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QUANTUM-MECHANICAL ANALOG OF THE ZEROTH LAW OF THERMODYNAMICS (TO THE PROBLEM OF INCORPORATING THERMODYNAMICS INTO THE QUANTUM-MECHANICAL THEORY)[1]

The presented approach to incorporate the stochastic thermodynamics into the quantum theory is based on the idea, proposed earlier by the authors, to consistently consider the stochastic influence by the environment considered as the whole and described by the wave functions of arbitrary vacua. In this research, a possibility of the explicit incorporation of the zeroth law of stochastic thermodynamics into the quantum-mechanical theory in the form of the saturated Schrödinger uncertainty relation is realized. This allows a comparative analysis between the sets of arbitrary vacuum states, namely, squeezed coherent (SCSs) and correlated coherent (CCSs) states, to be carried out. A possibility to establish a relation between SCSs and CCSs, on the one hand, and thermal states, on the other hand, is discussed.

K e y w o r d s: uncertainty relation, thermal equilibrium, the zeroth law, invariance, squeezed coherent states, correlated coherent states.

1. Introduction

The concept of thermal equilibrium in thermodynamics is usually associated with the zeroth law, i.e. with the equality – at least, on the average – between the Kelvin temperatures of the object, T, and the environment, T_0, the latter being related to a model of classical thermostat. At the zero temperature, the concept of thermal equilibrium cannot be introduced, of course, because no thermostat in the conventional representation, i.e. as a warm environment, is meant. Under those conditions, the stochastic thermal influence of the environment is not taken into account, and the quantum stochastic influence of the environment is naturally not considered in thermodynamics.

Meanwhile, at low enough temperatures, when the thermal action of the environment has already to be taken into consideration, the quantum stochastic influence remains to be a significant factor. Hence, the simultaneous thermal and quantum fluctuations, which are non-additive, emerge. To describe this situation arising at low temperatures, we introduced the concept of quantum thermostat as a model of the environment (in terms of quantum mechanics, this is an arbitrary vacuum). In order to extend the concept of

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thermal equilibrium to the case of the contact with the quantum thermostat, we also introduced [1], on the basis of empirical reasons, the effective temperature

$$\mathbb{T} = \frac{\hbar\omega}{2k_{\mathrm{B}}} \coth \frac{\hbar\omega}{2k_{\mathrm{B}}T}, \qquad (1)$$

where k_{B} is the Boltzmann constant, and T the Kelvin temperature. We also proposed the generalized zeroth law in the form

$$\mathbb{T} = \mathbb{T}_0 \pm \Delta\mathbb{T}, \qquad (2)$$

where $\mathbb{T}_0$ is the effective temperature of the quantum thermostat, and $\Delta\mathbb{T}$ the standard deviation of the effective object temperature. In the limit as the Kelvin temperature $T \to 0$, this relation keeps its sense as a condition of equilibrium with the cold vacuum and acquires the form

$$\mathbb{T}^{\min} = \mathbb{T}_0^{\min} \pm \Delta\mathbb{T}^{\min}, \qquad (3)$$

where $\mathbb{T}_0^{\min} \equiv \frac{\hbar\omega}{2k_{\mathrm{B}}} \neq 0$ is the minimum effective temperature for a normal vacuum mode with frequency ω.

Now, let us consider a possibility for expression (2) to have a fundamental interpretation at the microscopic level. To this end, let us consider the Hamiltonian of an arbitrary vacuum introduced by us in work [1]:

$$\hat{\mathfrak{H}}_{\tau,\varphi} = \hat{\mathcal{H}}_{\tau,\varphi} - \hat{\mathfrak{H}}_{\tau,\varphi}^{\mathrm{inf}}. \qquad (4)$$

In this expression, $\hat{\mathcal{H}}_{\tau,\varphi}$ is the Hamiltonian of the system simulated as a quantum oscillator with the frequency ω_0, and $\hat{\mathfrak{H}}_{\tau,\varphi}^{\mathrm{inf}}$ is the energy operator of the entire, i.e. quantum and thermal, stochastic influence of the environment on the oscillator at an arbitrary Kelvin temperature. Recall that the subscripts τ and φ are the parameters of the Bogoliubov (u,v)-transformation, which allow a transition from the initial (cold) to arbitrary vacuum (including the warm one) to be made,

$$u = \cosh\tau \cdot e^{i\varphi}; \quad v = \sinh\tau \cdot e^{-i\varphi}. \qquad (5)$$

In terms of these parameters, the Hamiltonian $\hat{\mathcal{H}}_{\tau,\varphi}$ in Eq. (4) is expressed as follows:

$$\hat{\mathcal{H}}_{\tau,\varphi} \equiv (\cosh 2\tau - \sinh 2\tau \cdot \cos 2\varphi)\hat{K}_{\tau,\varphi} +$$

$$+(\cosh 2\tau + \sinh 2\tau \cdot \cos 2\varphi)\hat{\Pi}_{\tau,\varphi}, \qquad (6)$$

where $\hat{K}_{\tau,\varphi}$ and $\hat{\Pi}_{\tau,\varphi}$ are the operators of the kinetic and potential energies, respectively.

The second operator, $\hat{\mathfrak{H}}_{\tau,\varphi}^{\mathrm{inf}}$, in Eq. (4) consists of two terms corresponding to the contributions of the purely quantum action of cold vacuum, $\hat{\jmath}_0 = \frac{\hbar}{2}\hat{I}$, and the additional action $\hat{\sigma}_{\tau,\varphi}$ arising at the transition from the initial cold vacuum (i.e. at the environment temperature $T = 0$) to an arbitrary one, for which nonzero temperatures of the environment are allowed. In this case,

$$\hat{\mathfrak{H}}_{\tau,\varphi}^{\mathrm{inf}} = \omega\hat{\jmath}_0 + \omega\hat{\sigma}_{\tau,\varphi}, \qquad (7)$$

where

$$\hat{\sigma}_{\tau,\varphi} \equiv (\sinh 2\tau \cdot \sin 2\varphi)\frac{1}{2}(\hat{p}\hat{q} + \hat{q}\hat{p}). \qquad (8)$$

Of course, at $\tau = 0$ and $\varphi = 0$, operator (7) transforms into the energy operator for the initial cold vacuum.

In what follows, to calculate the average value of operator (4), we use the complex wave function of an arbitrary vacuum $\psi_{\tau,\varphi}$. In the coordinate representation, it looks like

$$\psi_{\tau,\varphi}(q,\omega) = \left[2\pi(\,\Delta q_{\tau,\varphi})^2\right]^{-1/4} \times$$

$$\times \exp\left\{-\frac{q^2}{4(\Delta q_{\tau,\varphi})^2}(1 - i\beta_{\tau,\varphi})\right\}, \qquad (9)$$

where $(\Delta q_{\tau,\varphi})^2$ is the coordinate variance for an arbitrary vacuum, and $\beta_{\tau,\varphi}$ is an important parameter determining the wave function phase. Function (9) is the eigenfunction of the Hamiltonian of an arbitrary vacuum $\hat{\mathfrak{H}}_{\tau,\varphi}$ (4) corresponding to its zero eigenvalue [2],

$$\hat{\mathfrak{H}}_{\tau,\varphi}\psi_{\tau,\varphi}(q,\omega) = 0 \cdot \psi_{\tau,\varphi}(q,\omega) = 0.$$

The quantities $(\Delta q_{\tau,\varphi})^2$ and $\beta_{\tau,\varphi}$ in Eq. (9) are expressed in terms of the parameters τ and φ as follows:

$$(\Delta q_{\tau,\varphi})^2 = (\Delta q_0)^2(\cosh 2\tau - \sinh 2\tau \cdot \cos 2\varphi);$$

$$(\Delta q_0)^2 = \frac{\hbar}{2\omega_0}; \qquad (10)$$

$$\beta_{\tau,\varphi} = \sinh 2\tau \cdot \sin 2\varphi.$$

The momentum variance in the state $|\psi_{\tau,\varphi}(q,\omega)\rangle$ looks like

$$(\Delta p_{\tau,\varphi})^2 = (\Delta p_0)^2(\cosh 2\tau + \sinh 2\tau \cdot \cos 2\varphi), \quad (11)$$

where $(\Delta p_0)^2 = \dfrac{\hbar\omega_0}{2}$.

In this work, we continue our studies concerning the criteria that would allow the states corresponding to the thermal equilibrium with an arbitrary vacuum to be separated from the set of states $\psi_{\tau,\varphi}(q,\omega)$ generated by the Bogoliubov (u,v)-transformation. Squeezed (SCSs) and correlated coherent states (CCSs) are candidates for this role, because the expressions for the internal energy of a quantum oscillator in those states can be transformed to the form coinciding with Planck's formula $U_T = \frac{\hbar\omega}{2}\coth\frac{\hbar\omega}{2k_BT}$ for the state of equilibrium, where k_B is the Boltzmann constant, and T the Kelvin temperature. For this purpose, we can formally put the parameter τ into relation with the temperature as

$$\cosh 2\tau \equiv \coth\left(\frac{\hbar\omega}{2kT}\right); \quad \sinh 2\tau \equiv \left(\sinh\frac{\hbar\omega}{2kT}\right)^{-1} (12)$$

and get convinced in the formal similarity between the obtained and Planck results. However, the fundamental concept of temperature has no prototype in the microworld, being associated with the idea of thermal equilibrium. Therefore, the procedure of introducing a temperature-dependent parameter different from τ still does not allow one to make an ultimate conclusion concerning the equilibrium character of the given states, as well as a possibility to interpret them as analogs of the thermal ones. Hence, our aim consists in the formulation of some condition with the use of quantum language. This condition should be similar to that adopted in thermodynamics for the thermal equilibrium with a thermostat at the temperature T. We will also verify that this condition is obeyed in the SCS and CCS cases.

2. Analysis of Squeezed Coherent States of an Arbitrary Vacuum

In work [2], we have already pointed to the fact that SCSs can be considered as thermal ones only conditionally, bearing in mind that they can be associated in thermodynamics only with the cases of contact with a cold vacuum, i.e. at the Kelvin temperature $T = 0$. Here are additional arguments in favor of this statement, which are based on the research of the form of the Schrödinger uncertainty relation (UR) for those states.

In SCSs, where $\varphi = 0$, the wave function (9) becomes real-valued because $\beta_{\tau,\varphi}$ vanishes; it will be designated as $\psi_{\tau,0} \equiv \psi_0$. Substituting relations (12) into formula (6), we formally change the parametrization of the Hamiltonian of the system. However, as will be shown below, despite that we introduce another notation for it, $\hat{\mathcal{H}}_\tau \equiv \hat{\mathcal{H}}_{\tau,0}$ instead of $\hat{\mathcal{H}}_{\tau,\varphi}$, this operation turns out to be physically senseless. Really, putting the oscillator mass $m = 1$, we obtain in this case that

$$\hat{\mathcal{H}}_\tau = \left[\coth\frac{\hbar\omega}{2k_BT} - \left(\sinh\frac{\hbar\omega}{2k_BT}\right)^{-1}\right]\frac{1}{2}\hat{p}^2 +$$

$$+ \left[\coth\frac{\hbar\omega}{2k_BT} + \left(\sinh\frac{\hbar\omega}{2k_BT}\right)^{-1}\right]\frac{1}{2}\omega^2\hat{q}^2. \quad (13)$$

Now, the operator $\hat{\sigma}_{\tau,0} \equiv (\sinh 2\tau \cdot \sin 2\varphi)\frac{1}{2}(\hat{p}\,\hat{q} + \hat{q}\hat{p})\big|_{\varphi=0}$ in formula (7), which is responsible for the correlation between the coordinate and momentum fluctuations, becomes equal to zero, because $\sin 2\varphi = 0$. As a result, the stochastic influence is characterized only by the operator $\hat{\jmath}_0$ typical of the initial cold vacuum, so that expression (7) is simplified to $H_{\tau,\varphi}^{\inf} = \omega\hat{\jmath}_0$.

Taking into account that the average value of the Hamiltonian of the vacuum $\hat{\mathfrak{H}}_{\tau,\varphi}$ equals zero, formula (4) yields the equality

$$\langle\psi_\tau|\hat{\mathcal{H}}_\tau|\psi_\tau\rangle = \langle\psi_\tau|\omega\hat{\jmath}_0|\psi_\tau\rangle. \quad (14)$$

It is worth noting that the left- and right-hand sides of expression (14) contain physically different quantities: $\mathcal{H}_\tau$ characterizes the system represented by a quantum oscillator, whereas $\hat{\jmath}_0$ describes its environment. Therefore, equality (14) means that the average energy of the system (the oscillator) coincides with the average energy of a quantum action of the environment. This statement formulated in the quantum language is actually equivalent to the zeroth law of thermodynamics for the limiting case of contact between the system and the cold vacuum.

From formulas (14) and (13), it follows that

$$\left[\cosh^2\left(\frac{\hbar\omega}{2k_\mathrm{B}T}\right) - \left(\sinh^2\left(\frac{\hbar\omega}{2k_\mathrm{B}T}\right)\right)^{-1}\right]\mathbb{U}_0 = \frac{\hbar\omega}{2}. \quad (15)$$

Note, however, that the expression in the square brackets in Eq. (15) is identically equal to 1, so that $\mathbb{U}_0 = \langle\psi_0|\hat{\mathcal{H}}_0|\psi_0\rangle = \dfrac{\hbar\omega}{2}$, the average energy of an oscillator in the cold vacuum. Hence, this expression does not depend on the parameter T. Therefore, the parameter T cannot be interpreted as the temperature. In other words, the expediency to change the parametrization given in the form (12) expectedly turns out to be rather doubtful. At the same time, this operation allows some useful information to be extracted from Eq. (15). For instance, in view of the comments to formulas (10) and (11), we may assert that

$$\frac{\mathbb{U}_0}{\omega} = \Delta q_0 \cdot \Delta p_0 = (\mathcal{UP})_0,$$

where the notation $(\mathcal{UP})_0$ is introduced for the uncertainties product $\Delta p_0 \cdot \Delta q_0$. Then, formula (15) is, in essence, a particular realization of the Schrödinger UR, namely the saturated Heisenberg UR,

$$(\mathcal{UP})_0 = \frac{\hbar}{2},$$

which is not related to thermal effects any way.

Hence, the set of SCSs describes a specific case of the equilibrium between the system and the cold vacuum only, i.e., at $T = 0$; this situation corresponds to a system that is isolated as much as possible (from the nonclassical viewpoint), i.e. to a system subjected to the stochastic quantum influence only. In other words, it is incorrect to raise the issue of equilibrium for an SCS at any nonzero Kelvin temperature, which has a standard physical sense, in the framework of the zeroth law of thermodynamics. In this case, there is no "warm" thermostat, which could provide a thermal contact. This fact confirms the conclusion that it may be not occasionally that Umezawa did not call the squeezed states as truly thermal, but only thermal-like ones.

In such a way, we come to the conclusion that the saturation of UR in the Heisenberg form is still not a sufficient condition for the description of a thermal equilibrium at $T \neq 0$. Below, we will demonstrate that it is the Schrödinger UR that plays this role.

3. Analysis of the Correlated Coherent States of an Arbitrary Vacuum on the Basis of the Schrödinger Uncertainty Relation

A different situation arises for CCSs, because the parameter $\varphi = \pi/4$. In this case, the average value of Hamiltonian (4) of the vacuum equals zero, and we obtain the relation

$$\langle\psi_{\tau,\varphi}|\mathcal{H}|\psi_{\tau,\varphi}\rangle = \langle\psi_{\tau,\varphi}|\mathfrak{H}^{\mathrm{inf}}|\psi_{\tau,\varphi}\rangle. \quad (16)$$

Here, according to (7) and (8), the operator $\mathfrak{H}^{\mathrm{inf}}$ contains two nonzero terms. If we now change the parametrization and introduce the temperature according to formula (12), expressions (10) and (11) for variances look like

$$(\Delta q_T)^2 = (\Delta q_0)^2 \coth\left(\frac{\hbar\omega}{2k_\mathrm{B}T}\right) = \frac{\hbar\omega_0}{2}\coth\left(\frac{\hbar\omega}{2k_\mathrm{B}T}\right);$$

$$(\Delta p_T)^2 = (\Delta p_0)^2 \coth\left(\frac{\hbar\omega}{2k_\mathrm{B}T}\right) = \frac{\hbar}{2\omega_0}\coth\left(\frac{\hbar\omega}{2k_\mathrm{B}T}\right). \quad (17)$$

Respectively, after a similar operation, we can calculate the product of variances $(\mathcal{UP})_T$

$$(\mathcal{UP})_T = (\Delta q_T)(\Delta p_T) = \frac{\hbar}{2}\coth\left(\frac{\hbar\omega}{2k_\mathrm{B}T}\right) = \frac{\mathbb{U}_{\mathrm{Pl}}}{\omega}, \quad (18)$$

where $\mathbb{U}_{\mathrm{Pl}} = \frac{\hbar\omega}{2}\coth\left(\frac{\hbar}{2k_\mathrm{B}}\frac{\omega}{T}\right)$ is Planck's energy of the oscillator.

Thus, the left-hand side of (16) takes the form

$$\langle\psi_{\tau,\varphi}|\hat{\mathcal{H}}|\psi_{\tau,\varphi}\rangle = \frac{\hbar\omega}{2}\coth 2\tau = \omega(\mathcal{UP})_T. \quad (19)$$

The operator of additional influence $\hat{\sigma}_{\tau,\varphi}$ (8), which enters the right-hand side of (16) and is responsible for the correlation of fluctuations of the coordinate and the momentum, transforms (at $\varphi = \frac{\pi}{4}$) into the form

$$\hat{\sigma}_T \equiv (\sinh 2\tau \cdot \sin 2\varphi)\frac{1}{2}(\hat{p}\,\hat{q} + \hat{q}\hat{p}) =$$

$$= \left[\frac{\hbar}{2}\frac{1}{\sinh}\frac{\hbar\omega}{2k_\mathrm{B}T}\right]\frac{1}{2}(\hat{p}\,\hat{q} + \hat{q}\hat{p}). \quad (20)$$

In view of (7) and (20), we obtain the modulus of the complex-valued quantity on the right-hand side of expression (16) as

$$\mathbb{J}_T^2 = \left|\langle\psi_{\tau,\varphi}|\hat{\mathfrak{H}}^{inf}|\psi_{\tau,\varphi}\rangle\right|^2 = \sigma_T^2 + \mathbb{J}_{\mathrm{qu}}^2 =$$

$$+ \left[\frac{\hbar}{2}\frac{1}{\sinh\frac{\hbar\omega}{2k_\mathrm{B}T}}\right]^2 + \left(\frac{\hbar}{2}\right)^2 = \left[\frac{\hbar}{2}\coth\left(\frac{\hbar\omega}{2k_\mathrm{B}T}\right)\right]^2. \quad (21)$$

Here, the quantity $\mathbb{J}_T = \frac{\hbar}{2} \operatorname{cth} \frac{\hbar\omega}{2k_{\mathrm{B}}T}$ is a macroparameter and has a sense of the holistic (i.e., thermal and quantum) effective stochastic influence from the side of the environment. On the microlevel, this corresponds an arbitrary vacuum and the Hermitian operators $\hat{\sigma}_T$ and $\hat{j}_0$.

With regard for formulas (17) and (19) and with the use of the notation $(\Delta p_T)(\Delta q_T) \equiv (\mathcal{UP})_T$, for the product of variances, the left-hand side of equality (16) takes the form

$$\langle \psi_{\tau,\varphi} | \hat{\mathcal{H}} | \psi_{\tau,\varphi} \rangle = \frac{\hbar\omega}{2} \coth\left(\frac{\hbar\omega}{2k_B T}\right) = \omega(\mathcal{UP})_T. \quad (22)$$

Thus, by comparing formulas (21) and (22), we may conclude that equality (16), which is typical of an arbitrary vacuum with the wave function ψ_T, is nothing else but a saturated Schrödinger uncertainty relation (SUR),

$$\omega^2(\mathcal{UP})_T^2 = \left| \langle \psi_T | \mathfrak{H}^{\mathrm{inf}} | \psi_T \rangle \right|^2. \quad (23)$$

At the same time, the direct comparison of the right-hand sides of formulas (21) and (22) allows the same formula (16) to be presented in the form

$$(\mathcal{UP})_T = \mathbb{J}_T. \quad (24)$$

It should be emphasized that the left- and right-hand sides of formula (24), which are determined by expressions (21) and (22), have different physical meanings, despite that their dimensionalities are identical. The quantity $(\mathcal{UP})_T$ can be interpreted as the response $\mathbb{J}_{\mathrm{syst}}$ of the system to the stochastic influence of the environment, $\mathbb{J}_T$, so that there is ultimately the equality between the action on the system and its response,

$$\mathbb{J}_{\mathrm{syst}} = \mathbb{J}_T. \quad (25)$$

We note that this relation can be interpreted as a thermodynamic analog of Newton's third law. By applying the general Boltzmann formula for the effective stochastic influence, $\mathbb{J} = \frac{k_{\mathrm{B}}}{\omega} \cdot \mathbb{T}$, to the left- (for the system) and the right-hand (for the quantum thermostat) side of Eq. (25), we arrive at the relation $\mathbb{T}_{\mathrm{syst}} = \mathbb{T}_T$ which is the zeroth law of stochastic thermodynamics written down for the effective temperatures of the environment and the object. Thus, the saturated SUR (23) for thermal CCSs, being closely connected with the fundamental description at the microscopic level, acquires the status of a quantum-mechanical analog of the zeroth law of stochastic thermodynamics. Therefore, equality (23) represents the essential requirement of the modified theory.

In connection with the zeroth law written down in form (24), we would like to point out the following circumstance that emphasizes the essential role of the wave function phase. Really, the right-hand side of Eq. (24) contains the contribution of an action of the quantum-thermostat:

$$(\mathbb{J}_T) = \sqrt{\left(\frac{\hbar}{2} \frac{1}{\sinh \frac{\hbar\omega}{2k_{\mathrm{B}}T}}\right)^2 + \left(\frac{\hbar}{2}\right)^2}. \quad (26)$$

The first term in this expression is determined by the average value of operator $\hat{\sigma}_T$ dependent on the wave function phase. It is easy to see that, except for the case $T \to 0$, it is the wave function phase that mainly determines the right-hand side of Eq. (26). Its role is especially significant at high temperatures, when the corresponding term takes the form

$$\left(\frac{\hbar}{2} \frac{1}{\sinh \frac{\hbar\omega}{2k_{\mathrm{B}}T}}\right)^2 \to \left(\frac{k_{\mathrm{B}}T}{\omega}\right)^2 \gg \left(\frac{\hbar}{2}\right)^2.$$

In this case, the zeroth law (24) itself is reduced to the condition of the equality between the Kelvin temperatures, $T = T_0$ (T_0 is the temperature of a thermostat), which is adopted as a definition of thermal equilibrium in classical thermodynamics and quantum statistical mechanics. It is of importance, however, to emphasize that, even in the cases where the fluctuations of the temperature of the system can be neglected in a zeroth approximation – e.g., when the system consists of a large number of particles, – the temperature definition, which is adequate to its limiting (asymptotic) sense, looks like

$$T \to \frac{\omega}{k_{\mathrm{B}}} (\mathcal{UP})_T. \quad (27)$$

Hence, this quantity depends on the momentum and coordinate uncertainties, which testifies to its inherently stochastic character.

If the phase is absent – e.g., when we use the real-valued wave functions of the SCS type – formula (25) reads

$$\mathbb{J}_{\mathrm{syst}} = \mathbb{J}_{\mathrm{qu}}, \quad (28)$$

where $\mathbb{J}_{\mathrm{qu}} = \frac{\hbar}{2}$ is the quantum action. In this case, the zeroth law does not depend on the parameter T, which allows, as was indicated above, the "thermal" equilibrium to be fixed only with the cold vacuum, i.e. to be interpreted in a "Pickwickian" sense.

Hence, two requirements – the definition of vacuum and the coincidence of the expression for the internal energy of a quantum oscillator formally written down in terms of the parameter T with Planck's formula – turn out to be insufficient for the description of the thermal equilibrium with an arbitrary vacuum. At the same time, both sets of SCS and CCS states satisfy those requirements. However, only the saturated Schrödinger UR makes allowance for the thermal action at the microscopic level. Therefore, we can ascribe a physical meaning adequate to the temperature concept to the quantity T only in the case of CCSs of the type $\left|\psi_{\tau,\varphi}\right\rangle = \left|\psi_{\tau,\frac{\pi}{4}}\right\rangle \equiv \left|\psi_T\right\rangle$, which can be regarded as "thermal" CCSs. In other words, to separate the states that characterize the thermal equilibrium with an arbitrary vacuum (at $T \neq 0$) from all the states generated by the Bogoliubov (u, v)-transformations, one more obligatory requirement must be introduced. Its essence consists in that the equivalent of the zeroth law of thermodynamic in the form of saturated SUR,

$$\Delta p \cdot \Delta q = \left|\langle\psi|\hat{p}\cdot\hat{q}|\psi\rangle\right|.$$

is included into the apparatus of quantum theory. In the "warm" vacuum state $\left|\psi_T(q)\right\rangle$, it is reduced to the condition

$$(\mathcal{U}\mathcal{P})_T = \frac{\hbar}{2}\coth\left(\frac{\hbar\omega}{2k_{\mathrm{B}}T_0}\right),$$

where we explicitly wrote down the Kelvin temperature of the thermostat, T_0. Note that the left- and right-hand sides of this equality includes, respectively, object's parameters and those of the environment.

4. Invariance of the Zeroth Law of Stochastic Thermodynamics

Let us now analyze the fundamental formulation of the zeroth law, which was obtained above, from the viewpoint of its invariance with respect to the Bogoliubov (u, v)-transformations. One should pay attention once more that the left- and the right-hand side of the corresponding equalities contain qualitatively different physical quantities, the dimensionalities of which, nevertheless, coincide. In particular, formula (24) means that, at the zero temperature,

$$(\mathcal{U}\mathcal{P})_0 \equiv \Delta p_0 \cdot \Delta q_0 = \frac{\hbar}{2} = \mathbb{J}_{\mathrm{qu}}, \tag{29}$$

where $(UP)_0$ is considered as a holistic quantity that characterizes the system under investigation.

Recall that the (u, v)-transformations preserving the canonical permutation relations have the sense of transformations for two symmetry groups simultaneously; these are the group $SU(1, 1)$ and its locally isomorphic Lorentz group $O(2, 1)$, the both having the common invariant $\hbar^2/4$. Let us discuss the influence of the corresponding invariance on the quantities that enter the left- and right-hand sides of formula (29). As follows from the aforesaid, the expression on the right-hand side of Eq. (29) is not changed if we apply the transformations with real u and v parameters to it, i.e. if $\varphi = 0$ in formula (5). It is so because, in this case, the average value of the operator of quantum-thermal stochastic influence $\hat{\sigma}$ remains equal to zero at any value of the parameter τ. At the same time, the invariant expression on the left-hand side of Eq. (29) can have different forms depending on the choice of the parameter $\tau \neq 0$. In other words, the general expression for the quantity $(\mathcal{U}\mathcal{P})^2$ may look like

$$\left.(\mathcal{U}\mathcal{P})^2\right|_T = \left.(\mathcal{U}\mathcal{P})^2\right|_{T=0}\left(\cosh^2 2\tau - \sinh^2 2\tau\right) = \left(\frac{\hbar}{2}\right)^2, \tag{30}$$

which corresponds to different ways of SCS realization.

In view of formulas (12), expression (30) can be written down as a determinant

$$\left.(\mathcal{U}\mathcal{P})^2\right|_T = \left.(\mathcal{U}\mathcal{P})^2\right|_{T=0} \times$$

$$\times \left|\begin{pmatrix}\left(\coth\frac{\hbar\omega}{2kT} + \frac{1}{\sinh\frac{\hbar\omega}{2kT}}\right) & 0 \\ 0 & \left(\coth\frac{\hbar\omega}{2kT} - \frac{1}{\sinh\frac{\hbar\omega}{2kT}}\right)\end{pmatrix}\right| =$$

$$= \left|\begin{matrix}(\Delta p_T)^2 & 0 \\ 0 & (\Delta q_T)^2\end{matrix}\right| = \left(\frac{\hbar}{2}\right)^2. \tag{31}$$

If the momentum and coordinate variances are calculated by the averaging with the use of a real-valued wave function obtained from formula (9) at $\beta_{\tau,\varphi} = 0$ and called thermal-like, then, according to Umezawa, we deal with single-mode squeezed states [3].

While attempting to generalize formula (31), Umezawa [3] introduced two independent sets of quanta: ordinary quanta are associated with the conventional annihilation, $\hat{a}$, and creation, $\hat{a}^+$, operators; and the so-called thermal quanta are associated with the tilded operators $\hat{\tilde{a}}$ and $\hat{\tilde{a}}^+$. In such a manner, he doubled the Hilbert space, which allowed him to introduce two-mode squeezed states. They can be obtained on the basis of creation operators constructed with the help of the Bogoliubov (u, v)-transformations, which entangle the operators from two sets introduced by Umezawa. As a result, expression (30) reads

$$(\mathcal{UP})^2 = \begin{vmatrix} (\Delta\hat{p})_T^2 & (\Delta\hat{p}\,\Delta\hat{\tilde{p}})_T \\ (\Delta\hat{q}\,\Delta\hat{\tilde{q}})_T & (\Delta\hat{q})_T^2 \end{vmatrix} = \left(\frac{\hbar}{2}\right)^2, \qquad (32)$$

where the averaging is carried out over the thermal-like states, as in formula (31).

It is worth emphasizing that the off-diagonal members in determinant (32) have the form of correlators between the homogeneous quantities, $(\hat{p}, \hat{\tilde{p}})$ or $(\hat{q}, \hat{\tilde{q}})$, but the correlators between the heterogeneous quantities, $(\hat{p}, \hat{q})$ and so on, remaining equal to zero at that. Therefore, the right-hand side of equality (29) is not changed, which means that the introduced states are squeezed.

Note also that the quantities entering formulas (31) and (32) are averaged with the use of real wave functions. At the same time, in Umezawa's opinion, similar results can also be obtained with the help of a real density matrix. Recently, Park [4] has undertaken a successful attempt of this kind with respect to a quantum oscillator in the thermal equilibrium. He proposed a procedure to calculate the members of determinant in formula (32) by averaging with the Gibbs–von Neumann density operator

$$\hat{\rho}_T = Z^{-1} \exp\left[-\frac{\hbar\omega}{2k_\mathrm{B}T} \left(\hat{N}_a + \frac{1}{2}\hat{I} \right) \right], \qquad (33)$$

where $Z = \mathrm{Sp}\,\exp\left[-\frac{\hbar\omega}{2k_\mathrm{B}T} \left(\hat{N}_a + \frac{1}{2}\hat{I} \right) \right]$, and $\hat{I}$ is the unit operator. The result obtained by Park allows

determinant (32) to be written down in the form

$$(\mathcal{UP})^2 = \begin{vmatrix} \mathrm{Sp}[(\Delta\hat{p})^2\hat{\rho}_T] & \mathrm{Sp}[\Delta\hat{p}\Delta\hat{\rho}_T^{\frac{1}{2}}\Delta\hat{p}\Delta\hat{\rho}_T^{\frac{1}{2}}] \\ \mathrm{Sp}[\Delta\hat{q}\Delta\hat{\rho}_T^{\frac{1}{2}}\Delta\hat{q}\Delta\hat{\rho}_T^{\frac{1}{2}}] & \mathrm{Sp}[(\Delta\hat{q})^2\hat{\rho}_T] \end{vmatrix}. \qquad (34)$$

We would like to attract attention that Park, to provide the invariance of $\mathcal{UP}$, added off-diagonal terms, which are absent in the traditional approaches to calculate $\mathcal{UP}$. From the mathematical viewpoint, the necessity of such a generalization is associated with the fact that, in this case, the operator pairs $(\Delta\hat{p})^2$ and $\hat{\rho}_T$ or $(\Delta\hat{q})^2$ and $\hat{\rho}_T$ under the trace operator do not commute. Therefore, the method used to calculate variances in the classical probability theory or in quantum mechanics, in which pure states are applied, has to be generalized; this was convincingly demonstrated as early as in the work by Wigner and Yanase [5].

According to Park, the off-diagonal members in determinant (34) can be transformed using formula (33) and the commutation rules

$$\hat{\rho}_T^{\frac{1}{2}}\,\hat{a} = \exp\left(\frac{\hbar\omega}{2k_\mathrm{B}T}\right)\hat{a}\hat{\rho}_T^{\frac{1}{2}}; \quad \hat{\rho}_T^{\frac{1}{2}}\,\hat{a}^+ = \exp\left(\frac{\hbar\omega}{2k_\mathrm{B}T}\right)\hat{a}^+\hat{\rho}_T^{\frac{1}{2}}. \qquad (35)$$

For this purpose, we have to take into account that $\overline{(\Delta\hat{p})^2} = \overline{(\hat{p})^2}$ and $\overline{(\Delta\hat{q})^2} = \overline{(\hat{q})^2}$ in this case and express $\hat{p}$ and $\hat{q}$ in terms of $\hat{a}$ and $\hat{a}^+$. As a result, we obtain

$$\mathrm{Sp}[\hat{p}\hat{\rho}_T^{\frac{1}{2}}\hat{p}\hat{\rho}_T^{\frac{1}{2}}] = \mathrm{Sp}[\hat{p}\hat{p}_T\hat{\rho}_T], \qquad (36)$$

where

$$\hat{p}_T = \frac{i}{\sqrt{2}}\left(e^{\frac{1}{2}\frac{\hbar\omega}{2k_\mathrm{B}T}}\hat{a} - e^{-\frac{1}{2}\frac{\hbar\omega}{2k_\mathrm{B}T}}\hat{a}^+ \right) \qquad (37)$$

and, analogously,

$$\mathrm{Sp}[\hat{q}\hat{\rho}_T^{\frac{1}{2}}\hat{q}\hat{\rho}_T^{\frac{1}{2}}] = \mathrm{Sp}[\hat{q}\hat{q}_T\hat{\rho}_T], \qquad (38)$$

where

$$\hat{q}_T = \frac{1}{\sqrt{2}}\left(e^{\frac{1}{2}\frac{\hbar\omega}{2k_\mathrm{B}T}}\hat{a} + e^{-\frac{1}{2}\frac{\hbar\omega}{2k_\mathrm{B}T}}\hat{a}^+ \right). \qquad (39)$$

Expressions (37) and (39) can be considered as the renormalized momentum and coordinate operators,

respectively, which make allowance for the thermostat action. Using those quantities, the quantity $(\mathcal{UP})^2$ on the left-hand side of Eq. (34) can be written down as a determinant,

$$(\mathcal{UP})^2 = \begin{vmatrix} (\Delta\hat{p})_\rho^2 & (\Delta\hat{p}\,\Delta\hat{\tilde{p}})_\rho \\ (\Delta\hat{p}\,\Delta\hat{\tilde{p}})_\rho & (\Delta\hat{q})_\rho^2 \end{vmatrix}, \qquad (40)$$

in which the calculation of all averages with the density matrix $\hat{\rho}_T$ brings about the left-hand side of Eq. (34).

A comparison of formula (40) with the left-hand side of expression (32) testifies that the result of calculation of $(\mathcal{UP})^2$ by Park with the help of the real-valued density matrix $\hat{\rho}_T$ does not differ, in essence, from a similar result obtained by Umezawa with the use of real-valued two-mode squeezed states. It is important, however, to emphasize that the both results, (32) and (41), belong to the case of equilibrium between the system and the cold vacuum, because the right-hand side of the zeroth law (29) is not changed, when being averaged over the real–both pure and mixed–states. Therefore, the formal application of real states or real elements in the density matrix does not allow the equilibrium of the system with a warm vacuum to be described. This concerns not only the case of simple squeezed states, but also the cases of the Umezawa thermofield dynamics and the thermodynamics based on the quantum statistical mechanics, even if the latter is generalized in the spirit of Wigner and Yanase.

Now, let us discuss the invariance of the zeroth law with respect to the transitions between equilibrium thermal CCSs at nonzero temperatures. For this purpose, let us take advantage of the invariance of the zeroth law with respect to the Lorentz group $O(2, 1)$. It can be demonstrated most easily, by using the equality $\mathbb{J}_T^2 = \sigma_T^2 + \mathbb{J}_{qu}^2$, in (21). Then we obtain

$$\mathbb{J}_T^2 - \sigma_T^2 = \mathbb{J}_{qu}^2 = \left(\frac{\hbar}{2}\right)^2. \qquad (41)$$

From whence, it follows that the quantities $(\mathbb{J}_T, \sigma_T)$ for thermal CCSs can be regarded as a two-dimensional time-like vector in the pseudo-Euclidean space of states, with the quantity $\hbar/2$ playing the role of the length of this vector or the invariant of the Lorentz group $O(1, 1)$. It is analogous to the proper time in the space of events in the conventional special

theory of relativity (the group dimensionality is decreased, since the average value of Lagrangian equals 0 in thermal CCSs). In this case, the quantities

$$\beta_{\text{term}} = \left[\coth\frac{\hbar\omega}{2k_{\text{B}}T}\right]^{-1}; \quad \gamma_{\text{term}} = \left[\coth\frac{\hbar\omega}{2k_{\text{B}}T}\right] \quad (42)$$

play the role of the traditional Lorentzian factors β_L and γ_L, respectively. The limits of the parameter β_{term} as $T \to \infty$ and $T = 0$ in the space of states correspond to the limiting values $\beta_L = 0$ and $\beta_L \to 1$, respectively, in the space of events. As a result, the state of cold vacuum in the Bogoliubov transformation group corresponds to the proper inertial reference frame (IRF) in the special theory of relativity for the group $O(1, 1)$ in the space of states.

Different states of an arbitrary vacuum at finite temperatures are related with other IRFs, which are equivalent to the proper one. From this point of view, the zeroth law of stochastic thermodynamics in form (20) at $T \neq 0$ has the sense of the equality

$$(\mathbb{J}_T)^2 \equiv \left(\frac{\hbar}{2}\right)^2 \coth^2\frac{\hbar\omega}{2k_{\text{B}}T}, \qquad (43)$$

in which the left- and right-hand sides must be calculated independently, by averaging over the thermal CCSs. Note that the zero values of the off-diagonal members of the determinant in formula (43) follow from the fact that the averaging is carried out over pure complex states. The same circumstance gives rise to the appearance of the nonzero term σ_T^2 on the right-hand side of formula (43). This term is explicitly expressed in terms of the wave function phase, and it makes allowance for the quantum thermal stochastic influence of the environment.

Hence, we got more evidence that, among the existing theoretical approaches, only the $(\hbar, k)$-dynamics with complex temperature-dependent wave functions ensures the validity of the zeroth law at nonzero temperatures. Certainly, a possibility of constructing an adequate theory with the help of the complex density matrix remains open.

Note by the way that the authors who developed approaches to the description of thermal phenomena on the basis of real wave functions or real density matrix members intuitively understood the importance of the thermal equilibrium condition in form (24) at $T \neq 0$. However, this condition always has the same

trivial form – (31), (32), or (34) – in the corresponding theories,

$$\left(\frac{\hbar}{4}\right)^2 \left[\coth^2\left(\frac{1}{2}\beta\hbar\omega\right) - \left(\sinh^2\left(\frac{1}{2}\beta\hbar\omega\right)\right)^{-1}\right]\mathcal{E}_0 = \frac{\hbar\omega}{2} = \left(\frac{\hbar}{4}\right)^2. \quad (44)$$

Here, the parameter β was ascribed to be the same value equal to $\frac{1}{kT}$ in both hyperbolic functions. To achieve the required result, which would allow the parameter T in formula (44) to be interpreted as the temperature and relation (44) to be considered as the uncertaity relation, the authors of the cited works simply rewrote equality (44), by transposing one of the terms from the left- to the right-hand side. From the mathematical viewpoint, this operation is eligible, of course. However, it is incorrect from the physical viewpoint, since it means the *a priori* exclusion of differences in the behaviors of the temperatures of the thermostat and an object.

We see a fundamental difference between formula (44) and the following expression obtained by us:

$$\left(\frac{\hbar}{4}\right)^2\coth^2\frac{\hbar\omega}{2k_{\mathrm{B}}T} = \left(\frac{\hbar}{4}\right)^2 + \left(\frac{\hbar}{4}\right)^2\sinh^2\left(\frac{\hbar\omega}{2k_{\mathrm{B}}T_0}.\right)^{-1}, \quad (45)$$

It is very important that the left- and the right-hand side of equality (45) are associated with different physical entities: to the left, we have a parameter of the system with the temperature T that can fluctuate; and, to the right, the parameter of the stochastic environment with a fixed temperature T_0, which does not fluctuate because of the infinitely large number of degrees of freedom for the quantum thermostat. The invalidity of the mentioned formal procedure becomes especially evident in the high-temperature limit, when formula (44) degenerates into the identity

$$\coth^2\frac{\hbar\omega}{2k_{\mathrm{B}}T} \to \left(\sinh^2\frac{\hbar\omega}{2k_{\mathrm{B}}T}\right)^{-1}. \quad (46)$$

In this aspect, the approach, which is proposed by us and is based on the separate calculation of characteristics of the object and the thermostat, to the derivation of formula (45) is free from the mentioned arbitrariness and allows one to use the zeroth law of thermodynamics in the form of a "soft" condition admitting fluctuations of the object temperature.

5. Conclusions

1. Physically significant subgroups of the group of Bogoliubov (u, v)-transformations are demonstrated to generate two types of states: real-valued squeezed coherent states, which provide the saturation of the Heisenberg UR "coordinate–momentum" at the zero temperature, and complex-valued correlated coherent states, which provide the saturation of the Schrödinger UR "coordinate–momentum" at finite temperatures.

2. A quantum analog of the zeroth law of stochastic thermodynamics is formulated at the microscopic level in the form of the saturated Schrödinger UR.

3. The invariance of the saturated Schrödinger UR with respect to the Bogoliubov (u, v)-transformations is substantiated.

4. The saturated Schrödinger UR is proposed as a cornerstone of modified quantum-mechanical theory for finite temperatures.

5. It was shown that there is no correlation between the coordinate and momentum fluctuations in the theories, where the real wave functions or real density matrix members are used. Therefore, the concept of thermal equilibrium arising owing to the correlation between coordinate and momentum fluctuations can be introduced in this case only conditionally, at the zero temperature, when the thermal action of the environment is absent.

6. A correct incorporation of thermodynamics into the quantum theory is possible with arbitrary temperatures in the framework of the theory operating with complex wave functions of the vacuum, which are adequate to thermal CCSs.

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КВАНТОВОМЕХАНИЧНИЙ АНАЛОГ НУЛЬОВОГО ПОЧАТКУ ТЕРМОДИНАМІКИ (ДО ПРОБЛЕМИ ІНКОРПОРАЦІЇ ТЕРМОДИНАМІКИ В КВАНТОВІЙ ТЕОРІЇ)

Р е з ю м е

В основі даного підходу до інкорпорації стохастичної термодинаміки в квантову теорію лежить концепція послідовного обліку цілісного стохастичного впливу оточення, описуваного хвильовими функціями довільних вакуумів, запропонована нами раніше. У цьому дослідженні ми реалізуємо можливість явної інкорпорації в квантову теорію нульового початку стохастичної термодинаміки в формі насиченого співвідношення невизначеностей Шредінгера. Це дозволяє провести порівняльний аналіз сукупностей станів довільних вакуумів – стислих когерентних (СКС) і корельованих когерентних (ККС) станів. Крім того, ми обговорюємо можливість зіставити СКС і ККС тепловим станам.