distribution function in the BG statistics can be defined as [47]

$$\rho^{(n)}\left(\mathbf{r}_1,\ldots,\mathbf{r}_n\right) = \frac{N!}{(N-n)!}\,\frac{\int\cdots\int e^{-\beta U_N}\,d\mathbf{r}_{n+1}\cdots d\mathbf{r}_N}{Z_N}, \tag{4}$$

where U_N is the N-body interaction potential, and Z_N denotes the configuration integral, $Z_N = \int\cdots\int e^{-\beta U_N} d\mathbf{r}_1\cdots d\mathbf{r}_N$. Note that $\rho^{(n)}\left(\mathbf{r}_1,\ldots,\mathbf{r}_n\right)$ is only a function of the coordinates and not of the momenta. The N-particle correlation function $g^{(n)}\left(\mathbf{r}_1,\ldots,\mathbf{r}_n\right)$ is expressed in terms of the corresponding particle distributions by

$$g^{(n)}\left(\mathbf{r}_1,\ldots,\mathbf{r}_n\right) = \frac{\rho^{(n)}\left(\mathbf{r}_1,\ldots,\mathbf{r}_n\right)}{\rho^n}, \tag{5}$$

where ρ is the bulk density. This is noticeable that, in non-equilibrium statistical mechanics, RDF, in addition to the coordinate, is a function of the momentum [48,49]. RDF shows the structure of a liquid in terms of the probability of finding other particles at a certain distance from the central molecule. Also, RDFs can be inferred indirectly from X-ray spectra [50].

Over the past few decades, extensive studies have been conducted on RDF of dense fluids and liquids systems. The distribution functions calculated in the Tsallis statistics apply to weakly interacting systems and ionic solutions [51]. In Ref. [52], the correlation function for Boson systems has been calculated within the non-extensive quantum statistics. As far as we know, no report has been published regarding a proper RDF within the framework of the Tsallis statistics. The main purpose of this study is to use the probability distribution functions of Tsallis in order to obtain the RDF of N-particles systems. Given that the probability distribution in the BG statistics has an exponential form, as in Eq. (4), the momenta are eliminated from the numerator and the denominator of the fraction, and the momentum portion is removed from the probability density function by integrating over all the momenta. More importantly, compared to power-law distributions in Tsallis [53–56], achievement of the same result with BG statistics requires more discussion and contemplation. This is one of the remarkable aspects of this research.

The paper is organized as follows. Section 2 focuses on the theoretical formalism of the RDF in the first version of the Tsallis statistics. Also, a closed form is derived for the RDF in the first version. In Section 3, a closed formula is proposed for the RDF in the fourth version of the Tsallis statistics. Section 4 is devoted to the numerical results of RDF under low-density conditions. Finally, Section 5 is dedicated to the conclusion.

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