Comments on *Superstatistical properties of the one-dimensional Dirac oscillator* by Abdelmalek Boumali et al.

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In this comment, we discuss the mathematical formalism used in Phys. A 553, 124207 (2020) by Boumali et al., which describes the superstatistical thermal properties of a one-dimensional Dirac oscillator. In particular, we point out the importance of remain unaltered the Legendre structure to ensure an accurate description of the thermodynamic observables. Also, we remark that all the negative poles have to take into account to calculate the Gibbs-Boltzmann partition function. Our findings show that the divergences obtained by the authors in the Helmholtz free energy, which are propagated to the other thermal properties, are a consequence of an incomplete partition function. Moreover, we prove that the restrictions over the \(q\)-parameter are no needed if the correct partition function describes the system.

I. INTRODUCTION

The recently published paper by A. Boumali et al.\(^1\) shows the calculation of the thermal properties of a one-dimensional Dirac oscillator, in the framework of the superstatistics theory using the Gamma function as the distribution for the fluctuating inverse temperature. They computed the Helmholtz free energy, average energy, entropy, and specific heat capacity from an extension of the canonical formalism, i.e., by performing derivatives on the natural logarithm of the partition function \(Z\). By applying the well-known Beck and Cohen expansion, the authors write the superstatistical partition function \(Z_q\) in terms of the Boltzmann-Gibbs partition function \(Z_0\). The latter is computed by an analytical treatment of the Cahen-Mellin integral transformation. In this comment, we revised their calculations, which in our opinion, do not have a rigorous treatment. We list the main aspects to improve:

1. The Legendre structure of the thermodynamic necessarily has to be conserved to ensure an accurate description of the system. It is achieved by choosing the correct generalized logarithm function.

2. The expansion of the partition function in terms of powers of the parameter \(q\) is incomplete.

3. The canonical partition function \(Z_0\) presented by the authors is incomplete, given that in the Cahen-Mellin integral transformation, they have ignored all the poles located at the negative real axis.

The above corrections impact directly in the thermodynamic functions. In particular, we center our discussion into the specific heat, which is not positive definite in the author’s description.

II. THE SUPERSTATISTICAL FORMALISM REVISITED

The work published by Castaño et al.\(^2\), emphasize the importance of maintaining the Legendre structure of the potentials, even in a superstatistical description, i.e., the thermodynamic functions can be calculated from the derivatives of the logarithm of the partition function. In particular, when the Gamma distribution function models the fluctuation in the intensive parameter \(\bar{\beta}\), the Tsallis formalism for non-extensive thermodynamics appears, so that the superstatistical partition function reads:

\[
Z_q(\beta) \equiv \sum_n \left[1 - (1 - q)\beta E_n\right]^{1/(1-q)},
\]

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where \( q \) is a parameter which takes into account the grade of non-extensivity \([3, 4]\), and to simplify the notation we set \( \beta = \langle \beta \rangle \). The Legendre structure is given in terms of the \( q \)-logarithm

\[
\ln_q x = \frac{x^{1-q} - 1}{1 - q},
\]

which means that the thermodynamic functions can be written as:

\[
\begin{align*}
F_q(\beta) &\equiv U_q(\beta) - TS_q = -\frac{1}{\beta} \ln_q Z_q(\beta), \\
U_q(\beta) &= -\frac{\partial}{\partial \beta} \ln_q Z_q(\beta), \\
C_q(\beta) &= \frac{\partial U_q(\beta)}{\partial T},
\end{align*}
\]

and

\[
S_q = k_B \frac{1}{q} \left( 1 - \sum_n p_n^q \right) \forall q \in \mathbb{R}.
\]

As is shown in Ref. [2], the use of \( \ln Z \) instead of \( \ln_q Z \) in the presented Laguerre structure implies that the specific heat becomes negative, and spurious phase transitions may occur.

### A. Expansion of the partition function

By defining the parameter \( a = q - 1 \), the authors used Beck-Cohen expansion (around \( a = 0 \)) \([5]\):

\[
Z_a \approx \sum_n \left[ 1 + a \beta^2 E_n^2 - \frac{a^2}{3} \beta^3 E_n^3 \right] e^{-\beta E_n},
\]

which from the fact that

\[
\beta^k E_n^k = (-1)^k \beta^k \frac{\partial^k Z_0}{\partial \beta^k}, \quad Z_0 = \sum_n e^{-\beta E_n},
\]

can be written as

\[
Z_a \approx \left[ 1 + a \beta \frac{\partial^2 Z_0}{\partial \beta^2} + a^2 \beta^3 \frac{\partial^3 Z_0}{\partial \beta^3} \right] Z_0,
\]

which its third term has a different sign compared with Ec. (26) of the named paper. Moreover, the formula presented in Ref. [5] is not complete in the sense that in such work, Beck and Cohen want to discuss the equality of the first expansion term for all the distribution functions. Thus, a complete expansion at order \( O(a^2) \) takes the form:

\[
Z_a \approx \left[ 1 + a \beta \frac{\partial^2 Z_0}{\partial \beta^2} + a^2 \beta^3 \frac{\partial^3 Z_0}{\partial \beta^3} + \frac{1}{2} \beta^4 \frac{\partial^4 Z_0}{\partial \beta^4} \right] Z_0,
\]

which constitutes our first correction.

Our second correction is about the logarithmic prescription. The authors calculate the thermal functions from derivatives of

\[
\ln Z = \ln Z_0 + \ln \left[ 1 + a \beta \frac{\partial^2 Z_0}{\partial \beta^2} + a^2 \beta^3 \frac{\partial^3 Z_0}{3 \partial \beta^3} + \frac{1}{8} \beta^4 \frac{\partial^4 Z_0}{\partial \beta^4} \right] Z_0,
\]

which is

\[
\ln Z = \ln Z_0 + \frac{1}{2} a \left( \frac{\beta^2 \frac{\partial^2 Z_0}{\partial \beta^2}}{Z_0} - \ln^2 Z_0 \right) + \frac{1}{6} a^2 \left( \frac{\beta^3 \frac{\partial^3 Z_0}{\partial \beta^3}}{Z_0} - 3 \ln \frac{Z_0}{Z_0} \frac{\beta^2 \frac{\partial^2 Z_0}{\partial \beta^2}}{Z_0} + \ln^3 Z_0 \right).
\]
The authors calculate the partition function $Z_0$ starting from the positive energy spectrum of the 1D-Dirac oscillator [6]:

$$E_n = mc^2 \sqrt{1 + 2rn}, \quad n = 0, 1, 2, \cdots,$$

(10)

where $r = \hbar \omega / mc^2$. To perform the summation, they call the well-known Cahen-Mellin transformation in the form:

$$e^{-x} = \frac{1}{2\pi i} \int_C ds \Gamma(s) x^{-s},$$

(11)

so that, by identifying $x = \sqrt{2r} \beta mc^2$, is straightforward to get

$$Z_0 = \sum_{n=0} e^{-\beta E_n} = \frac{1}{2\pi i} \int_C ds \left( \sqrt{2r} \beta mc^2 \right)^{-s} \Gamma(s) \zeta_H \left( s, \frac{1}{2} \right),$$

(12)

where $\zeta_H(s, v)$ is the Hurwitz-zeta function. To perform the integral, the authors use the Cauchy’s residue theorem by identifying such residues at $s = 0$ and $s = 2$. However, as it is established in Ref. [7], the integration limits have the form:

$$\int_C \rightarrow \int_{c-i\infty}^{c+i\infty} \text{ with } c \in \mathbb{R}^+.$$

(13)

![FIG. 1: Poles of the integrand of Eq. (12). The integration contour $C$ is given by the location of $c$. In order to apply the Cauchy’s residue theorem, the semicircle of radius $R$ is closed on the left.](image)

Therefore, given the form of the integrand, the result is convergent if $s/2 > 1$, which implies $c > 2$. The latter is implemented by a closed contour with the form depicted in Fig. 1, which forces to take into account all the poles located in the negative real axis. Thus, the correct application of the Cauchy’s residue theorem yields:

$$Z_0 = \frac{e^{\tilde{\beta}}}{2} - \frac{1}{2} + \frac{1}{2r} \left( \frac{2}{\tilde{\beta}^2} - 1 \right) + \sum_{n=1} \frac{(-\sqrt{2r} \tilde{\beta})^n}{n!} \zeta_H \left( -\frac{n}{2}, 1 + \frac{1}{2r} \right),$$

(14)

where the ground state $n = 0$ was isolated and $\tilde{\beta} \equiv mc^2 \beta$.

IV. RESULTS

In the Boumal’s paper, the authors show the functional behavior of the Helmholtz free energy, the average energy, the entropy, and the specific heat. The last one is of particular interest in this comment, given that for some parameter
configurations, their specific heat is not positive definite, and it does not vanish when the temperature goes to zero. To clarify this, Fig. 2 shows the specific heat capacity without the superstatistics prescription $C^0_v$, calculated from the Boumali’s partition function:

$$Z^B_0 = \frac{1}{2r\tilde{\beta}^2} + \zeta_H \left(0, \frac{1}{2r}\right),$$

and compared with our results obtained from Eq. (14). The results were computed for values of the parameter $r$, which have been studied by several authors, namely, $r = 1, 0.5$. Although the specific heat of the authors has an expected functional shape for some parameter configurations, the construction of $Z_0$ implies that it has to work for any other parameter selection, nevertheless, as Fig. 2 (a) and (b) show, changing the energy scale (controlled by $r$) implies an $C^0_v$ which does not vanish when $\tilde{\tau} \equiv 1/\tilde{\beta} \to 0$, with negative regions, a not well-defined limit for high-temperatures ($\tilde{\beta} \to 0$) and an apparently singularity. On the other hand, if the specific heat is computed from Eq. (14) such features are recovered. The latter implies that the results starting from $Z^B_0$ do not give a proper thermodynamic treatment.

![Figure 2](image-url)

**FIG. 2**: Specific heat $C^0_v$ computed from Eq. (14) (continuous lines) and compared with the results of Eq. (15) (dashed lines) as a function of (a) $\tilde{\tau}$ and (b) $\tilde{\beta}$ for $r = 1$ (blue) and $r = 0.5$ (red).

The authors report a series of discontinuities present in $F$, $U$, and $S$, directly impacting the functional form of $C_v$. They argue that that undesirable behavior is removed by imposing restrictions over the parameter $q$. To clarify this point, the Helmholtz free energy $F_0$ computed from $Z_0$ and $Z^B_0$ is shown in Fig. 3. Note that the discussed discontinuities are present for values of $r \neq 1$, which are related to divergences into the natural logarithm of the partition function. Also, there is not a priori argument to establish restrictions over $q$; thus, the logical conclusion is that such non-analytical regions come from a wrong choice of $Z^B_0$. 
FIG. 3: Helmholtz free energy $F_0$ computed from Eq. (14) (continuous lines) compared with the results obtained from Eq. (15) (dashed lines) for $r = 1, 0.5, 0.7$.

Finally, in order to give the result in accordance to Eq. (9), Fig. 3 shows the specific heat capacity as a function of temperature for $r = 0.5, r = 1$, and for $q$ values out of the restricted interval that the authors refers. Here, we demonstrate that such values are physically accessible, which is a consequence of the validity of the Tsallis non-extensive statistics for all values of $q$. Also, the shape and analytic behavior of the specific heat validate the choice of $\ln a Z$ instead of the common natural logarithm.
V. CONCLUSIONS

Based on the preceding arguments, we infer that the results for the superstatistical thermal properties of the one-dimensional Dirac oscillator presented in Ref [1] are mistaken. In the first instance, the formalism used by the authors did not conserve the Legendre structure of the thermodynamics, leading to a wrong description of the observables. Moreover, the canonical partition function calculation did not consider all the poles in the negative real axis, which means it was incomplete. Hence, anomalous behaviors in the thermodynamical properties are observed in the results of the authors.

The results in this work have corrected their calculations by using the $q$-logarithm and implementing a proper partition function for the system. We have demonstrated that anomalies in $F$, $U$, and $S$ come from a wrong choice in partition function, which introduces the divergences observed, instead of an interval of possible values for the parameter $q$ imposed by the choosing of the Gamma distribution. As we have shown, well-behaved thermodynamical functions are obtained out of the interval mentioned by the authors; thus, a restriction over $q$ is not needed.

Finally, the authors’ analysis of the super statistical properties of graphene is also mistaken, given the fact that it was performed under a wrong formalism and with an incomplete partition function.

AUTHOR CONTRIBUTIONS

Jorge David Castaño-Yepes: Conceptualization, Methodology, Formal analysis, Investigation, Data curation, Writing - original draft, Visualization, Supervision, Project administration. I. A. Lujan-Cabrera: Validation, Formal analysis, Data curation. C.F. Ramirez-Gutierrez: Conceptualization, Validation, Data curation, Writing - original draft, Visualization.

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