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NONEQUILIBRIUM QUANTUM STATISTICAL OPERATOR. GENERAL DEFINITION OF NONEQUILIBRIUM REAL-TIME GREEN'S FUNCTION

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We observe the nonequilibrium system. By introducing the unitary transformation operator $U_{IS}(t, t')$ we defined the interaction representation, which made us able to derive the fundamental relation of quatum statistical physics. Using this equation we found the accurate expression for the statistical operator ϱ_H, in the Heisenberg representation, which enabled us to find out the general definition for nonequilibrium real-time Green's function.

1. Introduction

If we observe a statistical system affected by the external field, which can be taken to be sufficiently small, then the Hamiltonian of the perturbed system can be represented as a sum of time-independent Hamiltonian H_0 and the time-dependent term $V(t)$, the latter expressing the system interaction with the external field. Such a representation of a total Hamiltonian enables the definition of an interaction representation by means of a simple factor e^{iH_0t} and finding the formal solutions to motion equations.

However, if we observe the statistical system which under the action of an external field deviates to any arbitrary extent from a state of thermodynamical equilibrium, then both terms of the total Hamiltonian of the perturbed system are time--dependent; the first term $H_0(t)$ representing the energy of the non-interacting particles in an external field, and the second term $V(t)$ representing the energy of interacting particles in the external field. Since both terms of the total Hamiltonian are time-dependent, the problem arises how to define the interaction representation without using the factor e^{iH_0t}.

Keldysh[1] and Murayama[2] solved partially this problem by relying on the analogy with the usual manner of defining the interaction representation for the case of the small perturbation.

Having in view the role played by the statistical operator in the treatment of the quantum-mechanical problems and particularly in that of quatum-statistical physics, the present paper shows how all three representations and statistical operators in them are defined for the perturbed Hamiltonian of the most general form. Factor e^{iH_0t} is substituted by the transformation operator $U_{IS}(t, t')$ in the general form describing the transition from the Schrödinger representation into interaction. It made possible the derivation of the fundamental relation of quantum statistical physics relation connecting the equilibrium statistical operator to nonequilibrium statistical operator (equation (2.11″)) i. e., (3.17), Chapters 2, 3 and 4.

Apart from that we clarified the dilemma about the choice of values of the statistical operator in the Heisenberg representation which made us able to set up a general definition for nonequilibrium real-time Green's function (equation (5. 4)).

Having in view this definition of Green's function we could make a critical analysis of the hitherto definitions[1,3], Chapter 5.

2. *Nonequilibrium statistical operator in Schrödinger representation*

Let us observe the system of interacting particles affected by an external time--dependent field. The total Hamiltonian of the system $H_S(t)$ will be divided into two terms. The first term $H_{0S}(t)$ is the Hamiltonian of free particles in the external field, while the second term $V_S(t)$ represents the term describing the particle interaction in the external field:

$$H_S(t) = \begin{cases} H_{0S} + V_S & t < t_0 \\ H_{0S}(t) + V_S(t) & t > t_0, \end{cases} \tag{2.1}$$

where t_0 is the initial moment of the inclusion of the external field, and index S denotes Schrödinger representation. The change of the state of the perturbed system represented in Schrödinger representation by a ket $|, t\rangle_S$ is given by the equation of motion:

$$\mathrm{i}\frac{\mathrm{d}}{\mathrm{d}t}|, t\rangle_S = H_S(t)|, t\rangle_S, \quad \hbar = 1, \tag{2.2}$$

where

$$H_S(t) = H_{0S}(t) + V_S(t). \tag{2.3}$$

Besides

$$|, t\rangle_S = U_S(t, t')\, |, t'\rangle_S, \tag{2.4}$$

where t' is any moment $t' < t$, while the unitary operator $U_S(t, t')$ according to (2.2) is the solution of the equation:

$$\mathrm{i}\frac{\mathrm{d}}{\mathrm{d}t} U_S(t, t') = H_S(t)\, U_S(t, t'), \tag{2.5}$$

with the initial condition

$$U_S = (t', t') = 1 \tag{2.6}$$

which follows immediately from Eq. (2.4).

The system under observation can, at any moment, be in any state with some probability. Let the normalized ket vector, corresponding to discrete possible states be $|\,a\rangle$, and let the probability for the system to be in a definite state a, be $P_a > 0$. The statistical operator in the Schrödinger representation is then defined as[4]:

$$\varrho_S(t) \equiv \sum_a |a, t\rangle_S\, P_a\, {}_S\langle a, t|. \tag{2.7}$$

If the system at the initial moment t_0, prior to the inclusion of the external field, was distributed over non-perturbed states, $\{a\}$, with probability $\{P_a\}$ the statistical operator corresponding to these distributions is, according to (2.7):

$$\varrho_S(t_0) \equiv \sum_a |\, a, t_0\rangle_S\, P_a\, {}_S\langle a, t_0\,|, \tag{2.8}$$

where $|\, a, t_0\rangle_S$ are the eigenstates of the equilibrium Hamiltonian $H_S = H_{0S} + V_S$.

If we assume that the system, prior to action of the external field was in equilibrium, then

$$\varrho_S(t_0) = \varrho_{S\,eq}, \tag{2.9}$$

where $\varrho_{S\,eq}$ is equilibrium statistical operator.

The external field provokes the change of the equilibrium state according to (2.4) so that the statistical operator at any moment t:

$$\varrho_S(t) = \sum_a U_S(t, t_0)\, |\, a, t_0\rangle_S\, P_a\, {}_S\langle a, t_0\,|\, U_S^+(t, t_0), \tag{2.10}$$

which is, according to (2.8) and (2.9):

$$\varrho_S(t) = U_S(t, t_0)\, \varrho_S(t_0)\, U_S^+(t, t_0), \tag{2.11'}$$

$$\varrho_S(t) = U_S(t, t_0)\, \varrho_{S\,eq}\, U_S^+(t, t_0). \tag{2.11''}$$

By differentiating expression (2.7) with respect to time and using equation (2.2) we obtain the equation of motion for $\varrho_S(t)$:

$$\mathrm{i}\frac{\mathrm{d}}{\mathrm{d}t}\varrho_S(t) = -[\varrho_S(t), H_S(t)]_- . \tag{2.12}$$

3. Nonequilibrium statistical operator in the interaction representation

Other representations besides the Schrödinger may be used to describe a quantum system. But a new representation will only then be regarded as equivalent to Schrödinger if it keeps the observed quantities — the eigenvalues of the operators, the average values, the transition probabilities, etc. — invariant.

In the Schrödinger representation a full Hamiltonian $H(t)$ determines the time variation of the state vectors and operators stay temporally unchanged. We will now look for such a representation in which time-dependence is partially transformed from the state vector to the operator — interaction representation.

We will require that time dependence of the state vectors is determined by the Hamiltonian $V(t)$ and that Hamiltonian $H_0(t)$ determines the time-variation of the operators. The transition from the Schrödinger to such an interaction representation can be made via a unitary transformation operator $U_{IS}(t, t')$.

The corresponding change in the state vector is given by

$$|, t\rangle_I \equiv U^{+}_{IS}(t, t')\, |, t\rangle_S, \tag{3.1}$$

and the change in the operator of any particular quantity ξ by

$$\xi_I(t) = U^{+}_{IS}(t, t')\, \xi_S\, U_{IS}(t, t'). \tag{3.2}$$

If we choose that t' in the moment where interaction representation is equivalent to Schödinger representation:

$$|, t'\rangle_I \equiv |, t'\rangle_S, \tag{3.3}$$

then from (3.1) follows that operator $U_{IS}(t, t')$ satisfies the condition

$$U_{IS}(t', t') = 1. \tag{3.4}$$

Having in view that the Hamiltonian $V(t)$ determines the temporal evolution of state vectors we postulate the new form of the Schrödinger equation:

$$\mathrm{i}\frac{\mathrm{d}}{\mathrm{d}t}|, t\rangle_I = V_I(t, t')\, |, t\rangle_I, \tag{3.5}$$

where

$$V_I(t, t') = U_{IS}^{+}(t, t')\, V_S(t)\, U_{IS}(t, t'). \tag{3.6}$$

The formal solution of these equation has a form:

$$|, t\rangle_I = U_I(t, t')\, |, t'\rangle_I, \tag{3.7}$$

where time evolution operator $U_I(t, t')$ is unitary. From (3.7) follows that this operator satisfies the initial condition

$$U_I(t' t') = 1. \tag{3.8}$$

Substituting (3.7) in (3.5) we found equation of motion for $U_I(t, t')$:

$$\mathrm{i}\frac{\mathrm{d}}{\mathrm{d}t} U_I(t, t') = V_I(t, t')\, U_I(t, t'). \tag{3.9}$$

Differentiating (3.1) with respect to time and using (2.2), (3.5) and (3.6) we found equation of motion for $U_{IS}(t, t')$:

$$\mathrm{i}\frac{\mathrm{d}}{\mathrm{d}t} U_{IS}(t, t') = H_{0S}(t)\, U_{IS}(t, t'). \tag{3.10}$$

Initial condition needed for solving this differential equation is given by equation (3.4).

Using (3.1), (2.4), (3.3), and (3.7) we found relationship satisfying time-evolution operators and transformation operator:

$$U_{IS}(t, t') = U_S(t, t')\, U_I^{\dagger}(t, t'). \tag{3.11}$$

By differentiating equation (3.2) with respect to time and employing equation (3.10) we get the equation of motion for $\xi_I(t)$:

$$\mathrm{i}\frac{\mathrm{d}}{\mathrm{d}t} \xi_I(t) = [\xi_I(t), H_{0I}(t)]_-, \tag{3.12}$$

where

$$H_{0I}(t) = U_{IS}^{\dagger}(t, t')\, H_{0S}\, U_{IS}(t, t'). \tag{3.13}$$

In the Schrödinger representation the temporal evolution of statistical operator determines a full Hamiltonian. We will show now that when one defines interaction representation as we did, the temporal evolution of statistical operator determines only interaction term $V(t)$.

$$\varrho_I(t) = \sum_{\alpha} |\alpha, t\rangle_I\, P_{\alpha\, I}\langle \alpha, t\,|. \tag{3.14}$$

Differentiating (3.14) with respect to time and using Eq. (3.5) we get equation which covers time-evolution of $\varrho_I(t)$:

$$i \frac{d}{dt} \varrho_I(t) = -[\varrho_I(t), V_I(t, t')]_-. \tag{3.15}$$

To find the formal solution of this equation we start from the definition (3.1) and (3.14) and found:

$$\varrho_I(t) = U_{IS}^{\dagger}(t, t')\, \varrho_S(t)\, U_{IS}(t, t'). \tag{3.16}$$

If in the above expression we substitute expression (2.11″) and use relation (3.11) we get:

$$\varrho_I(t) = U_I(t, t')\, U_S(t', t_0)\, \varrho_{S\,eq}\, U_S^{\dagger}(t', t_0)\, U_I^{\dagger}(t, t'). \tag{3.17}$$

If we differentiate (3.17) with respect to time and use (3.9) we get equation (3.15) which means that expression (3.17) is really the solution of equation (3.15) with initial condition:

$$\varrho_I(t') = U_S(t', t_0)\, \varrho_{S\,eq}\, U_S^{\dagger}(t', t_0). \tag{3.18}$$

Using (3.18) relation (3.17) may be written in the form:

$$\varrho_I(t) = U_I(t, t')\, \varrho_I(t')\, U_I^{\dagger}(t, t'). \tag{3.19}$$

Relation (3.17) i. e. (3.19) as we have seen, connecting the equilibrium statistical operator to nonequilibrium statistical operator and themselves is the fundamental relation of quantum-statistical physics.

To prove that interaction representation defined in such a manner as we did is really equivalent to Schrödinger representation, we need to show that expectation value of an arbitrary observable ξ at the time t is the same as in Schrödinger representation.

The expectation value of arbitrary observable ξ at the time t in nonequilibrium system is defined as:

$$\bar{\xi}_S = \sum_{\alpha} {}_S\langle \alpha, t \mid \varrho_S(t)\, \xi_S \mid \alpha, t \rangle_S, \tag{3.20}$$

so that in interaction representation:

$$\bar{\xi}_I = \sum_{\alpha} {}_I\langle \alpha, t \mid \varrho_I(t)\, \xi_I(t) \mid \alpha, t \rangle_I. \tag{3.21}$$

Using equations (3.1), (3.2) and (3.16) we can prove that:

$$\bar{\xi}_I = \bar{\xi}_S, \tag{3.22}$$

which means that the observable quantity remains invariant.

To sum up: To define interaction representation in nonequilibrium case we use instead of factor $e^{iH_0(t-t')}$ the unknown unitary transformation operator $U_{IS}(t, t')$ where t' is the moment where interaction representation is equivalent to Schrödinger and can be any moment later than t_0, the moment of switching on of perturbation. The decomposition of the Hamiltonian $H(t)$ in part $H_0(t)$ and $V(t)$ so that $V(t)$ determines evolution of state vector and $H_0(t)$ evolution of operators yields for $U_{IS}(t, t')$ simple equation of motion (3.10) with initial condition (3.4). But the equation of motion for time evolution operator $U_I(t, t')$ has no more simple form and can be resolved only indirectly via the solution of equation (3.10).

4. Nonequilibrium statistical operator in the Heisenberg representation

In the Heisenberg representation the state $|\rangle_H$ is defined as:

$$|\rangle_H \equiv U_S^+(t, t')\, |, t\rangle_S. \tag{4.1}$$

Since $U_S(t', t') = 1$, it is:

$$|\rangle_H = |, t'\rangle_S, \tag{4.2}$$

so that according to (3.3):

$$|\rangle_H = |, t'\rangle_I = |, t'\rangle_S = U_S(t', t_0)\, |, t_0\rangle_S, \tag{4.3}$$

which means that all three representations are equal at moment $t' > t_0$.

In the Heisenberg representation the transformed observable will be defined as:

$$\xi_H(t) \equiv U_S^+(t, t')\, \xi_S\, U_S(t, t'). \tag{4.4}$$

On the basis of Eqs. (3.2) and (3.11) we get that:

$$\xi_H(t) = U_I^+(t, t')\, \xi_I(t)\, U_I(t, t'). \tag{4.5}$$

Differentiating expression (4.4) with respect to time and using Eq. (2.5) we get the equation of motion for $\xi_H(t)$:

$$\mathrm{i}\frac{\mathrm{d}}{\mathrm{d}t}\xi_H(t) = [\xi_H(t), H_H(t)]_-, \tag{4.6}$$

$$H_H(t) = U_S^+(t, t')\, H_S(t)\, U_S(t, t'). \tag{4.7}$$

The statistical operator in the Heisenberg representation will be defined as:

$$\varrho_H \equiv \sum_\alpha |\, \alpha\rangle_H\, P_\alpha\, {}_H\langle \alpha\, |. \tag{4.8}$$

From the above expression and definition (4.1) it stems that:

$$\varrho_H = U_S^{+}(t, t')\, \varrho_S(t)\, U_S(t, t'). \tag{4.9}$$

Substituting expression (2.11″) into (4.9) we get that:

$$\varrho_H = U_S(t', t_0)\, \varrho_{S\,eq}\, U_S^{+}(t', t_0). \tag{4.10}$$

On the basis of expressions (4.8) and (4.3) it follows that:

$$\varrho_H = \varrho_I(t') = \varrho_S(t'), \tag{4.11}$$

which means that the statistical operator in the Heisenberg representation is time--independent, and can be calculated from the fundamental equation of quantum--statistical physics, Eq. (3.17).

The expectation value of an arbitrary observable in the Heisenberg representation is:

$$\overline{\xi}_H = \sum_{\alpha} {}_H\langle \alpha \mid \varrho_H\, \xi_H(t) \mid \alpha \rangle_H. \tag{4.12}$$

Employing expressions (4.3), (4.4) and (4.11) we can prove that:

$$\overline{\xi}_H = \overline{\xi}_S \tag{4.13}$$

which means that this representation is equivalent to the Schrödinger representation.

5. *Definitions of real-time Green's function*

a. General definition

Since one particle Green's function is defined as an average value of the product of the field operators for two different times, t_1 and t_2, it must be defined in the Heisenberg representation in order to avoid the time dependence of the statistical operator. Let us observe, for the simplicity sake, the case when $t_1 > t_2$, which does not decrease the generality of the definition. One particle Green's function in that case should be defined as:

$$G(t_1, t_2) = \frac{1}{i} \sum_{\alpha} {}_H\langle \alpha \mid \varrho_H\, \Psi_H(t_1)\, \Psi_H^{+}(t_2) \mid \alpha \rangle_H. \tag{5.1}$$

To go from the Heisenberg representation to the interaction, we shall use expressions (4.3), (4.5) and (5.1) and we get:

$$G(t_1, t_2) = \frac{1}{i} \sum_{\alpha} {}_I\langle \alpha, t' \mid \varrho_I(t')\, U_I^{+}(t_1, t')\, \Psi_I(t_1) \times$$

$$\times\, U_I\, t_1, t_2)\, \Psi_I^{+}(t_2)\, U_I^{+}(t_2, t') \mid \alpha, t' \rangle_I. \tag{5.2}$$

Since our final aim is to express Green's function as an average over the equilibrium statistical operator $\varrho_{S\,eq}$ and equilibrium eigenstates $|\alpha, t_0\rangle_S$, by using expressions (4.3) and (3.16) we get:

$$G(t_1, t_2) = \frac{1}{i} \sum_{\alpha} {}_S\langle \alpha, t_0) \, U_S^+(t', t_0) \, U_S(t', t_0) \, \varrho_{S\,eq} \, U_S^+(t', t_0) \times$$
$$\times \, U_I^+(t_1, t') \, \Psi_I(t_1) \, U_I(t_1, t_2) \, \Psi_I^+(t_2) \, U_I^+(t_2, t') \, U_S(t', t_0) \, | \, \alpha, t_0, \rangle_S, \qquad (5.3)$$

which, further, due to the cyclic invariance of the trace, can be represented as:

$$G(t_1, t_2) = \frac{1}{i} \sum_{\alpha} {}_S\langle \alpha, t_0 \, | \, U_S(t', t_0) \, \varrho_{S\,eq} \, U_S^+(t', t_0) \, U_I^+(t_1, t') \times$$
$$\times \, \Psi_I(t_1) \, U_I(t_1, t_2) \, \Psi_I^+(t_2), \, U_I(t_2, t') \, | \, \alpha, t_0 \rangle_S. \qquad (5.4)$$

We have so obtained the most general definition of Green's function for the nonequilibrium system which deviates to any arbitrary extent from a state of thermodynamical equilibrium.

b. Comment to Kadanoff-Baym's definition of Green's function[3]

From general definition (5.4) it is easy to derive the definition of Green's function used by Kadanoff and Baym. These authors take that $t' = t_0$, which on the basis of the initial condition (2.6) yields:

$$G(t_1, t_2) = \frac{1}{i} \sum_{\alpha} {}_S\langle \alpha, t_0 \, | \, \varrho_{S\,eq} \, U_I^+(t_1, t_0) \, \Psi_I(t_1) \, U_I(t_1, t_2) \times$$
$$\times \, \Psi_I^+(t_2) \, U_I(t_2, t_0) \, | \, \alpha, t_0 \rangle_S, \qquad (5.5)$$

which is equivalent to the definition of Kadanoff and Baym (Ref. 4, Eq. (8.18)) provided $t_0 \to -\infty$ is chosen as a moment of the beginning of external field action. We have shown that Kadanoff-Baym's definition, of Green's function is correct in general and so if we wish to derivate the transport equation of Kadanoff and Baym without resorting to an analytic continuation from imaginary times and without the correction terms of Fujita[7] we must start from it, too. The preparation of the system in thermodynamical equilibrium state in early remote time $t_0 \to -\infty$, as shown by the author[5] leads to the explicit incorporation of the causality principle in the derivation of the quantum-mechanical kinetical equation.

c. Comment to Keldysh's definition of Green's function[1]

Keldysh takes for equation (3.15) the boundary condition

$$\varrho_I(-\infty) = \varrho_0 = \exp\{\Psi_0 - H_0(-\infty)\}/kT, \qquad (5.6)$$

where $H_0(-\infty)$ is the non-interacting Hamiltonian in remote early time and Ψ_0 is the initial free energy. Through such a choice for the initial value of the statistical operator Keldysh ignores the initial particle correlation. For the beginning of external field action Keldysh takes $t_0 \to -\infty$ and for the moment when all three representations are equivalent, he takes $t' = 0$.

The initial statistical operator $\varrho_I(-\infty)$ must be defined as:

$$\varrho_I(-\infty) = \sum_{\alpha} |a, -\infty\rangle_I P_{a\ I}\langle a, -\infty|, \tag{5.7}$$

where $|a, -\infty\rangle_I$ is the state of the system prior to the beginning of external field action and it can be found only approximately by applying the adiabatic hypothesis[6].

By means of the boundary condition (5.6) the formal solution of equation (3.15) may be written in the form:

$$\varrho_I(t) = U_I(t, -\infty)\, \varrho_I(-\infty)\, U_I^\dagger(t, -\infty). \tag{5.8}$$

Using this expression and Eq. (4.11) we find that for $t' = 0$

$$\varrho_H = U_I(0, -\infty)\, \varrho_I(-\infty)\, U_I^\dagger(0, -\infty). \tag{5.9}$$

On the basis of expression (4.3) it follows that:

$$|\,\rangle_H = U_I(0, -\infty)\, |, -\infty\rangle_I. \tag{5.10}$$

Using relations (4.5), (5.9) and (5.10) the general definition of Green's function can be reduced to the form equivalent to Keldysh's[1] definition:

$$G(t_1, t_2) = \frac{1}{i} \sum_{\alpha} {}_I\langle a, -\infty\,|\, \varrho_I(-\infty)\, U_I(-\infty, t_1)\, \Psi_I(t_1) \times$$
$$\times\, U_I(t_1, t_2)\, \Psi_I^\dagger(t_2)\, U_I(t_2, -\infty)\, |\, a, -\infty\rangle_I. \tag{5.11}$$

The comparison of expression (5.11) with Kadanoff-Baym's definition (5.5) shows that in expression (5.11) instead of the exact eigenstates of equilibrium systems and equilibrium statistical operators appear their approximate values obtained when the possibility of initial particle correlation is ignored. We have also seen that Keldysh preparated the system in equilibrium in a remote earlier time, $t_0 \to -\infty$, as did Kadanoff and Baym, which is the reason of the incorporation of the causality principle in the derivation of quantum mechanical kinetical equations[8].

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NERAVNOTEŽNI KVANTNI STATISTIČKI OPERATOR. GENERALNA DEFINICIJA NERAVNOTEŽNE VREMENSKI REALNE GRINOVE FUNKCIJE

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Posmatramo neravnotežni sistem. Uvođenjem unitarnog transformacionog operatora $U_{IS}(t, t')$ definisali smo interakcionu reprezentaciju, koja nam je omogućila da izvedemo fundamentalnu relaciju kvantne statističke fizike. Koristeći ovu relaciju našli smo tačan izraz za statistički operator ϱ_H u Hajzenbergovoj reprezentaciji što nam je omogućilo da postavimo generalnu definiciju za neravnotežnu realnu Grinovu funkciju.