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Non-extensive quantum statistics with particle–hole symmetry

T.S. Biró [a,*], K.M. Shen [b], B.W. Zhang [b]

[a] HIRG, HAS Wigner Research Centre for Physics, Budapest, Hungary
[b] IOPP, Central China Normal University, Wuhan, PR China

HIGHLIGHTS

- We generalize the KMS relation for non-exponential density matrices.
- We explore the requirement of the hole–antiparticle reinterpretation on smooth deformed exponential functions.
- We establish a connection between the mathematical forms of q-exponential and κ-exponential type approaches.
- We emphasize that the Sommerfeld expansion of a generalized Fermi distribution should contain only odd terms, beyond the leading 1/2.

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ABSTRACT

Based on Tsallis entropy (1988) and the corresponding deformed exponential function, generalized distribution functions for bosons and fermions have been used since a while Teweldeberhan et al. (2003) and Silva et al. (2010). However, aiming at a non-extensive quantum statistics further requirements arise from the symmetric handling of particles and holes (excitations above and below the Fermi level). Naive replacements of the exponential function or "cut and paste" solutions fail to satisfy this symmetry and to be smooth at the Fermi level at the same time. We solve this problem by a general ansatz dividing the deformed exponential to odd and even terms and demonstrate that how earlier suggestions, like the κ- and q-exponential behave in this respect.

1. Introduction

Since Tsallis suggested to use the non-extensive entropy formula, $S_T = \frac{1-\sum_{i=1}^{W} p_i^q}{q-1}$ in 1988 [1], the corresponding generalized statistical mechanics have been substantially developed and spread over many fields of application [2–9]. This non-logarithmic relation between entropy and probability is obviously non-additive, its non-additivity is comprised in the parameter q, differing from one. Its precise value is determined by the nature of the physical system under consideration. It smoothly reconstructs the Boltzmann–Gibbs–Shannon formula at $q = 1$. The application of non-extensive statistical mechanics becomes mandatory whenever finite size corrections to the thermodynamical limit are relevant. Non-extensive systems are those, which behave as final ones even at large size.

Several applications have been already investigated in a plethora of physical problems; both on the phenomenological level, by fitting power-law tailed distributions, and on the mathematical level, seeking for more and more general

* Corresponding author.
E-mail addresses: Biro.Tamas@wigner.mta.hu (T.S. Biró), shenkm@mails.ccnu.edu.cn (K.M. Shen), bwzhang@mail.ccnu.edu.cn (B.W. Zhang).

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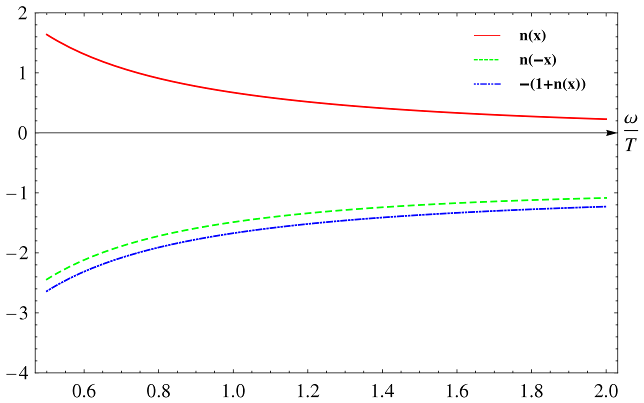

Fig. 1. The generalized KMS relation for bosons, tested by using original Tsallis' q-exponential function. The relation $n(-x) = -1 - n(x)$ breaks, since $e_q(x) \neq e_{2-q}(x) = 1/e_q(-x)$ appears in the respective formulas ($q = 0.8$).

construction rules and formulas. In particular the deformed exponential function, first identified by obtaining the canonical distribution to the Tsallis entropy, has been applied to a variety of physical problems.

Quantum statistics erects novel problems to be solved also in this respect. The naive replacement of the Euler-exponential with another, deformed exponential function namely can loose the particle–hole symmetry, inherent in the traditional Fermi distribution above and below the Fermi level. In many suggestions for the generalized Bose and Fermi distributions Tsallis' q-exponential function,

$$e_q(x) := [1 + (1-q)x]^{\frac{1}{1-q}} \tag{1}$$

is used instead of e^x at the corresponding place in the formulas [10–19] (see Fig. 1).

However, there is a fundamental problem with this ansatz: it does not satisfy the CPT invariant concept interpreting holes among the negative energy states as anti-particles with the corresponding positive energy [20],

$$n(-x) = \mp 1 - n(x) \tag{2}$$

with $x = \omega/T$. Here the upper sign is for bosons and the lower one for fermions, respectively. At a finite chemical potential (Fermi energy) one uses the argument $x = (\omega - \mu)/T$, and the above relation expresses a reflection symmetry to the $x = 0$ ($\omega = \mu$) case. In particular the original q-exponential, forming the Tsallis–Pareto cut power-law, is an incomplete approach in this respect, as long as $q \neq 2 - q$.

In this article we explore the general requirement on the deformed exponential function used in quantum statistics for satisfying the above symmetry. Starting by a generalized form of the Kubo–Martin–Schwinger (KMS) relation [21,22] we derive the desired property that a deformed exponential must satisfy. Based on this we formulate a suggestion how to "ph-symmetrize" an arbitrary function, $e_k(x)$.

2. Kubo–Martin–Schwinger relation

The KMS relation in its original form states that certain correlations between time dependent operators can be related to the reversed correlation at finite temperature by shifting the time difference variable, t, with a pure imaginary shift, $i\beta$:

$$\begin{aligned}\langle A_t B_0 \rangle &= \mathrm{Tr}\left(e^{-\beta H} e^{itH} A e^{-itH} B\right) \\ &= \mathrm{Tr}\left(e^{-\beta H} e^{itH} A e^{-itH} e^{\beta H} e^{-\beta H} B\right) \\ &= \mathrm{Tr}\left(e^{i(t+i\beta)H} A e^{-i(t+i\beta)H} e^{-\beta H} B\right) \\ &= \mathrm{Tr}\left(e^{-\beta H} B e^{i(t+i\beta)H} A e^{-i(t+i\beta)H}\right) \\ &= \langle B_0 A_{t+i\beta} \rangle. \end{aligned} \tag{3}$$

Considering generalized thermodynamical formulas we have to reconsider the KMS relation in a more general setting. Since this relation is proven simply by re-shuffling of operators under a trace, it holds very generally:

$$\begin{aligned}\langle A_t\, B_0 \rangle &= \mathrm{Tr}\left(\rho U A U^{-1} B\right) \\ &= \mathrm{Tr}\left(\rho U A U^{-1} \rho^{-1} \rho\, B\right) \\ &= \mathrm{Tr}\left(\rho\, B (\rho U) A (\rho U)^{-1}\right) \\ &= \langle B_0\, A_{t \oplus i\beta} \rangle. \end{aligned} \tag{4}$$

We note that for non-exponential H-dependence of the density matrix ρ the $\oplus$ operation is energy dependent. If we accept the requirement that $\rho(H)$ is the analytic continuation of a unitary function of H, then for a general $\rho = g(iH)$, from