

A WAY TO INCORPORATION OF THERMODYNAMICS INTO QUANTUM THEORY

*O.N. Golubeva*¹ and *A.D. Sukhanov*^{1,2*}

¹*Peoples' Friendship University of Russia, Moscow, Russia*

²*Joint Institute for Nuclear Research, Dubna, Russia*

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We suggest an approach allowing restrict a gap between macro- and micro descriptions of nature (i.e. between statistical thermodynamics and quantum mechanics) on the basis of a new heat bath model in the form of cold and heat vacua. Despite of standard quantum mechanics we start from microtheory in the form of \hbar, k -dynamics suggested by us earlier. Its concept, in general case, founds on use of complex wave function which amplitude and phase are depended on temperature.

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1. STATEMENT OF THE PROBLEM

At present, the interrelations between the macro- and microdescriptions of the nature attract special attention. Methods of equilibrium thermodynamics turn out to be very effective in the description of nano-objects. At the same time, methods of quantum mechanics are used more and more frequently to analyze macroscopic phenomena. Thus, the gap between the macro- and microtheories existing in the 19 and 20 centuries narrows continuously.

In this connection, a number of researchers formulated the problem of possible coordination between these theories by incorporating thermodynamics into quantum theory [1]. This idea suggests adapting the apparatus of quantum theory to the description of thermal phenomena, thus generating an illusion about the complete reduction of the macrodescription to the microdescription.

In our opinion, the idea of incorporating thermodynamics into quantum theory by combining statistical thermodynamics with quantum statistical mechanics is not very promising. The reason for this is that the types of statistical ensembles used in them (the Gibbs ensemble and the Boltzmann assembly, respectively) do not coincide.

We assume that it is much better to synthesize two other theories, namely, statistical thermodynamics without considering quantum effects and quantum mechanics without considering thermal effects. We are guided by the important fact that the same type of statistical collective (the Gibbs *ensemble*) is used in them. In the framework of the (\hbar, k) -dynamics, proposed by us [2], we managed to construct a more or less holistic description of equilibrium quantum-thermal phenomena, including macroparameter fluctuations. Thus, we propose to modify both theories

by moving in opposite directions.

To do this, the c -number apparatus of statistical thermodynamics, which makes it possible to take equilibrium thermal macroparameter fluctuations into account, must be incorporated into quantum mechanics with its operator formalism. Introducing the vacuum wave function at nonzero temperatures, we adapt quantum mechanics to the description of thermal effects.

From the other hand, the conceptual apparatus of statistical thermodynamics must be extended using c -number random quantities as previously. Matching the operator formalism with effective macroparameters [3], we adapt statistical thermodynamics to the description of quantum effects.

2. MODIFICATION OF QUANTUM MECHANICS FOR THE INCLUSION OF THERMAL EFFECTS

In this paper, we refuse completely the density matrix and have a deal with a complex wave function depending on temperature. We renounce also an attempt to introduce the notion of temperature for isolated system and consider only a system in the heat bath because there are no isolated system in nature. We generalize the classical model of heat bath to the quantum one and interpret it as quantum-thermal vacuum.

Generalizing the apparatus of quantum mechanics to take thermal effects into account, we assume that the zeroth law, i.e., the fundamental condition for the equilibrium of the object with the thermal-type stochastic environment, is initial in thermodynamics. Therefore, it would be natural to start with the determination of the *quantum* state that is adequate for

*Corresponding author E-mail address: ogol@mail.ru

the equilibrium if the stochastic thermal action at the minimal value of effective (but not Kelvin) temperature is additionally taken into account.

To do this, we turn to the universal geometric properties of the Hilbert state space, in which the Cauchy-Bunyakovsky-Schwarz *inequality* (CBSI) for vectors

$$|\delta p\rangle = \delta \hat{p}|\psi\rangle \quad \text{and} \quad |\delta q\rangle = \delta \hat{q}|\psi\rangle \quad (1)$$

holds. Here,

$$\delta \hat{p} \equiv \hat{p} - \langle \psi | \hat{p} | \psi \rangle; \quad \delta \hat{q} \equiv \hat{q} - \langle \psi | \hat{q} | \psi \rangle \quad (2)$$

are the operators of momentum and coordinate fluctuations.

The CBSI for these vectors has the form of the most general *Schrödinger uncertainties relation* (SUR) [4]:

$$\Delta p \cdot \Delta q \geq |\langle \psi | \delta \hat{p} \cdot \delta \hat{q} | \psi \rangle|, \quad (3)$$

where

$$(\Delta p)^2 \equiv \langle \psi | (\delta \hat{p})^2 | \psi \rangle; \quad (\Delta q)^2 \equiv \langle \psi | (\delta \hat{q})^2 | \psi \rangle \quad (4)$$

are the momentum and coordinate variances in the state $|\psi\rangle$, and

$$|\langle \psi | \delta \hat{p} \cdot \delta \hat{q} | \psi \rangle| = |\langle \delta p | \delta q \rangle| \quad (5)$$

has the meaning of the momentum and coordinate fluctuations correlator of the object in the same state expressed in terms of the fluctuation operators $\delta \hat{p}$ and $\delta \hat{q}$.

In thermodynamics, the equilibrium state is stable relative to small stochastic influence of environment. The correlation between corresponding typical quantities is a mechanism for preserving this stability in this case. In other words, it is necessary that: (a) the correlator (5) was non equal to zero; (b) the SUR had the form of equality, i.e. became saturated. (Some heuristic considerations confirming this statements will be stated below.)

Accordingly to the Schwarz-fon Neumann theorem the equality in the SUR (3) can be realized if the vectors $|\delta p\rangle$ and $|\delta q\rangle$ are proportional to each other, i.e.

$$\delta \hat{p}|\psi\rangle = (i\gamma \cdot e^{i\alpha})\delta \hat{q}|\psi\rangle. \quad (6)$$

Here, the real parameters $\gamma > 0$ and $\alpha \stackrel{\geq}{=} 0$. To simplify calculations, we assume that the average momentum and coordinate in this state are zero.

It is interesting that the equation

$$(\hat{p} - i\gamma e^{i\alpha} \hat{q})|\psi_\alpha\rangle = 0, \quad (7)$$

can be obtained from formula (6); it resembles the result of the action of the annihilation operator

$$\hat{a} = \frac{\hat{p} - i\zeta \hat{q}}{\sqrt{2\hbar\zeta}}$$

on the state $|\psi_\alpha\rangle$. In the coordinate representation, relation (7) takes the form of the differential equation for the unknown function $\psi_\alpha(q)$:

$$\frac{\hbar}{i} \frac{d}{dq} \psi_\alpha - (i\gamma e^{i\alpha})q \cdot \psi_\alpha = 0. \quad (8)$$

Solving it and using the normalization condition, in the general case, we obtain the complex function

$$\psi_\alpha(q) = \left[2\pi(\Delta q_0)^2 \frac{1}{\cos \alpha} \right]^{-1/4} \times \exp \left\{ -\frac{q^2}{4(\Delta q_0)^2} e^{i\alpha} \right\}, \quad \cos \alpha \neq 0 \quad (9)$$

as the universal wave function $\psi_\alpha(q)$; here,

$$(\Delta q_0)^2 = \frac{\hbar}{2\gamma}, \quad (10)$$

and respectively $(\Delta p_0)^2 = \frac{\hbar\gamma}{2}$.

The physical meaning of the function $\psi_\alpha(q)$ can be clarified if we take into account that, for $\alpha = 0$, Eq. (8) for the function ψ_0 is equivalent to the equation for the state $|0\rangle$, which is assumed to be called the *cold vacuum*. Accordingly, for arbitrary $\alpha \neq 0$, the state ψ_α describes an *arbitrary vacuum*. We note that the standard way of obtaining this state is related to the application of the Bogoliubov (u, v) -transformation.

In the state of the arbitrary vacuum, the equalities

$$(\Delta p_\alpha)^2 = \gamma^2 (\Delta q_\alpha)^2; \quad |\langle \delta p_\alpha | \delta q_\alpha \rangle| = |i\gamma e^{i\alpha}| \langle \delta q_\alpha | \delta q_\alpha \rangle = \gamma (\Delta q_\alpha)^2. \quad (11)$$

hold for the average quantities. Substituting formulas (11) to SUR (3), we see that the correlated state $|\psi_\alpha\rangle$ is marked, because the SUR becomes saturated:

$$\Delta p_\alpha \cdot \Delta q_\alpha = |\langle \psi_\alpha | \hat{p} \cdot \hat{q} | \psi_\alpha \rangle|. \quad (12)$$

In the cold-vacuum state $|\psi_0\rangle$ (for $\alpha = 0$), saturated SUR (12) transforms into the saturated Heisenberg uncertainties relation

$$\frac{\mathbb{U}_0}{\omega} = \Delta p_0 \cdot \Delta q_0 = |\langle \psi_0 | \frac{1}{2} [\hat{p}, \hat{q}] | \psi_0 \rangle| = \frac{\hbar}{2} \equiv \mathbb{J}_0. \quad (13)$$

Here, \mathbb{J}_0 is the measure of the purely quantum environmental action (for $\alpha = 0$). Thus, for $\alpha = 0$, the correlator $|\langle \psi_\alpha | \hat{p} \cdot \hat{q} | \psi_\alpha \rangle|$ has a minimum possible value. As it was to be expected, the state $|\psi_0\rangle$, in really, has the sense of equilibrium state with the cold vacuum for it answers the minimal value of the vacuum energy $\mathbb{U}_0 = \frac{\hbar\omega}{2}$. On this ground, from now on, we concede that saturated SUR (12) answers to equilibrium state with arbitrary vacuum $|\psi_\alpha\rangle$.

It is assumed to regard relation (13) as a fundamental equality reflecting the presence of unavoidable purely quantum effects in nature. This fact allows suggesting a hypothesis that the functions making it possible also to take into account thermal effects in addition to the quantum ones. They can be found

among the functions $\psi_\alpha(q)$ providing saturation of SUR (12) for $\alpha \neq 0$.

To confirm it, we pass from ψ_0 to the function ψ_α of the arbitrary vacuum. Then the correlator in the right-hand side of saturated SUR (12) can be represented in the form

$$|\langle \psi_\alpha | \hat{p} \cdot \hat{q} | \psi_\alpha \rangle| = \sqrt{\frac{\hbar^2}{4} \operatorname{tg}^2 \alpha + \mathbb{J}_0^2} = \frac{\hbar}{2} \frac{1}{\cos \alpha} \equiv \mathbb{J}_\alpha, \quad (14)$$

where the term in the radicand, which is additional if (14) is compared with (13), is related to the phase of the function ψ_α .

The expression (14) depends on the quantity \mathbb{J}_α , which generalizes the measure \mathbb{J}_0 of purely quantum effects. Under our assumption it is capable of taking additional thermal effects into account too. To do this, it is necessary to relate the obtained expressions to the Kelvin temperature, which has no direct preimage in quantum mechanics.

Of course, we did not infringe on the stability of the framework of quantum mechanics without thermal effects. We propose the solution only for a borderline area in which quantum and thermal effects cannot be neglected under equilibrium conditions.

3. INTERRELATION WITH KELVIN TEMPERATURE

We introduce the concept of thermal equilibrium with the Kelvin temperature T , which is typical of this state. To do this, we start from the experimentally confirmed Planck expression for the average energy of the quantum oscillator in a thermostat:

$$\mathbb{U}_T \equiv \mathcal{E}_{Pl} = \frac{\hbar\omega}{2} \coth\left(\varkappa \frac{\omega}{T}\right), \quad \varkappa = \frac{\hbar}{2k_B}, \quad (15)$$

where \varkappa has the meaning of fundamental world constant reflecting the simultaneous stochastic action of the quantum and thermal types.

Taking into account that, for the quantum oscillator in the equilibrium state, the average kinetic and potential energies coincide, we obtain the coordinate variance in this state:

$$(\Delta q_T)^2 = \frac{2}{\omega^2} \cdot \frac{1}{2} \mathcal{E}_{Pl} = \frac{\hbar}{2\omega} \coth\left(\varkappa \frac{\omega}{T}\right), \quad (16)$$

where we set $m = 1$ without loss of generality. Similarly, we have

$$(\Delta p_T)^2 = \frac{\hbar\omega}{2} \coth\left(\varkappa \frac{\omega}{T}\right); \quad \text{at } m = 1 \quad (17)$$

for the momentum variance.

In turn, calculating the coordinate variance in terms of the arbitrary-vacuum wave function ψ_α , we obtain

$$(\Delta q_\alpha)^2 = \frac{\hbar}{2\gamma \cos \alpha}. \quad (18)$$

We now compare two formulas (16) and (18) for the coordinate variance. They coincide if we set

$$\begin{aligned} \gamma = \omega; \quad \cos \alpha &= \left[\coth\left(\varkappa \frac{\omega}{T}\right) \right]^{-1}; \\ \sin \alpha &= \left[\operatorname{ch}\left(\varkappa \frac{\omega}{T}\right) \right]^{-1}. \end{aligned} \quad (19)$$

For such a choice of the parameter $\alpha \neq 0$, we choose only functions ψ_T such that correspond to the equilibrium with the environment at the temperature T :

$$\begin{aligned} \psi_T(q) &= [2\pi(\Delta q_T)^2]^{-1/4} \\ &\times \exp\left\{-\frac{q^2}{4(\Delta q_T)^2} \left(1 - i \frac{1}{\operatorname{sh} \varkappa \frac{\omega}{T}}\right)\right\}. \end{aligned} \quad (20)$$

They can be conditionally assumed to be the functions of the "thermal" vacuum. Accordingly, the correlator of coordinate and momentum fluctuations (14) becomes

$$|\langle \psi_T | \hat{p} \cdot \hat{q} | \psi_T \rangle| \equiv \mathbb{J}_T = \sqrt{\frac{\hbar^2}{4 \operatorname{sh}^2 \varkappa \frac{\omega}{T}} + \frac{\hbar^2}{4}}. \quad (21)$$

Here, the quantity $(\operatorname{sh} \varkappa \frac{\omega}{T})^{-1}$ in \mathbb{J}_T is directly related to the phase of the wave function ψ_T .

We now pay our attention to the fact that the quantity \mathbb{J}_T can also be immediately obtained from the correlator through the variance of coordinate:

$$|\langle \delta p_T | \delta q_T \rangle| = \omega(\Delta q_T)^2 = \mathbb{J}_T = \frac{\hbar}{2} \coth\left(\varkappa \frac{\omega}{T}\right). \quad (22)$$

Here, the dependence on the phase of the wave function ψ_T is *hidden*.

Together with the interrelation between momentum variance and coordinate variance

$$(\Delta p_T)^2 = \omega^2 \cdot (\Delta q_T)^2, \quad (23)$$

both sides of saturated "momentum-coordinate" SUR becomes

$$\Delta p_T \cdot \Delta q_T = \omega(\Delta q_T)^2 = \mathbb{J}_T. \quad (24)$$

Thus, they are expressed only in terms of one quantity, namely, the coordinate variance $(\Delta q_T)^2$; the ways of calculating it can be *various*.

To clarify the physical meaning of the quantity \mathbb{J}_T , we rewrite saturated SUR (12) in the "thermal-vacuum" state $\psi_T(q)$ in the form

$$\frac{\mathbb{U}_T}{\omega} = \Delta p_T \cdot \Delta q_T = \mathbb{J}_{T_0} = \frac{\hbar}{2} \coth\left(\varkappa \frac{\omega}{T_0}\right), \quad (25)$$

where we express the Kelvin thermostat temperature T_0 explicitly. We stress that, in this relation, the left-hand side of the equality is expressed in terms of the object characteristics and the right-hand side, in terms of the environmental characteristics.

At high temperatures, the saturated SUR Eq. (12) transforms into the equality $T = T_0$ having the meaning of the standard zero law (without considering temperature fluctuations), i.e., the thermal

equilibrium condition. This fact allows interpreting Eq. (12) as a generalized zero law in the case where the quantum and thermal effects are taken into account simultaneously. This law is valid at any temperature.

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СПОСОБ ВВЕДЕНИЯ ТЕРМОДИНАМИКИ В КВАНТОВУЮ ТЕОРИЮ

О.Н. Голубева, А.Д. Суханов

Мы предлагаем подход, позволяющий устранить разрыв между макро- и микроописаниями природы (т.е. между статистической термодинамикой и квантовой механикой) на основе новой модели термостата в форме холодного и теплого вакуумов. В отличие от стандартной квантовой механики мы исходим из микротерии в форме \hbar, k -динамики, предложенной нами ранее. Ее концепция, в общем случае, основана на использовании комплексной волновой функции, амплитуда и фаза которой зависят от температуры.

СПОСІБ ВВЕДЕННЯ ТЕРМОДИНАМІКИ У КВАНТОВУ ТЕОРІЮ

О.М Голубева, О.Д. Суханов

Ми пропонуємо підхід, що дозволяє усунути розрив між макро- й мікроописами природи (тобто між статистичною термодинамікою й квантовою механікою) на основі нової моделі термостата у формі холодного й теплого вакуумів. На відміну від стандартної квантової механіки ми виходимо з микротерії у формі \hbar, k -динаміки, запропонованої нами раніше. Її концепція, у загальному випадку, заснована на використанні комплексної хвильової функції, амплітуда й фаза якої залежать від температури.