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TIME-REVERSAL NONINVARIANCE OF GENERALIZED QUANTUM MECHANICAL BOLTZMANN KINETIC EQUATION DERIVED BY KELDYSH

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Considering the time-reversed system and using diagram techniques for anticausal Green function it was shown that the origin of time-reversal noninvariance of generalized quantum-mechanical Boltzmann kinetic equation derived by Keldysh stems from the selection of the boundary condition that the perturbed system was in the thermodynamical equilibrium at the moment $t = -\infty$.

1. Introduction

The application of the method of Green functions to the study of nonequilibrium processes yielded, among the other things, in 1963 (Kadanoff and Baym)$^{1)}$ the quantum mechanical kinetic equation describing irreversible processes in the system which deviates to small extent from equilibrium and in 1965 (Keldysh)$^{2)}$ it yielded the equation for the essentially nonequilibrium system.

Apart from providing us with a powerful means for solving the problems of the nonequilibrium statistical physics, the investigation of Kadanoff and Baym equation with respect to the time reversal noninvariance shed a new light to the problem of irreversibility.

Namely, the author$^{3)}$ in 1978 showed that the approximation of such a kind as Boltzmann *Stosszahlansatz* does not appear as a cause of time-reversal noninvariance of this equation, but that here the boundary condition of more cosmological nature having the form of *causal* initial condition is involved.

In the present paper we shall show that in the Keldysh quantum-mechanical kinetic equation appears the same *causal* boundary condition as a cause of time-reversal noninvariance though Keldysh does not use the method of analytical continuation, which in Kadanoff and Baym derivation has explicitly imposed the employment of the mentioned boundary condition.

In order to show it, we will use the same methodological approach as in the previous paper (Ref. 3), i. e., we consider the time-reversed situation described by anticausal Green function (*GF*) which represents the time-reversed solution of the corresponding equation of motion for causal *GF*.

Keldysh observed essentially nonequilibrum system with perturbed Hamiltonian of the most general form. To find such a definition for nonequilibrium causal *GF* which enables the use of the method of diagram technique Keldysh has assumed that the system was in thermodynamical equilibrium in the remote past, and that it was taken from it by switching in the external field at the time $t = -\infty$.

Using that definition of nonequilibrium *GF* and applying the diagram technique Keldysh derived the close equation of motion for one-particle causal *GF*.

For the time-reversed situation, we had to use *anticausal* initial condition, i. e., the condition that the system was in thermodynamical equilibrium at the time $t = +\infty$, in order to derive, by means of diagram technique, the close equation of motion for one-particle anticausal *GF*.

We have shown that by means of this equation we get the quantum-mechanical *Boltzmann equation* with erroneous sign of collision term which provided that the selection of the boundary condition that the system lies in thermodynamical equilibrium in far past, i. e., at the time $t = -\infty$, predetermines the irreversible motion of the system towards the equilibrium in the future.

2. *Definition of anticausal nonequilibrium real-time GF*

Let us observe a system of interacting particles affected by an external time dependent field. The total Hamiltonian of the system $H(t)$ will be divided into two terms. The first term $H_0(t)$ is the Hamiltonian of free particles in the external field, while the second term $V(t)$ represents the term describing the particle interaction in the external field:

$$H(t) = \begin{cases} H_0 + V & t < t_0 \\ H_0(t) + V(t), & t > t_0 \end{cases} \tag{2.1}$$

where t_0 is the initial moment of the inclusion of the external field.

Keldysh preparated the system in equilibrium in a remote earlier time $t_0 = -\infty$ taking the initial condition:

$$\varrho_I(t = -\infty) = \varrho_{eq} = \exp\{\Psi_0 - H_0(-\infty)\}/kT, \tag{2.2}$$

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 ϱ_I Keldysh ignores the initial particle correlation. For the beginning of the external field action Keldysh takes the moment $t_0 = -\infty$.

Keldysh defines causal one-particle GF in interaction representation as:

$$G(1,2) = \pm \frac{1}{\mathrm{i}} \mathrm{Tr}\{\varrho_I(-\infty)\, \mathrm{T}_C(S_C \psi_I(1)\, \psi_I^{\dagger}(2))\}, \tag{2.3}$$

where T_C indicates ordering along contour c going from $-\infty$ to $+\infty$ and then returning back to $-\infty$; S_c is complete S-matrix along the whole contour c; $1 = (\vec{r}_1, t_1)$, $2 = (\vec{r}_2, t_2)$.

Let us consider a time-reversed system. The external field can be observed as a time-dependent perturbation which starts to act the system which is in the thermodynamical equilibrium in the far future, i. e., at the time $t_0 = +\infty$.

For a time-reversed situation we have instead of (2.2) the initial condition:

$$\tilde{\varrho}_I(t = +\infty) = \varrho_{eq} = \exp\{\Psi_0 - H_0(+\infty)\}/kT. \tag{2.4}$$

By means of that initial condition we will define the anticausal nonequilibrium real-time GF as:

$$\tilde{G}(1,2) = \pm\, \mathrm{i}\, \mathrm{Tr}\{\tilde{\varrho}_I(+\infty)\, \tilde{\mathrm{T}}_{\tilde{c}}(\tilde{S}_{\tilde{c}} \psi_I(1)\, \psi_I^{\dagger}(2))\}, \tag{2.5}$$

where $\tilde{\mathrm{T}}_{\tilde{c}}$ indicates ordering along the contour $\tilde{c}$ going from $+\infty$ to the $-\infty$ and then returning back to $+\infty$, $\tilde{S}_{\tilde{c}}$ is the complete S-matrix defined along the whole contour $\tilde{c}$.

For such a defined anticausal GF we can prove that:

$$\tilde{G}^{>}(1,2) = (G^{<}(1,2))^{*}. \tag{2.6}$$

That means that anticausal GF defined as Eq. (2.5) really represents the time-reversed solution of the equation of motion for the causal GF.

3. *Equation of motion for the one-particle anticausal GF*

In order to derive the close equation of motion for the one-particle anticausal GF we proceed as Keldysh did using diagram techniques.

To go over the matrix form of writing the equations we defined a two-rowed matrix $\tilde{G}$ and $\tilde{\Sigma}$ in the following manner:

$$\tilde{G} = \begin{pmatrix} \tilde{G}^{c} & \tilde{G}^{-} \\ \tilde{G}^{+} & \tilde{\tilde{G}}^{c} \end{pmatrix}; \quad \tilde{\Sigma} = \begin{pmatrix} \tilde{\Sigma}'^{c} & \tilde{\Sigma}^{-} \\ \tilde{\Sigma}^{+} & \tilde{\tilde{\Sigma}}'^{c} \end{pmatrix}, \tag{3.1}$$

where

$$\tilde{G}^{-}(1,2) = -\mathrm{i}\,\langle \psi_H^{+}(2)\,\psi_H(1)\rangle, \tag{3.2}$$

$$\tilde{G}^{+}(1,2) = \mathrm{i}\,\langle \psi_H(1)\,\psi_H^{+}(2)\rangle, \tag{3.3}$$

$$\tilde{G}^{c}(1,2) = \mathrm{i}\,\langle \tilde{T}(\psi_H(1)\,\psi_H^{+}(2))\rangle, \tag{3.4}$$

$$\tilde{\tilde{G}}^{c}(1,2) = \mathrm{i}\,\langle T(\psi_H(1)\,\psi_H^{+}(2))\rangle, \tag{3.5}$$

and $\tilde{\Sigma}$ are anticausal self-energy operators satisfying relation

$$\tilde{\Sigma}^{c} + \tilde{\tilde{\Sigma}}^{c} = -(\tilde{\Sigma}^{+} + \tilde{\Sigma}^{-}). \tag{3.6}$$

We have here only a system of Fermi-particles.

The technique for evolution of any arbitrary graph is completely analogous with Keldysh's technique.

The summation of the diagrams for the complete *GF* leads to an equation of the type of Dyson's equation:

$$\tilde{G}(\vec{r}\,t;\vec{r}'\,t') = \tilde{G}_0(\vec{r}\,t;\vec{r}'\,t') + \mathrm{i}\,g^2 \int\limits_{+\infty}^{-\infty}\int\limits_{+\infty}^{-\infty} \tilde{G}_0(\vec{r}\,t;\vec{r}'\;t') \tag{3.7}$$

$$\times\,\tilde{\Sigma}(\vec{r}_1\,t_1,\vec{r}_2\,t_2)\,\tilde{G}(\vec{r}_2\,t_2,\vec{r}'\,t')\,\mathrm{d}\vec{r}_1\,\mathrm{d}\vec{r}_2\,\mathrm{d}t_1\,\mathrm{d}t_2.$$

Acting on this equation with operator

$$\hat{G}_0^{-1} = G_0^{-1}(x)\,G_z; \quad G_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \tag{3.8}$$

where

$$G_0^{-1}(x) = \mathrm{i}\frac{\partial}{\partial t} - \varepsilon\left(-\mathrm{i}\,\nabla - \frac{e}{c}\vec{A}(x)\right) - e\vec{\Phi}(x), \tag{3.9}$$

$\{\vec{A}(x), \vec{\Phi}(x)\}$ is external electromagnetic field: $x = (\vec{r}, t)$.

Proceeding in the same manner as Keldysh did we derived the equation of motion for one-particle anticausal *GF*:

$$\left\{\mathrm{i}\left(\frac{\partial}{\partial t} - \frac{\partial}{\partial t'}\right)\right\} - \varepsilon\left[-\mathrm{i}(\nabla_{\vec{r}} - \nabla_{\vec{r}'}) - \frac{e}{c}(\vec{A}(x) + \vec{A}(x'))\right]$$

$$- e(\vec{\Phi}(x) + \vec{\Phi}(x'))\}\,\tilde{G}^{-}(x,x')$$

$$= \mathrm{i}\,g^2 \int\limits_{-\infty}^{+\infty} \mathrm{d}x''\,\{\tilde{\Sigma}^{-}(x,x'')\,\tilde{G}^{+}(x'',x') - \tilde{G}^{-}(x,x'')\,\tilde{\Sigma}^{+}(x'',x')\}. \tag{3.10}$$

4. *Proof that the equation of motion for one-particle causal GF is time-reversal noninvariant*

For a function $G^+ (\vec{r}\, t, \vec{r}'\, t')$ which taken at coincident times $t' = t$ directly determines the distribution of electrons; Keldysh derived equation of motion which has the form:

$$\begin{aligned} &\left\{ \mathrm{i} \left(\frac{\partial}{\partial t} - \frac{\partial}{\partial t'} \right) - \varepsilon \left[- \mathrm{i} (\nabla_{\vec{r}} - \nabla_{\vec{r}'}) - \frac{e}{c} (\vec{A}(x) + \vec{A}(x')) \right] \right. \\ &\qquad \left. - e (\vec{\Phi}(x) + \vec{\Phi}(x')) \right\} G^+ (x, x') \qquad (4.1) \\ &= \mathrm{i} g^2 \int_{-\infty}^{+\infty} \mathrm{d}x'' \{ \Sigma^+ (x, x'') G^- (x'', x') - \Sigma^- (x, x'') G^- (x'', x') \}. \end{aligned}$$

If Wigner time-reversal is applied to equation (4.1), that is, if we first exchange the arguments x, x' and afterwards perform the complex conjugation of the equation using Eq. (2.6), we get:

$$\begin{aligned} &\left\{ \mathrm{i} \left(\frac{\partial}{\partial t} - \frac{\partial}{\partial t'} \right) - \varepsilon \left[- \mathrm{i} (\nabla_{\vec{r}} - \nabla_{\vec{r}'}) - \frac{e}{c} (\vec{A}(x) + \vec{A}(x')) \right] \right. \\ &\qquad \left. - e (\vec{\Phi}(x) + \Phi(x')) \right\} \widetilde{G}^- (x, x') \qquad (4.2) \\ &= - \mathrm{i} g^2 \int_{-\infty}^{+\infty} \mathrm{d}x'' \{ \widetilde{\Sigma}'^- (x, x'') \widetilde{G}^+ (x'', x') - \widetilde{G}^- (x, x'') \widetilde{\Sigma}^+ (x'', x') \}. \end{aligned}$$

This is not the same equation as equation (3.10), derived on the basis of the definition of one-particle causal *GF*. So that it follows that equation (4.1) is time-reversal nonivariant. As other assumption made at the derivation of equation (4.1) could not affect the time symmetry of this equation it follows that the cause of time-reversal noninvariant exclusively lies in the selection of causal boundary condition.

5. *Derivation of the quantum mechanical »anticausal Boltzmann equation«*

From Eq. (4.1) Keldysh derived quantum mechanical Boltzmann equation which describes the irreversible motion of perturbed system to the equilibrium in the future so that it could be expected that equation (3.10) referring to the time-reversed system should yield similar equation which would describe the motion of this system towards equilibrium in the past.

We are going over from variables x, x' to the new variables $(\vec{r}_s, t_s) = x_s = (x + x')/2$ and $(\vec{r}_a, t_a) = x_a = (x - x')/2$. By means of these new variables we define $\widetilde{G}^- (\vec{r}\, t, \vec{p}\, \varepsilon)$ as:

$$\widetilde{G}^- (\vec{r}_s\, t_s, \vec{p}\, \varepsilon) = \int_{-\infty}^{+\infty} \mathrm{d}\vec{r}_a \int_{-\infty}^{+\infty} \mathrm{d}t_a \exp(-\mathrm{i}\, \vec{p}_- \vec{r}_a + \mathrm{i}\, \varepsilon\, t_a) \times \widetilde{G}^- (\vec{r}_a\, t_a, \vec{r}_s\, t_s), \tag{5.1}$$

which can be interpreted as the particle density with the momentum $\vec{p}_- = -\vec{p}$ and by energy ε in the space-time point, $\vec{r}, t < 0$ of the time-reversed system. Therefrom stems the definition of the corresponding distribution function:

$$\widetilde{f}(\vec{p}_-, \vec{r}, t) = \frac{\mathrm{i}}{2\pi} \int_{-\infty}^{+\infty} \mathrm{d}\varepsilon\, \widetilde{G}^- (\vec{r}\, t, \vec{p}\, \varepsilon). \tag{5.2}$$

Inserting the new coordinates in (3.10) and by means of defining (5.1) and (5.2) using the quasi-classical nature of the external field and assuming that the interaction is small, upon a lengthy transformation we get the equation:

$$\begin{aligned}
&\left\{ \frac{\partial}{\partial t_-} - \vec{v}\, \nabla_{\vec{r}} + e \left(\vec{\mathscr{E}} + \frac{\vec{v} \times \vec{H}}{c} \right) \nabla_{\vec{p}_-} \right\} \widetilde{f}(\vec{p}_-, \vec{r}, t) \\
&= -2\pi g^2 \int_{-\infty}^{+\infty} |\, m_{\vec{k}_-} |^2 \{ [(1 + N_{\vec{k}_-})\, \delta\, (\varepsilon_{\vec{p}_-} - \varepsilon_{\vec{p}_- + \vec{k}_-} + \omega_{\vec{k}_-}) \\
&+ N_{\vec{k}_-}\, \delta\, (\varepsilon_{\vec{p}_-} - \varepsilon_{\vec{p}_- + \vec{k}_-} - \omega_{\vec{k}_-})]\, \widetilde{f}(\vec{p}_- + \vec{k}_-, \vec{r}\, t_-)\, [1 - \widetilde{f}(\vec{p}_-, \vec{r}, t_-) \\
&- [(1 + N_{\vec{k}_-})\, \delta\, (\varepsilon_{\vec{p}_-} - \varepsilon_{\vec{p}_- + \vec{k}_-} - \omega_{\vec{k}_-}) + N_{\vec{k}_-} \delta\, (\varepsilon_{\vec{p}_-} - \varepsilon_{\vec{p}_- + \vec{k}_-} + \omega_{\vec{k}_-})] \\
&\times [1 - \widetilde{f}(\vec{p}_- + \vec{k}_-, \vec{r}, t_-)]\, \widetilde{f}(\vec{p}_-, \vec{r}, t_-) \frac{\mathrm{d}\vec{k}_-}{(2\pi)^3}.
\end{aligned} \tag{5.3}$$

Equation (5.3) differs from the quantum-mechanical Boltzmann equation (Ref, 2.) Eq. (7)) only in the sign of the collision term and describes time-reversal of the original process described by this equation. Therefore we shell call it the *anticausal Boltzmann equation.*

6. Discussion

In the present paper we have shown that the selection of the boundary condition that the system was in a thermodynamical equilibrium at the time $t = -\infty$ predetermines the irreversible motion towards future, described by the distribution function fulfilling the causality condition[4].

If we observe time-reversed system choosing the boundary condition that the system was in equilibrium in the far future, i. e. at the time $t = + \infty$ we get the *Boltzmann equation* with erroneous sign of collision term. The solution of this equation violates the causality condition that is the value of the distribution function at moment t depends on the external field acting on the system after this moment.

That is why here as well in the Kadanoff and Baym method we reach the conclusion that the difference between the causal and anticausal behaviour of the system stems from the selection of the boundary condition and the irreversibility appears as a consequence of the causality condition.

Thereby we have unambigously proved that the quantum mechanical treatment of nonequilibrium process explicitly imposes the boundary condition as a cause of irreversible behaviour of the system unlike the classical approach, wherein they are implicitly contained in the hypothesis of molecular chaos.

Since these conditions can only be imposed on a system from the outisde, and since indeed it is impossible for a local system to be truly isolated from the influence of the rest of the universe one is inevitably led to cosmological considerations$^{5)}$.

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VREMENSKA NESIMETRIČNOST GENERALISANE KVANTNO-MEHANIČKE BOLTZMANNOVE KINETIČKE JEDNAČINE KOJU JE IZVEO KELDYSH

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Posmatrajući sistem u kome je izvršena inverzija vremena i koristeći tehniku dijagrama za antikauzalne Greenove funkcije, pokazano je da razlog vremenske nesimetričnosti generalisane kvantnomehaničke Boltzmannove kinetičke jednačine koju je izveo Keldysh, leži u izboru graničnog uslova da se perturbovani sistem nalazio u termodinamičkoj ravnoteži u trenutku $t = - \infty$.