ON THE COMPENSATION EQUATION IN SUPERCONDUCTIVITY THEORY

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A relation between the matrix elements of the variational derivatives of the scattering matrix and the energy operator is established. With its aid the kernel of the integral equation for the compensation of "dangerous" diagrams is expressed in terms of the usual Green functions.

1. INTRODUCTORY REMARKS

An analysis of the influence of the Coulomb interaction between electrons in superconductivity theory was given in a paper by Bogolyubov, Tolmachev, and the author.[1] The structure of the kernel $Q(k, k')$ of the integral equation for the compensation of dangerous electron diagrams was also investigated (§5). This kernel was expressed in terms of the characteristics of the auxiliary model problem which describes the Coulomb interaction between the electrons and also their interaction with the auxiliary classical external field. The above-mentioned characteristics of the model problem were strictly determined only in one case through the method of approximate second quantization (§6.1). In the remaining cases expressions for these characteristics, containing "radiative" Coulomb corrections, were estimated, in the region of the infrared catastrophe, from qualitative considerations (§6.2). The reason for this was that the method of expressing the kernel Q in terms of the energy operator

$$R = H_{\text{int}} T\left(\exp\left\{-i\int_{-\infty}^{0} H_{\text{int}}(t)dt\right\}\right) = H_{\text{int}} S^{0}_{-\infty} \quad (1.1)$$

which was used in that paper, leads for a number of cases to inconvenient and asymmetric expressions.

It is, however, well known that the energy characteristics of a many-body system can be expressed in terms of the "total" S-matrix[2,3]

$$S = S^{\infty}_{-\infty} = T\left(\exp\left\{-i\int_{-\infty}^{\infty} H_{\text{int}}(t)dt\right\}\right). \quad (1.2)$$

In the present investigation such an approach is used as the basis of the discussion. Through this the kernel $Q(k, k')$ is expressed in terms of the vacuum matrix elements of the variational derivatives of S, i.e., in terms of the usual Green functions for which explicit expressions can be obtained, for instance, by the method of approximate second quantization.[5]

2. THE RELATION BETWEEN THE OPERATORS S AND R AND THEIR VARIATIONAL DERIVATIVES

The connection of the energy levels of a system which has undergone second quantization and the total scattering matrix S was recently investigated by Sucher[2] and Rodberg.[3] The most convenient formula was obtained by Rodberg (Eq. (16) of reference 3).* From this formula follows, in particular, a connection between the matrix elements of the total S-matrix (1.2) and those of the energy operator R (1.1) which can be written in the form

$$\langle \Phi_n^* S \Phi_n \rangle_c = -2\pi i \delta(E - E_n) \langle \Phi_n^* R \Phi_n \rangle_c. \quad (2.1)$$

The index "c" indicates here that only connected diagrams are taken into account in the evaluation of the matrix elements.

Equations of the type (2.1) can also be established for the commutators of the quantities S, R with the particle creation and annihilation operators, and also for the variational derivatives of S and R with respect to those operators.

Let $a^+_{k,\sigma}$ be the creation operator for an electron with momentum k, energy $\epsilon(k)$ and spin σ. We can then connect the commutator [see Eq. (47.13) of reference 4]

$$[a^+_{k,\sigma}, S]_- = -\sum_{k',\sigma'}\int_{-\infty}^{\infty} \frac{\delta S}{\delta a_{k',\sigma'}(t)} [a^+_{k,\sigma}, a_{k',\sigma'}(t)]_+ dt$$

$$= -\int_{-\infty}^{\infty} \frac{\delta S}{\delta a_{k,\sigma}(t)} e^{-i\epsilon(k)t} dt \quad (2.2)$$

with the commutator

$$[a^+_{k,\sigma}, R] = -\int_{-\infty}^{0} \frac{\delta R}{\delta a_{k,\sigma}(t)} e^{-i\epsilon(k)t} dt \quad (2.3)$$

*A similar formula was independently obtained by V. V. Tolmachev (unpublished).

through the relation

$$[a^{+}_{k,\sigma}, S]\,\Phi_E = -i\int_{-\infty}^{\infty} e^{it(H_0+\varepsilon(k)-E)}\,dt\,[a^{+}_{k,\sigma}, R]\,\Phi_E. \quad (2.4)$$

To show that, we write (2.1) in the form

$$S\Phi_E = -i\int_{-\infty}^{\infty} e^{it(H_0-E)}\,dt R\Phi_E. \quad (2.5)$$

From (2.5) follows also that

$$Sa^{+}_{k,\sigma}\Phi_E = -i\int_{-\infty}^{\infty} e^{it(H_0-E-\varepsilon(k))}\,dt\,Ra^{+}_{k,\sigma}\Phi_E. \quad (2.6)$$

On the other hand,

$$a^{+}_{k,\sigma}S\Phi_E = -ia^{+}_{k,\sigma}\int_{-\infty}^{\infty} e^{it(H_0-E)}\,dt R\Phi_E$$

$$= -i\int_{-\infty}^{\infty} e^{it(H_0-\varepsilon(k)-E)}\,dt\,a^{+}_{k,\sigma}R\Phi_E. \quad (2.7)$$

The difference between Eqs. (2.6) and (2.7) gives (2.4).

Considering more complicated commutators we arrive at the formula

$$\int_{-\infty}^{\infty}\left\langle\Phi_1^{*}\frac{\delta^{n+m}S}{\delta a^{+}_{k_1\sigma_1}(t_1)\ldots\delta a^{+}_{k_n\sigma_n}(t_n)\,\delta a_{l_1s_1}(\tau_1)\ldots\delta a_{l_ms_m}(\tau_m)}\Phi_2\right\rangle_c$$

$$\times\exp\Big\{i\sum_i\varepsilon(k_i)\,t_i - i\sum_j\varepsilon(l_j)\tau_j\Big\}\,dt_1\ldots d\tau_m$$

$$= -2\pi i\delta\Big(E_1-\sum_i\varepsilon(k_i)+\sum_j\varepsilon(l_j)-E_2\Big)$$

$$\times\int_{-\infty}^{0}\left\langle\Phi_1^{*}\frac{\delta^{n+m}R}{\delta a^{+}_{k_1\sigma_1}(t_1)\ldots\delta a_{l_ms_m}(\tau_m)}\Phi_2\right\rangle_c$$

$$\times\exp\Big\{i\sum_i\varepsilon(k_i)\,t_i - i\sum\varepsilon(l_j)\tau_j\Big\}\,dt_1\ldots d\tau_m. \quad (2.8)$$

We note next that we can use the property of the translational invariance of the matrix element of the variational derivative of the S-matrix to perform in the left hand side one integration over time and to split off explicitly the δ-function. This gives

$$i\int_{-\infty}^{\infty}\left\langle\Phi_1^{*}\frac{\delta^{n+m}S}{\delta a^{+}_{k_1\sigma_1}(0)\,\delta a^{+}_{k_2\sigma_2}(t_2)\ldots\delta a_{l_ms_m}(\tau_m)}\Phi_2\right\rangle_c$$

$$\times\exp\Big\{i\sum_{i=2}^{n}\varepsilon(k_i)\,t_i - i\sum_j\varepsilon(l_j)\tau_j\Big\}\,dt_2\ldots d\tau_m$$

$$= \int_{-\infty}^{0}\left\langle\Phi_1^{*}\frac{\delta^{n+m}R}{\delta a^{+}_{k_1\sigma_1}(t_1)\ldots\delta a_{l_ms_m}(\tau_m)}\Phi_2\right\rangle_c$$

$$\times\exp\Big\{i\sum_{i=1}^{n}\varepsilon(k_i)\,t_i - i\sum_j\varepsilon(l_j)\tau_j\Big\}\,dt_1\,dt_2\ldots d\tau_m \quad (2.9)$$

where

$$\sum_{i=1}^{n}\varepsilon(k_i)-\sum_{j=1}^{m}\varepsilon(l_j) = E_1-E_2. \quad (2.10)$$

Equation (2.9) is most convenient for further applications.

3. TRANSFORMATIONS OF THE KERNEL Q OF THE COMPENSATION EQUATION

We go now to the transformation of the kernel $Q(k, k')$ of the equation of compensation of dangerous electron diagrams, determined by Eq. (I.5.36).* In reference 1 it was shown that the kernel Q can be written in the form of a sum of two terms

$$Q(k, k') = Q_c(k, k') + Q_{ph}(k, k'). \quad (3.1)$$

The first term Q_C corresponds to Coulomb effects only and can be obtained from (I.5.36) by replacing R by R_C [Eq. (I.5.49)], i.e., by assuming $H_{ph} = 0$. Using the fact that in the case considered the momenta k, k′ are near the Fermi surface, so that the energies $\tilde{\epsilon}(k)$, $\tilde{\epsilon}(k')$ are small, we obtain using (2.9)

$$Q_c(k, k') = \begin{cases} i\int_{-\infty}^{\infty}\langle\delta^4S_c/\delta a^{+}_{k',+}(0)\,\delta a^{+}_{-k',-}(t_1)\,\delta a_{k,+}(t_2)\,\delta a_{-k,-}(t_3)\rangle_c\,dt_1\,dt_2\,dt_3 & \text{if } k<k_F, \\ i\int_{-\infty}^{\infty}\langle\delta^4S_c/\delta a^{+}_{k,+}(0)\,\delta a^{+}_{-k,-}(t_1)\,\delta a_{k',+}(t_2)\,\delta a_{-k',-}(t_3)\rangle_c\,dt_1\,dt_2\,dt_3 & \text{if } k>k_F, \end{cases} \quad (3.2)$$

where

$$S_c = T\Big(\exp\Big\{-i\int_{-\infty}^{\infty}H_c(t)\,dt\Big\}\Big). \quad (3.3)$$

To transform the second term in (3.1) which is proportional to g^2 it is convenient to start not from Eq. (I.5.36) but from the earlier Eq. (I.5.31).

We shall use (2.9) to write the coefficient of u_k^2 on the right hand side of that equation which is according to (I.5.34) equal to

$$\int_{-\infty}^{0}dt\,dt'\exp\{i\tilde{\varepsilon}(k)(t+t')\}\,\langle\delta^2R'/\delta a^{+}_{k,+}(t')\,\delta a^{+}_{-k,-}(t)\rangle_c$$

$$= \sum_{k'}u_{k'},\,v_{k'}Q(k, k'), \quad (3.4)$$

in the form

$$i\int_{-\infty}^{\infty}\langle\delta^2S/\delta a^{+}_{k,+}(0)\,\delta a^{+}_{-k,-}(t)\rangle_c\,e^{i\tilde{\varepsilon}(k)t}\,dt.$$

In accordance with (2.10) this is possible, if

*I.e., Eq. (5.36) of reference 1.

$$\tilde{\varepsilon}(k)+\tilde{\varepsilon}(k)=2\tilde{\varepsilon}(k)=0, \tag{3.5}$$

i.e.,

$$\sum_{k'} u_{k'}v_{k'}\,Q(k,k')=i\int_{-\infty}^{\infty}\langle\delta^2 S/\delta a^+_{k,+}(0)\,\delta a^{\pm}_{-k,-}(t)\rangle_c\,dt \tag{3.6}$$

if (3.5) is satisfied.

The matrix element which enters into the right hand side can be written in the form of a time-ordered product of two "currents" $(\delta S/\delta a^+)S^+$:

$$\left\langle\frac{\delta^2 S}{\delta a^+_{k,+}(0)\,\delta a^{\pm}_{-k,-}(t)}\right\rangle_c=\left\langle\frac{\delta^2 S}{\delta a^+_{k,+}(0)\,\delta a^{\pm}_{-k,-}(t)}S^+\right\rangle_{\alpha_0}$$

$$=\left\langle T\left(\frac{\delta S}{\delta a^+_{k,+}(0)}S^+\right)\left(\frac{\delta S}{\delta a^{\pm}_{-k,-}(t)}S^+\right)\right\rangle_{\alpha_0} \tag{3.7}$$

if we take the causality properties of the S-matrix [see, for instance, Eq. (48.15) of reference 4] into account. The index α_0 denotes here an averaging over the α-vacuum.

The time-ordered product of "currents" thus obtained is for any fixed order of the time arguments $(t > 0$ or $t < 0)$ the ordinary product of these "currents". This product can be expanded in a series in terms of a complete set of functions. If we restrict ourselves in this expansion to terms corresponding to states containing one α-electron and one β-phonon we split off the "main terms" containing small denominators $\{\tilde{\omega}(q)+\tilde{\varepsilon}(k)+\tilde{\varepsilon}(k')\}$.

By this means we get, for instance for $t < 0$, using the property of translational invariance,

$$\left\langle\frac{\delta^2 S}{\delta a^+_{k,+}(0)\,\delta a^{\pm}_{-k,-}(t)}\right\rangle_c=\sum_{k',s}\left\langle\frac{\delta S}{\delta a^+_{k,+}(0)}S^+\alpha^+_{k',s}\beta^+_{k-k'}\right\rangle_{\alpha_0}$$

$$\left\langle\alpha_{k's}\beta_{k-k'}\frac{\delta S}{\delta a^{\pm}_{-k,-}(t)}S^+\right\rangle_{\alpha_0}=\sum_{k',s}\exp\{it\,[\tilde{\omega}(k-k')+\tilde{\varepsilon}(k')]\}$$

$$\times\left\langle\frac{\delta S}{\delta a^+_{k,+}(0)}\alpha^+_{k's}\beta^+_{k-k'}\right\rangle_{\alpha_c}\left\langle\alpha_{k's}\beta_{k-k'}\frac{\delta S}{\delta a^{\pm}_{-k,-}(t)}\right\rangle_{\alpha_c} \tag{3.8}$$

Commuting after that the operators α^+, α, β^+, β with $\delta S/\delta a^+$ we can go to the limit as $\alpha\to a$. Combining the results for $t < 0$ and $t > 0$, taking into account the symmetry of the Hamiltonian H_{ph} with respect to β and β^+ we get, using (3.7) and (3.8)

$$i\int_{-\infty}^{\infty}\langle\delta^2 S/\delta a^+_{k,+}(0)\,\delta a^{\pm}_{-k,-}(t)\rangle_c\,dt$$

$$=-2\sum_{k'}\frac{u_{k'}v_{k'}}{\tilde{\varepsilon}(k')+\tilde{\omega}(k-k')}\Gamma(k,k',q)\,\Gamma(-k,-k',-q);$$

$$(q=k-k'), \tag{3.9}$$

where

$$\Gamma(k,k',q)=\int_{-\infty}^{\infty}d\tau\,d\theta\,\langle\delta^3 S/\delta a_{k',+}(\tau)\,\delta a^+_{k,+}(0)\,\delta\beta_q(\theta)\rangle_{a_c}. \tag{3.10}$$

Expression (3.10) is written down in the limit of small $\tilde{\varepsilon}(k')$ and $\tilde{\omega}(q)$.

Before comparing Eqs. (3.6) and (3.9), we make the following substitution. According to condition (3.5), Eq. (3.6) permits us to evaluate Q in the limiting case $\tilde{\varepsilon}(k)=0$. Since the momentum k is near the Fermi surface, the energy $\tilde{\varepsilon}(k)$ will in actual fact be a small quantity. In the representation of the kind (I.5.57) which we have used, the energy $\tilde{\varepsilon}(k)$ is everywhere put equal to zero except in the energy denominator $\tilde{\omega}(q)+\tilde{\varepsilon}(k)+\tilde{\varepsilon}(k')$. To obtain the required expression for Q_{ph} we must thus add $\tilde{\varepsilon}(k)$ in the energy denominator of the right hand side of (3.9). In this way we get from (3.6) and (3.9)

$$Q_{ph}(k,k')=-2\frac{\Gamma(k,k',q)\,\Gamma(-k,-k',-q)}{\tilde{\omega}(q)+\tilde{\varepsilon}(k)+\tilde{\varepsilon}(k')}. \tag{3.11}$$

Performing in (3.10) the variation over β and the transition to the limit $g = 0$, we have also

$$Q_{ph}(k,k')=2\frac{g^2(q)\,\omega(q)\,(\lambda_q+\mu_q)^2}{\tilde{\omega}(q)+\tilde{\varepsilon}(k')+\tilde{\varepsilon}(k)}$$

$$\times\Lambda(k,k',q)\,\Lambda(-k,-k',-q), \tag{3.12}$$

where

$$\Lambda(k,k',q)$$

$$=\int_{-\infty}^{\infty}d\tau\,d\theta\,\langle\delta^2\,[T\,(H_q(\theta)S_c)]/\delta a_{k',+}(\tau)\,\delta a^+_{k,+}(0)\rangle_{a_c}, \tag{3.13}$$

$$H_q(\theta)=\frac{1}{\sqrt{2V}}\sum_{l,s}a^+_{l+q,s}(\theta)\,a_{l,s}(\theta). \tag{3.14}$$

The quantity Λ can be expressed simply in terms of one-electron Green functions of the above-mentioned model problem. On the other hand, performing explicitly in (3.13) the functional differentiation and using the "generalized Wick theorem" [see Eq. (34.11) of reference 4] we get a representation of Λ in terms of the one-electron Green functions and the four-vertex Green function of the pure Coulomb problem. We have

$$\Lambda=\frac{1}{\sqrt{2V}}\Big\{1+\int_{-\infty}^{\infty}dt\,d\tau\,\overline{a^+_{k',+}(t)\,a_{k',+}}(0)$$

$$\times\langle\delta^2 S_c/\delta a^+_{k',+}(t)\,\delta a_{k',+}(\tau)\rangle_c$$

$$+\int_{-\infty}^{\infty}dt\,d\tau\,\overline{a^+_{k,+}(\tau)\,a_{k,+}}(t)\,\langle\delta^2 S_c/\delta a^+_{k,+}(0)\,\delta a_{k,+}(t)\rangle_c$$

$$+\sum_{l,s}\int_{-\infty}^{\infty}d\theta\,d\tau\,dt_1dt_2\,\overline{a^+_{l+q,s}(\theta)\,a_{l+q,s}}(t_1)\,\overline{a^+_{l,s}(t_2)\,a_{l,s}}(\theta)$$

$$\times\langle\delta^4 S_c/\delta a^+_{l,s}(t_2)\,\delta a^+_{k,+}(0)\,\delta a_{l+q,s}(t_1)\,\delta a_{k',+}(\tau)\rangle_c\Big\}. \tag{3.15}$$

The time-ordered pairing which occurs here has the form

$$\overline{a_{k,+}^{+}(t)\,a_{k,+}(\tau)} = \begin{cases} \theta_F(k)\,e^{-i\tilde{\varepsilon}(k)(t-\tau)} & \text{if } t > \tau, \\ -\theta_G(k)\,e^{-i\tilde{\varepsilon}(k)(\tau-t)} & \text{if } t < \tau, \end{cases} \quad (3.16)$$

where

$$\theta_F(k) = 1 - \theta_G(k) = \begin{cases} 1 & \text{if } k < k_F, \\ 0 & \text{if } k > k_F. \end{cases} \quad (3.17)$$

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[1] Bogolyubov, Tolmachev, and Shirkov, Новый метод в теории сверхпроводимости (A New Method in Superconductivity Theory), Acad. Sci. Press, 1958; [Fortschr. Physik, in press].

[2] J. Sucher, Phys. Rev. **107**, 1448 (1957).

[3] L. S. Rodberg, Phys. Rev. **110**, 277 (1958).

[4] N. N. Bogolyubov and D. V. Shirkov, Введение в теорию квантованных полей (Introduction into the Theory of Quantum Fields) GTI, 1957 [translation published by Interscience, 1959].

[5] Chen Chun-Sian and Chow Shih-Hsun, J. Exptl. Theoret. Phys. (U.S.S.R.) **34**, (1958), Soviet Phys. JETP **7**, 1080 (1958).

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