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ON THE HIGHER-ORDER RESPONSE OF A SUPERCONDUCTOR

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ON THE HIGHER-ORDER RESPONSE OF A SUPERCONDUCTOR

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1. Introduction

We consider the response of a superconductor to the external fields ϕ , $\vec{A}$ (electromagnetic potential), Δ (superconducting order parameter treated as an external field) and Δ^{+} in arbitrary order. In calculating this response it is convenient first to solve an unphysical problem in an imaginary time interval (for which the boundary conditions for the Green functions are known) and then to go over to the physical problem by analytical continuation. There are different ways to do this.

Following Kadanoff and Baym[1] we solve in the present paper the equations of motion for the Green functions in the time interval $[t_0, t_0 - i\beta]$ (t_0 real, $\beta = 1/T$)[x]. The external fields are considered to be analytical functions in the domain $0 \geq \mathrm{Im}\, t \geq -\beta$ and to satisfy the condition

$$\lim_{\mathrm{Re}\, t \to -\infty} \phi(t) = 0 \qquad (1)$$

[x] Throughout the paper we use $\hbar = c = k_{\mathrm{Boltzmann}} = 1$.

(analogous for the other fields) describing the absence of the fields at very early times. The resulting correlation functions, for example $F^{+>}(12) = \langle \psi_{\downarrow}^{+}(1)\, \psi_{\uparrow}^{+}(2) \rangle$, are then analytically continued to real times. The physical problem is determined by correlation functions, for example $f^{+>}(12)$ [x/], which are defined for real times and which describe the response of the superconductor to the external fields turned on at an early time. In /1/ it is proven that the two types of correlation functions (for example $F^{+>}$ and $f^{+>}$) are both analytical functions and coincide in the limit $t_0 \to -\infty$.

Recently, Gorkov and Eliashberg/2/ treated the same problem in another way. They considered the Green functions and the external fields in the time interval $[0, -i\beta]$ with the usual boundary conditions (for example for the potential $\phi(t)|_{t=0} = \phi(t)|_{t=-i\beta}$). The coefficients $B^{(\ell)}(\omega_1, \ldots, \omega_\ell)$ (where $\omega_s = i 2\pi n_s / \beta$) describing the response of the correlation functions to the external fields, for example

$$\langle \psi_{\downarrow}^{+}(1)\, \psi_{\uparrow}(1) \rangle_{\omega} = B^{(1)}(\omega)\, \Delta_{\omega}^{+} + \ldots \qquad (2)$$
$$+ \sum_{\omega_1+\omega_2+\omega_3=\omega} B^{(3)}(\omega_1, \omega_2; \omega_3)\, \Delta_{\omega_1}^{+}\, \Delta_{\omega_2}\, \Delta_{\omega_3}^{+} + \ldots,$$

are then (in the upper half-plane) analytically continued to real frequencies. The corresponding coefficients $b^{(\ell)}$, which describe the physical response and which are first defined for real frequencies, are also analytical functions in the upper half-plane because of the causality condition. The method of Gorkov and Eliashberg/2/ is based on the probable, but not proven identity of the two types of analytical functions [xx/].

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x/ For the definition see equation (16).

xx/ We remark in this connection, that in each order the result is a certain sum of terms, where each term is an analytical function in the upper half-plane.

The Kadanoff-Baym method of analytical continuation in the time representation is not more complicated than the analytical continuation in the frequency representation and has the advantage over the latter, that for it exists an appropriate proof of the identity of the two types of analytical functions resulting from the physical and the unphysical problems. Because of the differences between the two methods it seemed easier to compare the results than to discuss the connection between these methods. The results of the present paper justify the treatment of Gorkov and Eliashberg /2/. The general considerations are also applicable to other similar problems.

2. Basic Formulae

The superconductor is described by the Hamiltonian $H = H_0 + H_1$, where

$$H_0 = \int d^3r \, \psi^+_\alpha \, h(\vec{r}) \, \psi_\alpha \quad , \tag{3}$$

$$\begin{aligned} H_1 = \int d^3r \{ & \rho \phi(\vec{r}\, t) - \vec{j}\, \vec{A}(\vec{r}\, t) + \\ & + \psi^+_\uparrow \psi^+_\downarrow \Delta(\vec{r}\, t) + \psi_\downarrow \psi_\uparrow \Delta^+(\vec{r}\, t) \} , \end{aligned} \tag{4}$$

$$h(\vec{r}) = -\frac{\vec{\nabla}^2}{2m} - \mu + \sum_{\vec{a}} u(\vec{r} - \vec{a}) . \tag{5}$$

μ is the chemical potential, $u(\vec{r}-\vec{a})$ is the potential of an impurity at $\vec{r} = \vec{a}$, ρ is the charge density and $\vec{j}$ the current density. For self-consistency it is necessary that for all times Δ and Δ^+ coincide with the averages of $|g| \psi_\uparrow \psi_\downarrow$ and $|g| \psi^+_\downarrow \psi^+_\uparrow$, respectively (g is the coupling constant).

We consider the Green functions

$$G_{\alpha\beta}(12) = \delta_{\alpha\beta} G(12) = \frac{1}{i} \frac{\langle TS \psi_\alpha(1) \psi^+_\beta(2) \rangle}{\langle TS \rangle} , \tag{6}$$

$$F^{+}_{\alpha\beta}(12) = I_{\alpha\beta}\, F^{+}(12) = \frac{\langle TS\, \psi^{+}_{\alpha}(1)\, \psi^{+}_{\beta}(2) \rangle}{\langle TS \rangle} \tag{7}$$

in the time interval $[t_0, t_0 - i\beta]$. Here means $\langle \ldots \rangle = \mathrm{tr}(\ldots e^{-\beta H_0})/\mathrm{tr}\, e^{-\beta H_0}$; $I_{\downarrow\uparrow} = 1$, $I_{\uparrow\downarrow} = -1$
(the other elements are zero), and S is given by

$$S = \exp\{-i \int_{t_0}^{t_0 - i\beta} dt\, H_1(t)\}. \tag{8}$$

The time dependence of the operators is given in the interaction picture x/.

The Green functions satisfy the equations of motion

$$\{ i \frac{\partial}{\partial t_1} - h(\vec{r}_1) - \Phi(1) \}\, G(12) + i\, \Delta(1)\, F^{+}(12) = \delta(1-2), \tag{9}$$

$$\{ i \frac{\partial}{\partial t_1'} + h(\vec{r}_1) + \Phi^{+}(1) \}\, F^{+}(12) - i\Delta^{+}(1)\, G(12) = 0, \tag{10}$$

with

$$\begin{aligned} \Phi(1) &= e\,\phi(1) + \frac{ie}{m} \vec{A}(1)\, \nabla, \\ \Phi^{+}(1) &= e\,\phi(1) - \frac{ie}{m} \vec{A}(1)\, \nabla \end{aligned} \tag{11}$$

x/ For example $\psi^{+}(t) = e^{iH_0 t}\, \psi^{+}(0)\, e^{-iH_0 t}$. For real times (or for quantities independent of time) + has the usual meaning of Hermitean (or complex) conjugate .

(we use a gauge for which $\nabla \vec{A} = 0$ and neglect the term containing A^2), and the boundary condition

$$G(12)\Big|_{t_1=t_0} = -G(12)\Big|_{t_1=t_0-i\beta} \tag{12}$$

and analogous for F^+ .

By help of the unperturbed Green functions $G_0^{(\mp)}$, satisfying the equations of motion

$$\{ i\frac{\partial}{\partial t_1} \mp h(\vec{r}_1)\} G_0^{(\mp)}(12) = \delta(1-2) \tag{13}$$

and the boundary condition (12), we convert equations (9) and (10) into integral equations:

$$\begin{aligned} G(11') = G_0^{(-)}(11') - i \int_{t_0}^{t_0-i\beta} G_0^{(-)}(12)\, \Delta(2)\, F^+(21') + \\ + \int_{t_0}^{t_0-i\beta} G_0^{(-)}(12)\, \Phi(2)\, G(21'), \end{aligned} \tag{14}$$

$$\begin{aligned} F^+(11') = i \int_{t_0}^{t_0-i\beta} G_0^{(+)}(12)\, \Delta^+(2)\, G(21') - \\ - \int_{t_0}^{t_0-i\beta} G_0^{(+)}(12)\, \Phi^+(2)\, F^+(21'). \end{aligned} \tag{15}$$

The integrals in these (and further) equations indicate space (or momentum) and time integrations over all internal variables.

Equations (14) and (15) can be iterated and lead to the following rules for the construction of the diagrams: One has to insert the vertex Φ between two $G_0^{(-)}$ functions, the vertex $-\Phi^+$ between two $G_0^{(+)}$ functions, the vertex $-i\Delta$ between $G_0^{(-)}$ and $G_0^{(+)}$, and the vertex $i\Delta^+$ between $G_0^{(+)}$ and $G_0^{(-)}$.

In this way we can calculate the corresponding correlation functions $F^{+>}$, $G^>$ and $F^{+<}$, $G^<$ in the time interval $[t_0, t_0 - i\beta]$.

The correlation functions $f^{+>}, g^{>}$ and $f^{+<}, g^{<}$ describing the physical problem of the response of the superconductor to the external fields, for example

$$f^{+>}(12) = \langle \tilde{\tilde{\psi}}_{\downarrow}^{+}(1) \; \tilde{\tilde{\psi}}_{\uparrow}^{+}(2) \rangle , \tag{16}$$

with

$$\tilde{\tilde{\psi}}_{\downarrow}^{+}(1) = U^{+}(1) \; \psi_{\downarrow}^{+}(1) \, U(1), \tag{17}$$

$$U(1) = T \exp\{ - i \int_{-\infty}^{t_1} dt \, H_1(t) \} \tag{18}$$

(t_1, t_2 real), can be calculated from $F^{+\gtrless}, G^{\gtrless}$, by means of analytical continuation.

3. Analytical Continuation

As already stated in the introduction the analytical continuation in the time representation is based on the following theorem of Kadanoff and Baym [1], valid for external fields which are analytical functions in the domain $0 \geq \mathrm{Im}\, t \geq -\beta$ and satisfy condition (1):

(i) The correlation functions $F^{+>}, G^{>}$ and $F^{+<}, G^{<}$ are analytical functions of their time variables in the domains

$$0 \geq \mathrm{Im}(t_1 - t_2) > -\beta \qquad \text{for} \quad F^{+>}, G^{>}, \tag{19a}$$

$$0 \leq \mathrm{Im}(t_1 - t_2) < \beta \qquad \text{for} \quad F^{+<}, G^{<}. \tag{19b}$$

(ii) The correlation functions $f^{+>}, g^{>}$ and $f^{+<}, g^{<}$ are also analytical functions in the domains (19a) and (19b), respectively. In the limit $t_0 \to -\infty$ the two types of analytical functions coincide, that means $f^{+>} = F^{+>}$, ...

The iterated equations (14) and (15) lead to integrals of the type

$$I_n(11') = \int_{t_0}^{t_0-i\beta} G_0^{(\pm)}(12)\, G_0^{(\pm)}(23) \ldots G_0^{(\pm)}(n,1'), \tag{20}$$

with
$$I_1(11') = G_0^{(\pm)}(11').$$

(In considering the process of analytical continuation we omit the vertices between the $G_0^{(\pm)}$). The corresponding correlation functions satisfy the recursion formulae

$$\begin{aligned} I^{>}_{n+1}(11') &= \int_{t_0}^{t_1'} I^{>}_n(12)\, G^{<}_0(21') + \\ &+ \int_{t_1'}^{t_1} I^{>}_n(12)\, G^{>}_0(21') + \int_{t_1}^{t_0-i\beta} I^{<}_n(12)\, G^{>}_0(21') \end{aligned} \tag{21}$$

and analogous for $I^{<}_{n+1}$. In (21) and the following formulae we have omitted the indices $\pm$ from G_0. The analytical continuation of (21) to real times leads to

$$\begin{aligned} I^{\gtrless}_{n+1}(11') &= \int_{-\infty}^{\infty} I^{\gtrless}_n(12)\, G^{A}_0(21') + \\ &+ \int_{-\infty}^{\infty} I^{R}_n(12)\, G^{\gtrless}_0(21'), \end{aligned} \tag{22}$$

where

$$G_0^{R,A}(12) = \left\{ \begin{matrix} \theta(t_1 - t_2) \\ -\theta(t_2 - t_1) \end{matrix} \right\} (G_0^{>}(12) - G_0^{<}(12)) \tag{23}$$

and analogous for $I^{R,A}$. With the help of the recursion formula (22) we get for the equal-time correlation functions the result

$$\begin{aligned} I^{\gtrless}_n(11) = \int_{-\infty}^{\infty} \{ & G_0^{\gtrless}(12) G_0^{A}(23)\, G_0^{A}(34) \ldots G_0^{A}(n1) + \\ & + G_0^{R}(12)\, G_0^{\gtrless}(23)\, G_0^{A}(34) \ldots G_0^{A}(n1) + \end{aligned} \tag{24}$$

$$+ G_0^R(12)\, G_0^R(23)\, G^R_0(34) \ldots G_0^{\gtrless}(n1)\},$$

where all times are real.

As example we consider the physical response of Δ^+ to the external fields, which is given by the analytical continuation to real times of

$$\Delta^+(1) = |g|\, F^{+>}(11) = \frac{1}{2}|g|\,(F^{+>}(11) + F^{+<}(11)). \tag{25}$$

For a term $\Lambda^{+(n)}$ of the n-th order we get from (24) (going over to the frequency representation)

$$\Delta^{+(n)}_\omega = \frac{1}{2}|g| \int d\omega_1 \frac{d\omega'}{2\pi} \cdots \frac{d\omega^{(n)}}{2\alpha}\, \delta(\omega - \omega' - \ldots - \omega^{(n)}) \times$$

$$\times\{ -\mathrm{th}\frac{\beta\omega_1}{2} G_0^A(\omega_1) f_{\omega'} G_0^A(\omega_1 - \omega') \ldots f_{\omega^{(n)}} G_0^A(\omega_1 - \omega) +$$

$$+\mathrm{th}\frac{\beta(\omega_1-\omega)}{2} G_0^R(\omega_1) f_{\omega'} G_0^R(\omega_1 - \omega') \ldots f_{\omega^{(n)}} G_0^R(\omega_1 - \omega) +$$

$$+G_0^R(\omega_1)\left[\mathrm{th}\frac{\beta\omega_1}{2} - \mathrm{th}\frac{\beta(\omega_1-\omega')}{2}\right] f_{\omega'} G_0^A(\omega_1 - \omega') \ldots f_{\omega^{(n)}} G_0^A(\omega_1 - \omega) + \tag{26}$$

$$+ G_0^R(\omega_1) f_{\omega'} G_0^R(\omega_1 - \omega')\left[\mathrm{th}\frac{\beta(\omega_1-\omega')}{2} - \mathrm{th}\frac{\beta(\omega_1-\omega'-\omega'')}{2}\right] f_{\omega''} G_0^A(\omega_1 - \omega' - \omega'') \ldots f_{\omega^{(n)}} G_0^A(\omega_1 - \omega) +$$

$$+ G_0^R(\omega_1) f_{\omega'} G_0^R(\omega_1 - \omega') \ldots \left[\mathrm{th}\frac{\beta(\omega_1 - \omega' - \ldots - \omega^{(n-1)})}{2} - \mathrm{th}\frac{\beta(\omega_1-\omega)}{2}\right] f_{\omega^{(n)}} G_0^A(\omega_1 - \omega)\},$$

where we have used

$$G_0^{>}(\omega) + G_0^{<}(\omega) = \operatorname{th}\frac{\beta\omega}{2}\left(G_0^R(\omega) - G_0^A(\omega)\right). \qquad (27)$$

The vertex functions f_ω in (26) stand for $-i\Delta_\omega$, $i\Delta^+_\omega$, Φ_ω and $-\Phi^+_\omega$ in accordance with the rules given at the end of section 2.

It is possible, formally to sum up all terms for Δ^+ with the help of the retarded and advanced solutions of the equations (all times are real)

$$\left\{ i\frac{\partial}{\partial t_1} - h(\vec{r}_1) - \Phi(1)\right\} G^{(-)}(12) + i\,\Delta(1)F^+(12) = \delta(1-2),$$
$$\left\{ i\frac{\partial}{\partial t_1} + h(\vec{r}_1) + \Phi^+(1)\right\} F^+(12) - i\,\Delta^+(1)G^{(-)}(12) = 0, \qquad (28)$$

and

$$\left\{ i\frac{\partial}{\partial t_1} + h(\vec{r}_1) + \Phi^+(1)\right\} G^{(+)}(12) - i\,\Delta^+(1)F(12) = \delta(1-2),$$
$$\left\{ i\frac{\partial}{\partial t_1} - h(\vec{r}_1) - \Phi(1)\right\} F(12) + i\,\Delta(1)G^{(+)}(12) = 0. \qquad (29)$$

We get the final result

$$\Delta^+_\omega = \frac{1}{2}|g| \int \frac{d\omega_1}{2\pi}\left\{ -\operatorname{th}\frac{\beta\omega_1}{2} F^{+A}_{\omega_1,\omega_1-\omega} + \operatorname{th}\frac{\beta(\omega_1-\omega)}{2} F^{+R}_{\omega_1,\omega_1-\omega}\right\} +$$
$$+\frac{1}{2}|g| \int \frac{d\omega_1}{2\pi}\frac{d\omega_2}{2\pi}\frac{d\omega'}{2\pi}\left[\operatorname{th}\frac{\beta\omega_2}{2} - \operatorname{th}\frac{\beta(\omega_2-\omega')}{2}\right]\times$$
$$\times\left\{ i\,G^{(+)R}_{\omega_1\omega_2}\Delta^+_{\omega'}\,G^{(-)A}_{\omega_2-\omega',\omega_1-\omega} - i\,F^{+R}_{\omega_1\omega_2}\Delta_{\omega'}\,F^{+A}_{\omega_2-\omega',\omega_1-\omega} - \right. \qquad (30)$$
$$\left. - G^{(+)R}_{\omega_1\omega_2}\Phi^+_{\omega'}F^{+A}_{\omega_2-\omega',\omega_1-\omega} + F^{+R}_{\omega_1\omega_2}\Phi_{\omega'}\,G^{(-)A}_{\omega_2-\omega',\omega_1-\omega}\right\}.$$

In (26) and (30) we have not indicated the necessary integrations over the coordinates or the momenta.

The results (26) and (30) coincide[x] with the results of Gorkov and Eliashberg[2] and, therefore, justify their treatment.

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References

1. L.P.Kadanoff and G.Baym. Quantum Statistical Mechanics, Chapter 8-2, New York 1962.
2. L.P.Gorkov and G.M.Eliashberg. Zh. eksper. teor. Fiz. 54, 612 (1968).

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[x] Note slight differences in the notation.