Deformed Density Matrix and Generalized Uncertainty Relation in Thermodynamics

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Abstract

A generalization of the thermodynamic uncertainty relations is proposed. It is done by introducing of an additional term proportional to the interior energy into the standard thermodynamic uncertainty relation that leads to existence of the lower limit of inverse temperature. The authors are of the opinion that the approach proposed may lead to proof of these relations. To this end, the statistical mechanics deformation at Planck scale. The statistical mechanics deformation is constructed by analogy to the earlier quantum mechanical results. As previously, the primary object is a density matrix, but now the statistical one. The obtained deformed object is referred to as a statistical density pro-matrix. This object is explicitly described, and it is demonstrated that there is a complete analogy in the construction and properties of quantum mechanics and statistical density matrices at Plank scale (i.e. density pro-matrices). It is shown that an ordinary statistical density matrix occurs in the low-temperature limit at temperatures much lower than the Plank's. The associated deformation of a canonical Gibbs distribution is given explicitly.

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1 Introduction

In this paper generalization of the thermodynamic uncertainty relations is proposed. It is done by introducing of an additional term proportional to the interior energy into the standard thermodynamic uncertainty relation that leads to existence of the lower limit of inverse temperature. Consequently, statistical mechanics at Planck scale should be deformed. As is known, at Planck scale Quantum Mechanics (QM) undergoes variation: it should be subjected to deformation also. This is realized due to the presence of the Generalized Uncertainty Relations (GUR) and hence the fundamental length [1],[2]. The deformation in Quantum Mechanics at Planck scale takes different paths: commutator deformation (Heisenberg's algebra deformation) [4],[5] or density matrix deformation [9], [10]. In the present work the second approach is extended by the authors to the Statistical Mechanics at Plank scale. To this end, a deformed statistical density matrix, also called a statistical density pro-matrix, is constructed as a complete analog to the deformed quantum mechanics matrix. In Quantum Mechanics with fundamental length (QMFL) the deformation parameter was represented by the value $\alpha = l_{min}^2/x^2$ where x is the scale, whereas in case of the Statistical Mechanics this value will be $\tau = T^2/T_{max}^2$ where T_{max} is a maximum temperature of the order of the Planck's. Existence of T_{max} follows from (GUR) for the "energy - time" pair. The limitations on the parameter variation interval are the same. In this way it is demonstrated that there exists a complete analogy in the construction and properties of quantum mechanics and statistical density matrices at Planck scale (density pro-matrices). It should be noted that an ordinary statistical density matrix appears in the low-temperature limit (at temperatures much lower than the Planck's). The associated deformation of a canonical Gibbs distribution is described explicitly.

2 Generalized Uncertainty Relation in Thermodynamics

It is well known that in thermodynamics an inequality for the pair interior energy - inverse temperature, which is completely analogous to the standard uncertainty relation in quantum mechanics [11] can be written down [12] – [14]. The only (but essential) difference of this inequality from the

quantum mechanical one is that the main quadratic fluctuation is defined by means of classical partition function rather than by quantum mechanical expectation values. In the last 14 - 15 years a lot of papers appeared in which the usual momentum-coordinate uncertainty relation has been modified at very high energies of order Planck energy E_p [1]–[7]. In this note we propose simple reasons for modifying the thermodynamic uncertainty relation at Planck energies. This modification results in existence of the minimal possible main quadratic fluctuation of the inverse temperature. Of course we assume that all the thermodynamic quantities used are properly defined so that they have physical sense at such high energies.

We start with usual Heisenberg uncertainty relations [11] for momentum - coordinate:

$$\Delta x \geq \frac{\hbar}{\Delta p}. \tag{1}$$

It was shown that at the Planck scale a high-energy term must appear:

$$\Delta x \geq \frac{\hbar}{\Delta p} + \alpha' L_p^2 \frac{\Delta p}{\hbar} \tag{2}$$

where L_p is the Planck length $L_p^2 = G\hbar/c^3 \simeq 1,6 \ 10^{-35} m$ and α' is a constant. In [3] this term is derived from the string theory, in [1] it follows from the simple estimates of Newtonian gravity and quantum mechanics, in [4] it comes from the black hole physics, other methods can also be used [5],[6]. Relation (2) is quadratic in Δp

$$\alpha' L_p^2 (\Delta p)^2 - \hbar \, \Delta x \Delta p + \hbar^2 \leq 0 \tag{3}$$

and therefore leads to the fundamental length

$$\Delta x_{min} = 2\sqrt{\alpha'} L_p \tag{4}$$

Using relations (2) it is easy to obtain a similar relation for the energy - time pair. Indeed (2) gives

$$\frac{\Delta x}{c} \geq \frac{\hbar}{\Delta pc} + \alpha' L_p^2 \frac{\Delta p}{c\hbar}, \tag{5}$$

then

$$\Delta t \geq \frac{\hbar}{\Delta E} + \alpha' \frac{L_p^2}{c^2} \frac{\Delta pc}{\hbar} = \frac{\hbar}{\Delta E} + \alpha' t_p^2 \frac{\Delta E}{\hbar}. \tag{6}$$

where the smallness of L_p is taken into account so that the difference between ΔE and $\Delta(pc)$ can be neglected and t_p is the Planck time $t_p =$

$L_p/c = \sqrt{G\hbar/c^5} \simeq 0,54\ 10^{-43}sec$. Inequality (6) gives analogously to (2) the lower boundary for time $\Delta t \geq 2t_p$ determining the fundamental time

$$\Delta t_{min} = 2\sqrt{\alpha'}t_p \qquad (7)$$

Thus, the inequalities discussed can be rewritten in a standard form

$$
\begin{cases}
\Delta x \geq \dfrac{\hbar}{\Delta p} + \alpha'\left(\dfrac{\Delta p}{P_{pl}}\right)\dfrac{\hbar}{P_{pl}} \\[4mm]
\Delta t \geq \dfrac{\hbar}{\Delta E} + \alpha'\left(\dfrac{\Delta E}{E_p}\right)\dfrac{\hbar}{E_p}
\end{cases}
\qquad (8)
$$

where $P_{pl} = E_p/c = \sqrt{\hbar c^3/G}$. Now we consider the thermodynamics uncertainty relations between the inverse temperature and interior energy of a macroscopic ensemble

$$\Delta\frac{1}{T} \geq \frac{k}{\Delta U}. \qquad (9)$$

where k is the Boltzmann constant.

N.Bohr [12] and W.Heisenberg [13] first pointed out that such kind of uncertainty principle should take place in thermodynamics. The thermodynamic uncertainty relations (9) were proved by many authors and in various ways [14]. Therefore their validity does not raise any doubts. Nevertheless, relation (9) was proved in view of the standard model of the infinite-capacity heat bath encompassing the ensemble. But it is obvious from the above inequalities that at very high energies the capacity of the heat bath can no longer to be assumed infinite at the Planck scale. Indeed, the total energy of the pair heat bath - ensemble may be arbitrary large but finite merely as the universe is born at a finite energy. Hence the quantity that can be interpreted as the temperature of the ensemble must have the upper limit and so does its main quadratic deviation. In other words the quantity $\Delta(1/T)$ must be bounded from below. But in this case an additional term should be introduced into (9)

$$\Delta\frac{1}{T} \geq \frac{k}{\Delta U} + \eta\,\Delta U \qquad (10)$$

where η is a coefficient. Dimension and symmetry reasons give

$$\eta \sim \frac{k}{E_p^2} \quad or \quad \eta = \alpha'\frac{k}{E_p^2}$$

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As in the previous cases inequality (10) leads to the fundamental (inverse) temperature.

$$T_{max} = \frac{\hbar}{2\sqrt{\alpha'}t_p k} = \frac{\hbar}{\Delta t_{min}k}, \quad \beta_{min} = \frac{1}{kT_{max}} = \frac{\Delta t_{min}}{\hbar} \qquad (11)$$

It should be noted that the same conclusion about the existence of the maximal temperature in Nature can be made also considering black hole evaporation [8].

Thus, we obtain the system of generalized uncertainty relations in a symmetric form

$$
\begin{cases}
\Delta x & \geq \quad \frac{\hbar}{\Delta p} + \alpha' \left(\frac{\Delta p}{P_{pl}} \right) \frac{\hbar}{P_{pl}} + ... \\[2ex]
\Delta t & \geq \quad \frac{\hbar}{\Delta E} + \alpha' \left(\frac{\Delta E}{E_p} \right) \frac{\hbar}{E_p} + ... \\[2ex]
\Delta \frac{1}{T} & \geq \quad \frac{k}{\Delta U} + \alpha' \left(\frac{\Delta U}{E_p} \right) \frac{k}{E_p} + ...
\end{cases} \qquad (12)
$$

or in the equivalent form

$$
\begin{cases}
\Delta x & \geq \quad \frac{\hbar}{\Delta p} + \alpha' L_p^2 \frac{\Delta p}{\hbar} + ... \\[2ex]
\Delta t & \geq \quad \frac{\hbar}{\Delta E} + \alpha' t_p^2 \frac{\Delta E}{\hbar} + ... \\[2ex]
\Delta \frac{1}{T} & \geq \quad \frac{k}{\Delta U} + \alpha' \frac{1}{T_p^2} \frac{\Delta U}{k} + ...
\end{cases} \qquad (13)
$$

where the dots mean the existence of higher order corrections as in [23]. Here T_p is the Planck temperature: $T_p = \frac{E_p}{k}$.

In the conclusion of this section we would like to note that the restriction on the heat bath made above turns the equilibrium partition function to be non-Gibbsian [15].

Note that the last inequality is symmetrical to the second one with respect to the substitution [17]

$$t \mapsto \frac{1}{T}, \hbar \mapsto k, \triangle E \mapsto \triangle U.$$

However this observation can by no means be regarded as a rigorous proof of the generalized uncertainty relation in thermodynamics.

There is a reason to believe that a rigorous justification for the last (thermodynamic) inequalities in systems (12) and (13) may be made by means of a certain deformation of Gibbs distribution.

Let us outline the main aspects of above-considered deformation. In our opinion it could be obtained as the result of density-matrix deformation in Statistical Mechanics (see [18], Section 2, Paragraph 3):

$$\rho = \sum_n \omega_n |\varphi_n><\varphi_n|, \tag{14}$$

where probability is given by

$$\omega_n = \frac{1}{Q} \exp(-\beta E_n).$$

Deformation of density matrix ρ (14) can be carried out similarly to deformation of density matrix (density pro-matrix) in Quantum Mechanics at Planck's scale (see [9],[10]). Proceeding with this analogy density matrix ρ in (14) should be changed by $\rho(\tau)$, where τ is a parameter of deformation. Deformed density matrix must fulfill the condition $\rho(\tau) \approx \rho$ when $T \ll T_p$. By analogy with [9],[10], only probabilities ω_n are subject of deformation in (14), changing by $\omega_n(\tau)$ and correspondingly deformed statistical density matrix is

$$\rho(\tau) = \sum_n \omega_n(\tau)|\varphi_n><\varphi_n|. \tag{15}$$

This approach in our opinion could give us the possibility to obtain Deformed Canonical Distribution as well as a rigorous proof of thermodynamical general uncertainty relations. In section 4 the construction of such a deformed statistical mechanics at Planck scale is demonstrated. However, first it seems expedient to outline briefly the principal features of the corresponding deformation in QM.

3 Deformation of Quantum-Mechanics Density Matrix at Planck Scale

In this section the principal features of QMFL construction with the use of the density matrix deformation are briefly outlined [10].

As mentioned above, for the fundamental deformation parameter we use $\alpha = l_{min}^2/x^2$ where x is the scale. In contrast with [10], for the deformation parameter we use α rather than β to avoid confusion, since quite a distinct value is denoted by β in Statistical Mechanics:$\beta = 1/kT$.

Definition 1. (Quantum Mechanics with Fundamental Length)
Any system in QMFL is described by a density pro-matrix of the form

$$\rho(\alpha) = \sum_{\mathbf{i}} \omega_{\mathbf{i}}(\alpha)|\mathbf{i} >< \mathbf{i}|,$$

where

1. $0 < \alpha \leq 1/4$;

2. The vectors $|i >$ form a full orthonormal system;

3. $\omega_i(\alpha) \geq 0$ and for all i the finite limit $\lim_{\alpha \to 0} \omega_i(\alpha) = \omega_i$ exists;

4. $Sp[\rho(\alpha)] = \sum_i \omega_i(\alpha) < 1$, $\sum_i \omega_i = 1$;

5. For every operator B and any α there is a mean operator B depending on α:

$$< B >_\alpha = \sum_i \omega_i(\alpha) < i|B|i > .$$

Finally, in order that our definition 1 agree with the result of section 2, the following condition must be fulfilled:

$$Sp[\rho(\alpha)] - Sp^2[\rho(\alpha)] \approx \alpha. \tag{16}$$

Hence we can find the value for $Sp[\rho(\alpha)]$ satisfying the condition of definition 1:

$$Sp[\rho(\alpha)] \approx \frac{1}{2} + \sqrt{\frac{1}{4} - \alpha}. \tag{17}$$

According to point 5), $< 1 >_\alpha = Sp[\rho(\alpha)]$. Therefore for any scalar quantity f we have $< f >_\alpha = f Sp[\rho(\alpha)]$. In particular, the mean value $< [x_\mu, p_\nu] >_\alpha$ is equal to

$$< [x_\mu, p_\nu] >_\alpha = i\hbar\delta_{\mu,\nu} Sp[\rho(\alpha)]$$

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We denote the limit $\lim_{\alpha \to 0} \rho(\alpha) = \rho$ as the density matrix. Evidently, in the limit $\alpha \to 0$ we return to QM.

As follows from definition 1, $< (j >< j) >_\alpha = \omega_j(\alpha)$, from whence the completeness condition by α is $< (\sum_i |i >< i|) >_\alpha = < 1 >_\alpha = Sp[\rho(\alpha)]$. The norm of any vector $|\psi >$ assigned to α can be defined as $< \psi|\psi >_\alpha = < \psi|(\sum_i |i >< i|)_\alpha |\psi >=< \psi|(1)_\alpha |\psi >=< \psi|\psi > Sp[\rho(\alpha)]$, where $< \psi|\psi >$ is the norm in QM, i.e. for $\alpha \to 0$. Similarly, the described theory may be interpreted using a probabilistic approach, however requiring replacement of ρ by $\rho(\alpha)$ in all formulae.

It should be noted:

I. The above limit covers both Quantum and Classical Mechanics. Indeed, since $\alpha \sim L_p^2/x^2 = G\hbar/c^3 x^2$, we obtain:

  a. $(\hbar \neq 0, x \to \infty) \Rightarrow (\alpha \to 0)$ for QM;

  b. $(\hbar \to 0, x \to \infty) \Rightarrow (\alpha \to 0)$ for Classical Mechanics;

II. As a matter of fact, the deformation parameter α should assume the value $0 < \alpha \leq 1$. However, as seen from (17), $Sp[\rho(\alpha)]$ is well defined only for $0 < \alpha \leq 1/4$, i.e. for $x = il_{min}$ and $i \geq 2$ we have no problems at all. At the point, where $x = l_{min}$, there is a singularity related to complex values assumed by $Sp[\rho(\alpha)]$, i.e. to the impossibility of obtaining a diagonalized density pro-matrix at this point over the field of real numbers. For this reason definition 1 has no sense at the point $x = l_{min}$.

III. We consider possible solutions for (1). For instance, one of the solutions of (1), at least to the first order in α, is

$$\rho^*(\alpha) = \sum_i \alpha_i exp(-\alpha)|i >< i|,$$

where all $\alpha_i > 0$ are independent of α and their sum is equal to 1. In this way $Sp[\rho^*(\alpha)] = exp(-\alpha)$. Indeed, we can easily verify that

$$Sp[\rho^*(\alpha)] - Sp^2[\rho^*(\alpha)] = \alpha + O(\alpha^2). \qquad (18)$$

Note that in the momentum representation $\alpha \sim p^2/p_{pl}^2$, where p_{pl} is the Planck momentum. When present in matrix elements, $exp(-\alpha)$

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can damp the contribution of great momenta in a perturbation theory.

IV. It is clear that within the proposed description the states with a unit probability, i.e. pure states, can appear only in the limit $\alpha \to 0$, when all $\omega_i(\alpha)$ except for one are equal to zero or when they tend to zero at this limit. In our treatment pure state are states, which can be represented in the form $|\psi><\psi|$, where $<\psi|\psi>= 1$.

V. We suppose that all the definitions concerning a density matrix can be transferred to the above-mentioned deformation of Quantum Mechanics (QMFL) through changing the density matrix ρ by the density pro-matrix $\rho(\alpha)$ and subsequent passage to the low energy limit $\alpha \to 0$. Specifically, for statistical entropy we have

$$S_\alpha = -Sp[\rho(\alpha)\ln(\rho(\alpha))]. \tag{19}$$

The quantity of S_α seems never to be equal to zero as $\ln(\rho(\alpha)) \neq 0$ and hence S_α may be equal to zero at the limit $\alpha \to 0$ only.

Some Implications:

I. If we carry out measurement on the pre-determined scale, it is impossible to regard the density pro-matrix as a density matrix with an accuracy better than particular limit $\sim 10^{-66+2n}$, where 10^{-n} is the measuring scale. In the majority of known cases this is sufficient to consider the density pro-matrix as a density matrix. But on Planck's scale, where the quantum gravitational effects and Plank energy levels cannot be neglected, the difference between $\rho(\alpha)$ and ρ should be taken into consideration.

II. Proceeding from the above, on Planck's scale the notion of Wave Function of the Universe (as introduced in [19]) has no sense, and quantum gravitation effects in this case should be described with the help of density pro-matrix $\rho(\alpha)$ only.

III. Since density pro-matrix $\rho(\alpha)$ depends on the measuring scale, evolution of the Universe within the inflation model paradigm [20] is not a unitary process, or otherwise the probabilities $p_i = \omega_i(\alpha)$ would be preserved.

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4 Deformation of Statistical Density Matrix

It follows that we have a maximum energy of the order of Planck's from an inequality (6):

$$E_{max} \sim E_p$$

Proceeding to the Statistical Mechanics, we further assume that an internal energy of any ensemble U could not be in excess of E_{max} and hence temperature T could not be in excess of $T_{max} = E_{max}/k \sim T_p$. Let us consider density matrix in Statistical Mechanics :

$$\rho_{stat} = \sum_n \omega_n |\varphi_n >< \varphi_n|, \qquad (20)$$

where the probabilities are given by

$$\omega_n = \frac{1}{Q} \exp(-\beta E_n)$$

and

$$Q = \sum_n \exp(-\beta E_n)$$

Then for a canonical Gibbs ensemble the value

$$\overline{\Delta(1/T)^2} = Sp[\rho_{stat}(\frac{1}{T})^2] - Sp^2[\rho_{stat}(\frac{1}{T})], \qquad (21)$$

is always equal to zero, and this follows from the fact that $Sp[\rho_{stat}] = 1$. However, for very high temperatures $T \gg 0$ we have $\Delta(1/T)^2 \approx 1/T^2 \geq 1/T_{max}^2$. Thus, for $T \gg 0$ a statistical density matrix ρ_{stat} should be deformed so that in the general case

$$Sp[\rho_{stat}(\frac{1}{T})^2] - Sp^2[\rho_{stat}(\frac{1}{T})] \approx \frac{1}{T_{max}^2}, \qquad (22)$$

or

$$Sp[\rho_{stat}] - Sp^2[\rho_{stat}] \approx \frac{T^2}{T_{max}^2}, \qquad (23)$$

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In this way ρ_{stat} at very high $T \gg 0$ becomes dependent on the parameter $\tau = T^2/T^2_{max}$, i.e. in the most general case

$$\rho_{stat} = \rho_{stat}(\tau)$$

and

$$Sp[\rho_{stat}(\tau)] < 1$$

and for $\tau \ll 1$ we have $\rho_{stat}(\tau) \approx \rho_{stat}$ (formula (20)) .
This situation is identical to the case associated with the deformation parameter $\alpha = l^2_{min}/x^2$ of QMFL given in section 3. That is the condition $Sp[\rho_{stat}(\tau)] < 1$ has an apparent physical meaning when:

I. At temperatures close to T_{max} some portion of information about the ensemble is inaccessible in accordance with the probability that is less than unity, i.e. incomplete probability.

II. And vice versa, the longer is the distance from T_{max} (i.e. when approximating the usual temperatures), the greater is the bulk of information and the closer is the complete probability to unity.

Therefore similar to the introduction of the deformed quantum-mechanics density matrix in section 3 of [10] and in previous section of this paper, we give the following
Definition 2. (Deformation of Statistical Mechanics)
Deformation of Gibbs distribution valid for temperatures on the order of the Planck's T_p is described by deformation of a statistical density matrix (statistical density pro-matrix) of the form

$$\rho_{\mathbf{stat}}(\tau) = \sum_{\mathbf{n}} \omega_{\mathbf{n}}(\tau)|\varphi_{\mathbf{n}} >< \varphi_{\mathbf{n}}|$$

having the deformation parameter $\tau = T^2/T^2_{max}$, where

I. $0 < \tau \leq 1/4$;

II. The vectors $|\varphi_n >$ form a full orthonormal system;

III. $\omega_n(\tau) \geq 0$ and for all n at $\tau \ll 1$ we obtain $\omega_n(\tau) \approx \omega_n = \frac{1}{Q}\exp(-\beta E_n)$
In particular, $\lim\limits_{T_{max}\to\infty(\tau\to 0)} \omega_n(\tau) = \omega_n$

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IV. $Sp[\rho_{stat}(\tau)] = \sum_n \omega_n(\tau) < 1$, $\sum_n \omega_n = 1$;

V. For every operator B and any τ there is a mean operator B depending on τ

$$< B >_\tau = \sum_n \omega_n(\tau) < n|B|n > .$$

Finally, in order that our Definition 2 agree with the formula (23), the following condition must be fulfilled:

$$Sp[\rho_{stat}(\tau)] - Sp^2[\rho_{stat}(\tau)] \approx \tau. \tag{24}$$

Hence we can find the value for $Sp[\rho_{stat}(\tau)]$ satisfying the condition of Definition 2 (similar to Definition 1):

$$Sp[\rho_{stat}(\tau)] \approx \frac{1}{2} + \sqrt{\frac{1}{4} - \tau}. \tag{25}$$

It should be noted:

I. The condition $\tau \ll 1$ means that $T \ll T_{max}$ either $T_{max} = \infty$ or both in accordance with a normal Statistical Mechanics and canonical Gibbs distribution (20)

II. Similar to QMFL in Definition 1, where the deformation parameter α should assume the value $0 < \alpha \leq 1/4$. As seen from (25), here $Sp[\rho_{stat}(\tau)]$ is well defined only for $0 < \tau \leq 1/4$. This means that the feature occurring in QMFL at the point of the fundamental length $x = l_{min}$ in the case under consideration is associated with the fact that **highest measurable temperature of the ensemble is always $T \leq \frac{1}{2}T_{max}$**.

III. The constructed deformation contains all four fundamental constants: $G, \hbar, c, k$ as $T_{max} = \varsigma T_p$, where ς is the denumerable function of α' (2) and T_p, in its turn, contains all the above-mentioned constants.

IV. Again similar to QMFL, as a possible solution for (9) we have an exponential ansatz

$$\rho^*_{stat}(\tau) = \sum_n \omega_n(\tau)|n >< n| = \sum_n exp(-\tau)\omega_n|n >< n|$$

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$$Sp[\rho_{stat}^*(\tau)] - Sp^2[\rho_{stat}^*(\tau)] = \tau + O(\tau^2). \qquad (26)$$

In such a way with the use of an exponential ansatz (26) the deformation of a canonical Gibbs distribution at Planck scale (up to factor $1/Q$) takes an elegant and completed form:

$$\omega_{\mathbf{n}}(\tau) = \mathbf{exp}(-\tau)\omega_{\mathbf{n}} = \mathbf{exp}(-\frac{\mathbf{T^2}}{\mathbf{T_{max}^2}} - \beta\mathbf{E_n}) \qquad (27)$$

where $T_{max} = \varsigma T_p$

5   Conclusion

It has been demonstrated that a nature of deformations in Quantum and Statistical Mechanics at Plank scale is essentially identical. Still further studies are required to look into variations of the formulae for entropy and other quantities in this deformed Statistical Mechanics. Of particular interest is the problem of a rigorous proof for the Generalized Uncertainty Relations (GUR) in Thermodynamics (section 2 of the present paper and [16],[21]) as a complete analog of the corresponding relations in Quantum Mechanics [1], [3, 4, 5, 6], in turn necessitating the deformation of Gibbs distribution. The present paper as an integration of [21],[22]is aimed at the solution of this problem.

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