THERMODYNAMIC POTENTIALS GENERALIZED FROM A λ-DEFORMED EXPONENTIAL FUNCTION

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Abstract - In the transformation of the effective Hamiltonian for the case of a spatially dependent mass, into its canonical form, a generalized (λ-deformed) Hermitian linear momentum operator $p_\lambda$is deduced. Added to this, a spatial canonical transformation $x_\lambda$to solve the resulting differential equation leads to a λ-deformed quantum mechanics.In this scenario it is possible to propose a λ-deformed exponential function $exp_\lambda(x) = exp(x_\lambda)$ and its correspondingλ-deformed logarithmic partner$ln_\lambda(x)$.From these results, and the definition of the internal energy $U = -k\frac{\partial}{\partial\beta}ln(Z)$, it is straightforward to get the generalized internal energy$U_\lambda = -k\frac{\partial}{\partial\beta}ln_\lambda(Z_\lambda)$ which enables a natural generalization of others thermodynamic functions such as the EntropyS_λ, the Helmholtz free energy F_λ and the heat capacity C_λ.Some particular mass distributions$m(\lambda;x)$ are used as example to illustrate the proposal. Besides, in the case of $m(\lambda;x) = m_0(1+\lambda x)^{-2}$ our proposal leads straightforwardly to the Tsallis results obtained by solving a variational problem with suitable Lagrange parameters.

Keywords - Schrödinger Equation, Position-dependent Mass, Generalized Exponential Function, Internal Energy, Thermodynamic Functions.

I. INTRODUCTION

The exactly solvable position dependent mass Schrödinger equation (PDMSE) is very important for the multiple applications that it has in material science and condensed matter, such as semiconductor heterostructures [1], quantum wells and quantum dots [2], quantum liquids [3] just for mentionsome of these. On the other hand, in this work we are interested in solving the PDMSE, by insert deformation parameters. Namely, through a canonical transformation as well as in the interaction potentials to have new quantum deformed variables from which a λ-deformed quantum mechanics is identified [4]. From there, we leads to a straightforwardly generalization of thermodynamic properties. At this regard, it should be noticed that a generalization of the statistics mechanics has been already demonstrated from the celebrated paper of Tsallis [5] based on the κ-exponential function, preserving the main features of ordinary Boltzmann-Gibbs statistical mechanics. For this reason, it has attracted the interest of many researchers who have studied its foundations and mathematical aspects [6], as well as specific applications of the theory to various fields including. quantum entanglement [7], plasma physics [8], in genomics[9]. Very recently The κ-deformed exponential function has been used by Tsallis to Predicting COVID-19 peaks around the world, [10]. In that case, in spite on their multiple applications, the Tsallis κ-deformed exponential function has been proposed empirically and does not relation with the PDMSE. However, the concept of deformed quantum mechanics has been related with a change in the linear momentum operator [11-12] which means the existence of a relationship with the PDMSE. So, in this work our deformed exponential function is related with the position dependent mass distribution which makes a great difference with the Tsallis proposal. In short, with the aim to accomplish the objective of this work in section 2 it is presented the generalization of the linear momentum operator where generalization means linear momentum operator for the PDMSE.As a result, section 3is devoted to the generalization of thermodynamic potentials and section 4 is deserved to applications where two different position dependent mass distributions are considered as well a comparative studio of our findings with other already published results.

II. THE GENERALIZED LINEAR MOMENTUM OPERATOR

2.1. Theλ-deformed quantum mechanics with position-dependent mass

The most general position-dependent mass Schrödinger equation, is given by [13]

$$-\frac{\hbar^2}{4}\left(m^\alpha(\lambda;x)\frac{d}{dx}m^\beta(x)\frac{d}{dx}m^\gamma(\lambda;x) + m^\gamma(\lambda;x)\frac{d}{dx}m^\beta(\lambda;x)\frac{d}{dx}m^\alpha(\lambda;x)\right)\psi_n(u) + V(x)\psi_n(u) = E_n\psi_n(x) \tag{1}$$

which, with$m(\lambda;x) = m_0M(\lambda;x)$and the restriction $\alpha+\beta+\gamma = -1$, may adopt different hermitian forms [14]. The Eq.(1) can be rewritten as [15]

$$\left[-\frac{d}{dx}\left(\frac{\hbar^2}{2m(\lambda;x)}\right)\frac{d}{dx} + U(x)\right]\psi_n(x) = E_n\psi_n(x) \tag{2}$$

where

$$U(x) = V(x) + \frac{\hbar^2}{4}(\beta+1)\frac{m''(\lambda;x)}{m^2(\lambda;x)} - \frac{\hbar^2}{2}[\alpha(\alpha+\beta+1)+\beta + 1]\frac{(m'(\lambda;x))^2}{m^3(\lambda;x)} \tag{3}$$

Now we are going to transform the Eq.(2) into a canonical form, namely $H = \frac{\hat{p}^2}{2m_0} + u$. To that, we rewrite the Hamiltonian in Eq.(2) as

$$\widehat{H} = \frac{d}{dx}\left(\frac{i\hbar}{\sqrt{2m(x)}}\right)\left(\frac{i\hbar}{\sqrt{2m(x)}}\right)\frac{d}{dx} + U(x) \tag{4}$$

such that

$$\widehat{H} = \left[\frac{i\hbar}{\sqrt{2m(x)}}\frac{d}{dx} + i\hbar\left(\frac{1}{\sqrt{2m(x)}}\right)'\right]\left[\frac{i\hbar}{\sqrt{2m(x)}}\frac{d}{dx}\right] + U(x) \tag{5}$$

where we have used the commutator $\left[\frac{d}{dx},\ f(x)\right] = f'(x)$ with $f(x) = \frac{i\hbar}{\sqrt{2m(x)}}$.

Thus, after some operational calculations one gets

$$\begin{aligned}\widehat{H} &= \left(\frac{i\hbar}{\sqrt{2m(\lambda;x)}}\frac{d}{dx}\right)^2 - \frac{i\hbar m'(\lambda;x)}{4m(\lambda;x)\sqrt{2m(x)}}\left(\frac{i\hbar}{\sqrt{2m(\lambda;x)}}\frac{d}{dx}\right) \\ &\quad - \left(\frac{i\hbar}{\sqrt{2m(\lambda;x)}}\frac{d}{dx}\right)\left(\frac{i\hbar m'(\lambda;x)}{4m(\lambda;x)\sqrt{2m(\lambda;x)}}\right) \\ &\quad - \frac{\hbar^2\left(\frac{m'(\lambda;x)}{4m(\lambda;x)\sqrt{m(\lambda;x)}}\right)'}{\sqrt{2m(\lambda;x)}} + U\end{aligned} \tag{6}$$

where now we have used the commutator

$$\left[F(x)\frac{d}{dx}, Q(x)\right] = F(x)Q'(x) \tag{7}$$

with $F(x) = \frac{i\hbar}{\sqrt{2m(\lambda;x)}}$ and $Q(x) = \frac{i\hbar m'(\lambda;x)}{4m(\lambda;x)\sqrt{2m(\lambda;x)}}$.

Finally, the Hamiltonian can adopt the canonical form

$$\widehat{H} = \frac{1}{2m_0}\hat{p}_\lambda^2 + u_{eff}(x) \tag{8}$$

where

$$\hat{p}_\lambda = -\frac{i\hbar}{\sqrt{M(\lambda;x)}}\frac{d}{dx} - \frac{i\hbar}{2}\left(\frac{1}{\sqrt{M(\lambda;x)}}\right)' \tag{9}$$

would be the λ-deformed (generalized) linear momentum operator and $u_{eff}(x)$ is the *effective* potential

$$u_{eff}(x) = U(x) + \frac{\hbar^2}{2m_0}\left[\left(\left(\frac{1}{2\sqrt{M(\lambda;x)}}\right)'\right)^2 + \frac{\hbar^2}{\sqrt{M(\lambda;x)}}\left(\frac{1}{2\sqrt{M(\lambda;x)}}\right)''\right] \tag{10}$$

that, after using Eq.(3), becomes

$$u_{eff}(x) = V(x) + \frac{\hbar^2}{4m_0}\left(\beta+\frac{1}{2}\right)\frac{M''(\lambda;x)}{M^2(\lambda;x)} - \frac{\hbar^2}{2m_0}\left[\alpha(\alpha+\beta+1)+\beta + \frac{9}{16}\right]\frac{\left(M'(\lambda;x)\right)^2}{M^3(\lambda;x)} \tag{11}$$

At this point, it should be noted that the particular case of constant mass $m(0;x) = m_0$ ($M(0;x) = 1$) leads to

$$\hat{p}_0 = \hat{p} \text{ and } u_{eff}(x) = V(x) \tag{12}$$

where $\hat{p} = -i\hbar(d/(dx))$ is the standard linear momentum operator.

2.2. Canonical transformation

To solve the Eq.(8)for some solvable potential $V$and mass distribution $m(\lambda;x)$, we propose the point canonical transformation

$$x_\lambda = \int\sqrt{M(\lambda;x)}dx \tag{13}$$

such that

$$\begin{aligned}&\frac{\hbar^2}{2m_0}\frac{d^2\psi}{dx_\lambda^2} - \frac{\hbar^2}{2m_0}\frac{d\ ln\sqrt{m(\lambda;x_\lambda)}}{dx_\lambda}\frac{d\psi}{dx_\lambda} - (V-E)\psi \\ &\quad - \frac{\hbar^2}{2m_0}(\beta+1)\frac{d^2\ ln\sqrt{m(\lambda;x_\lambda)}}{dx_\lambda^2}\psi \\ &+ \frac{\hbar^2}{2m_0}(4\alpha(\alpha+\beta+1)+\beta + 1)\left(\frac{d\ ln\sqrt{m(\lambda;x_\lambda)}}{dx_\lambda}\right)^2\psi = 0.\end{aligned} \tag{14}$$

After apply the similarity transformation

$$\psi = exp\left(\frac{1}{2}ln\left(\sqrt{m(\lambda;x_\lambda)}\right)\right)\phi(x_\lambda) \tag{15}$$

we have

$$\begin{aligned}&\frac{\hbar^2}{2m_0}\frac{d^2\phi}{dx_\lambda^2} - (V-E)\phi \\ &\quad - \frac{\hbar^2}{2m_0}\left(\beta+\frac{1}{2}\right)\frac{d^2\ ln\sqrt{m(\lambda;x_\lambda)}}{dx_\lambda^2}\phi \\ &+ \frac{\hbar^2}{2m_0}\left(4\alpha(\alpha+\beta+1)+\beta + \frac{3}{4}\right)\left(\frac{d\ ln\sqrt{m(\lambda;x_\lambda)}}{dx_\lambda}\right)^2\phi = 0\end{aligned} \tag{16}$$

It is worth mentioning that the particular case of good ambiguity [16]$\alpha = -1/4 \quad , \beta = -1/2$ leads to

$$\frac{\hbar^2}{2m_0}\frac{d^2\phi}{dx_\lambda^2} - (V-E)\phi = 0 \tag{17}$$

Indicating that any solvable potential $V(x)$ is related to a position-dependent mass regardless its form.
Another possibility is the case $\alpha = 0 \quad , \beta = -1$ such that

$$\frac{\hbar^2}{2m_0}\frac{d^2\phi}{dx_\lambda^2} - (V-E)\phi + \frac{\hbar^2}{2m_0}\left(\frac{d^2 ln\sqrt{m(\lambda;x_\lambda)}}{dx_\lambda^2}\right)\phi - \frac{\hbar^2}{4m_0}\left(\frac{dln\sqrt{m(\lambda;x_\lambda)}}{dx_\lambda}\right)^2\phi = 0 \tag{18}$$

which, after defining $w = -\frac{1}{2}ln\left(\sqrt{m(\lambda;x_\lambda)}\right)$ the above equation writes down as

$$-\frac{\hbar^2}{2m_0}\frac{d^2\phi}{dx_\lambda^2} + \left[V(x_\lambda) + \frac{\hbar^2}{2m_0}\left(\frac{d\,w}{dx_\lambda} + w^2\right)\right] = E\phi \tag{19}$$

in accordance with [17].
Eqs.(17) and (19) are ready to be solved for some mass distribution $m(\lambda;x)$ and interaction potential$V(x)$ [18], but for the purpose of this work, it is not necessary to solve the PDMSE.

III. GENERALIZATION OF THERMODYNAMIC POTENTIALS

3.1. The λ-deformed quantum dynamical variables with position-dependent mass

It is straightforward to show, from the generalized dynamic variables of the quantum mechanics, namely theλ-deformed linear momentum operator p_λ and the canonical transformationx_λ introduced in Eqs.(9) and (13) respectively, that the commutation relationship $[x,p] = ih$ keeps invariant under this transformation, namely

$$[x_\lambda\ , p_\lambda] = ih \tag{20}$$

Also, it is possible to introduce the generalized (λ-deformed) exponential function

$$exp_\lambda(x) = exp(x_\lambda) \tag{21}$$

fulfilling the condition

$$\lim_{\lambda\to 0} exp_\lambda(x) = exp(x) \tag{22}$$

$exp(x)$beingthe standard exponential function.
So, if there existsthe inverse function x_λ^{-1} of the canonical transformation x_λ, it is possible to get a generalized(λ-deformed) logarithmic function as follow

$$ln_\lambda(x) = x_\lambda^{-1}\big(ln(x)\big) \tag{23}$$

In fact

$$ln_\lambda(exp_\lambda(x)) = x_\lambda^{-1}\Big(ln\big(exp(x_\lambda)\big)\Big) = x_\lambda^{-1}(x_\lambda) = x \tag{24}$$

3.2. Generalized thermodynamic potentials

The canonical partition function $Z(T)$ could be considered as the corner stone in statistical physics due that all the thermodynamic functions associated to a statistical system, such as the internal energy$U$, entropy S, free energy$F$, heat capacity$C$ and others are obtained in terms of $Z(T)$ and its derivatives [19]. It is defined as

$$Z = \sum_i^W exp(-\beta\epsilon_i) \tag{25}$$

where W is the total number of microscopic configurations whose probabilities are P_i such that

$$P_i = C\ exp(-\beta\epsilon_i) \tag{26}$$

with $\beta = k/T$ and C being a normalization constant.The condition$\sum_i^W P_i = 1$ leads to

$$P_i = \frac{1}{Z}exp(-\beta\epsilon_i). \tag{27}$$

Thus, the internal energy U is

$$U = \sum_i^W P_i\,\epsilon_i = \sum_i^W \frac{1}{Z}exp(-\beta\epsilon_i)\,\epsilon_i$$

$$= -\frac{1}{Z}\sum_i^W \frac{\partial}{\partial\beta}exp(-\beta\epsilon_i)$$

$$= -\frac{\partial}{\partial\beta}lnZ \tag{28}$$

From the expression for the partition function given in Eq.(25), the λ-deformed exponential function $exp_\lambda(x)$ given Eq.(21) and the λ-deformed logarithm function $ln_\lambda(x)$ given Eq.(23), it is natural to introduce a generalized (λ-deformed) partition function Z_λ and consequently the internal energy U_λ.Namely

$$Z_\lambda = \sum_i^W exp_\lambda(-\beta\epsilon_i) \tag{29}$$

and

$$U_\lambda = -\frac{\partial}{\partial\beta}ln_\lambda(Z_\lambda) \tag{30}$$

where$ln_\lambda(x)$ is the λ-deformed logarithmic function given in Eq.(23) for some mass distribution $m(\lambda;x)$ involved is the solution of the position-dependent mass Schrödinger equation. Likewise, as the internal energy U is involved with others thermodynamic potentials, it is straightforward to calculate the corresponding generalization of them. For example [19] the Entropy$S = k\ln(Z) + k\beta U$, theHelmholtz free energy $F = -\frac{1}{\beta} ln(Z)$and theheat capacity $C = -k\beta^2 \frac{d\,U}{d\beta}$.

IV. APPLICATION TOTHERMODYNAMIC POTENTIALS

4.1. Mass distribution $m(\lambda;x) = m_0(1+\lambda x\ )^{-2}$

In this case $M(\lambda;x) = (1+\lambda x)^{-2}$ such that, from Eq.(9) and (13) the λ-deformed quantum dynamic variables are

$$\hat{p}_\lambda = -i\hbar(1+\lambda x)\frac{d}{dx} + i\hbar\frac{\lambda}{2} \tag{31}$$

$$x_\lambda = \frac{1}{\lambda} ln(1+\lambda x) \tag{32}$$

Thus,in accordance with Eqs.(13) and (21), the generalized λ-deformed exponential function is

$$exp_\lambda(x) = exp\left(\frac{1}{\lambda} ln(1+\lambda x)\right) \tag{33}$$

that is to say

$$exp_\lambda(x) = (1+\lambda x)^{\frac{1}{\lambda}} \tag{34}$$

whose inverse function is defined as the generalized λ-deformed logarithmic function

$$ln_\lambda(x) = \frac{x^\lambda\ -\ 1}{\lambda} \tag{35}$$

Then from the Eq.(29) we can write the λ-deformed partition function $Z_\lambda(T)$as

$$Z_\lambda = \sum_i^W (1-\beta\lambda\epsilon_i)^{\frac{1}{\lambda}}\,. \tag{36}$$

Hence, the generalized (λ-deformed) internal energy comes from the Eq.(30) as

$$U_\lambda = -\frac{\partial}{\partial\beta}\left(\frac{Z_\lambda^\lambda\ -\ 1}{\lambda}\right) \tag{37}$$

$$U_\lambda = -\frac{\partial}{\partial\beta}\left(\frac{\left(\sum_i^W (1-\beta\lambda\epsilon_i)^{\frac{1}{\lambda}}\right)^\lambda\ -\ 1}{\lambda}\right) \tag{38}$$

Eqs.(36) and (37) match with Eqs.(11) and (12) given in Ref.[20]by identifying a shift of the parameter λ as $\lambda \longrightarrow q-1$. It is worth mentioning that the results in [20] where obtained by solving a variational problem with suitable Lagrange parameters, while in this work where obtained straightforwardly from λ-deformed quantum variables, particularly from the transformation x_λ given in Eq.(32). In addition the limit case $\lambda\longrightarrow 0$ leads to the standard results

$$\lim_{\lambda\to 0} exp_\lambda(x) = exp(x) \tag{39}$$

$$\lim_{\lambda\to 0} ln_\lambda(x) = ln(x) \tag{40}$$

and consequently

$$\lim_{\lambda\to 0} Z_\lambda = Z \tag{41}$$

$$\lim_{\lambda\to 0} U_\lambda = U = -\frac{\partial}{\partial\beta}(lnZ). \tag{42}$$

The generalization of others thermodynamic potentials are as follow:

a.- Entropy $S_\lambda = k\,ln_\lambda(Z_\lambda) + k\beta U_\lambda$,
b.- the Helmholtz free energy $F_\lambda = -\frac{1}{\beta} ln_\lambda(Z_\lambda)$ and
thec.- the heat capacity $C_\lambda = -k\beta^2 \frac{d\,U_\lambda}{d\beta}$.

4.2. Mass distribution $m(\lambda;x) = m_0(1+\lambda^2x^2\ )^{-1}$

In this new situation the unitless mass distribution is$M(\lambda;x) = (1+\lambda^2x^2)^{-1}$ such that, from Eq.(9) and (13) the λ-deformed quantum variables are

$$\hat{p}_\lambda = -i\hbar\sqrt{1+\lambda^2x^2}\,\frac{d}{dx} - \frac{i\hbar\lambda^2 x}{2\sqrt{1+\lambda^2x^2}} \tag{43}$$

$$x_\lambda = \frac{1}{\lambda} senh^{-1}(\lambda x) \tag{44}$$

Thus, the generalized λ-deformed exponential function results fromEqs. (13) and (21) as

$$exp_\lambda(x) = exp\left(\frac{1}{\lambda} senh^{-1}(\lambda x)\right) \tag{45}$$

If we use the identity

$$senh^{-1}(x) = ln\left(x+\sqrt{x^2+1}\right) \tag{46}$$

then

$$exp_\lambda(x) = \left(\lambda x + \sqrt{\lambda^2 x^2 + 1}\right)^{\frac{1}{\lambda}} \tag{47}$$

and the corresponding inverse function is

$$ln_\lambda(x) = \frac{x^\lambda - x^{-\lambda}}{2\lambda} \tag{48}$$

Eq.(29) together with Eq.(47) leads to the λ-deformed partition function Z_λ

$$Z_\lambda = \sum_i^W \left(-\beta\epsilon_i\lambda + \sqrt{\lambda^2(\beta\epsilon_i)^2 + 1}\right)^{\frac{1}{\lambda}}. \tag{49}$$

Hence, the generalized (λ-deformed) internal energy comes from the Eq.(30) as

$$U_\lambda = -\frac{\partial}{\partial\beta}\left(\frac{\left(\sum_i^W \left(-\beta\epsilon_i\lambda + \sqrt{\lambda^2(\beta\epsilon_i)^2 + 1}\right)^{\frac{1}{\lambda}}\right)^\lambda - 1}{\lambda}\right) \tag{50}$$

Expression given in Eq.(48) can be rewritten as

$$ln_\lambda(x) = x^{-\lambda}\left(\frac{x^{2\lambda} - 1}{2\lambda}\right) \tag{51}$$

that, under the shift $2\lambda \longrightarrow 1 - q$ leads to

$$ln_{\frac{1-q}{2}}(x) = x^{-\frac{1-q}{2}}\left(\frac{x^{1-q} - 1}{1-q}\right) \tag{52}$$

from which it is possible to express the Tsallis entropyS_q[5, 21] as

$$S_q = k\frac{W^{1-q} - 1}{1-q} = k\, W^{1-q}\, ln_{\frac{1-q}{2}}(W) \tag{53}$$

with the limit case $q \longrightarrow 1$ ($\lambda \longrightarrow 0$)

$$\lim_{q\to 1} S_q = k\, ln(W). \tag{54}$$

Likewise, as expected, from expressions given in Eqs.(45) and (48) the limit case $\lambda \longrightarrow 0$ leads to the standard results

$$\lim_{\lambda\to 0} exp_\lambda(x) = exp(x) \tag{55}$$

$$\lim_{\lambda\to 0} ln_\lambda(x) = ln(x) \tag{56}$$

and consequently Eqs.(49) and (50) reduce to

$$\lim_{\lambda\to 0} Z_\lambda = Z \tag{57}$$

$$\lim_{\lambda\to 0} U_\lambda = U = -\frac{\partial}{\partial\beta}(lnZ). \tag{58}$$

Thus recovering the standard expressions for the thermodynamic potentials as Entropy S ,Helmholtz free energy$F$and the heat capacity C.

V. CONCLUDING REMARKS

The purpose of this work has been to find a class of generalized λ-deformed quantum mechanics that can be used to generalize thermodynamic potentials. To attain this objective, we have used the canonical form of the position-dependent mass Hamiltonian from where the generalized Hermitian linear momentum operator, λ-deformed,p_λ is obtained. From there, with the aim to generalize thermodynamicfunctions, it is proposed a λ-deformed exponential function and its corresponding λ-deformed logarithmic partner. With that, the generalization of thermodynamic functions is direct. That is, from the λ-deformed generalized internal energy $U_\lambda = -k\frac{\partial}{\partial\beta} ln_\lambda(Z_\lambda)$ all the other related thermodynamic functions are straightforward generalized. In order to show the usefulness of our proposal, we have considered two different position dependent mass distributions. From the application of one of them it is recovered the results of Tsallis which means that their findings are related with specific position dependent mass distributions. Our method can be easily extended to other$m(\lambda; x)$.

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