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Abstract

Full Text

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ON THE THEORY OF SUPERCONDUCTIVITY

(Presented by Academician N. N. Bogolyubov on 18 XII 1959)

The method of two-time temperature Green functions (retarded and advanced) is very convenient for considering various problems of statistical physics (¹⁻³). We shall apply it to the problem of the thermodynamics of the superconducting state on the basis of the Fröhlich Hamiltonian. We shall use Green functions of the type

$$\begin{aligned} \langle\langle A(t); B(t') \rangle\rangle_r &= -i\theta(t-t')\langle[A(t), B(t')]\rangle, \\ \langle\langle A(t); B(t') \rangle\rangle_a &= i\theta(t'-t)\langle[A(t), B(t')]\rangle, \end{aligned} \quad \theta(t) = \begin{cases} 1, & t > 0, \\ 0, & t < 0, \end{cases} \quad (1)$$

where $\langle\cdots\rangle$ denotes averaging over the grand canonical ensemble; $[A, B] = AB + BA$. The indices r, a will henceforth be omitted, since the Fourier components of the Green functions (1) can be analytically continued into the region of complex energy and regarded as a single analytic function with a cut along the real axis (^{1,3}).

For the Green functions we have a chain of equations:

$$\begin{aligned} i\frac{d}{dt}\langle\langle a_{k\sigma}(t); a_{k\sigma}^+(t') \rangle\rangle &= \delta(t-t') + T_k\langle\langle a_{k\sigma}; a_{k\sigma}^+ \rangle\rangle \\ &+ \sum_q A_q\langle\langle a_{k-q,\sigma}b_q; a_{k\sigma}^+ \rangle\rangle + \sum_q A_q\langle\langle a_{k-q,\sigma}b_q^+; a_{k\sigma}^+ \rangle\rangle; \end{aligned} \quad (2a)$$

$$\begin{aligned} i\frac{d}{dt}\langle\langle a_{k-q,\sigma}(t)b_q(t); a_{k\sigma}^+(t') \rangle\rangle &= (T_{k-q} + \omega_q)\langle\langle a_{k-q,\sigma}b_q; a_{k\sigma}^+ \rangle\rangle \\ &+ \sum_{q_1} A_{q_1}\langle\langle a_{k-q-q_1,\sigma}(b_{q_1} + b_{-q_1}^+)b_q; a_{k\sigma}^+ \rangle\rangle \\ &+ \sum_{k_1\sigma_1} A_q\langle\langle a_{k-q,\sigma}a_{k_1-q,\sigma_1}^+a_{k_1\sigma_1}; a_{k\sigma}^+ \rangle\rangle; \end{aligned} \quad (2)$$

$$\begin{aligned}
i \frac{d}{dt} \langle \langle a_{k-q,\sigma}(t) b_{-q}^+(t); a_{k\sigma}^+(t') \rangle \rangle &= (T_{k-q} - \omega_q) \langle \langle a_{k-q,\sigma} b_{-q}^+; a_{k\sigma}^+ \rangle \rangle \\
&+ \sum_{q_1} A_{q_1} \langle \langle a_{k-q-q_1,\sigma} (b_{q_1} + b_{-q_1}^+) b_{-q}^+; a_{k\sigma}^+ \rangle \rangle \quad (2) \\
&- \sum_{k_1 \sigma_1} A_q \langle \langle a_{k-q,\sigma} a_{k_1-q,\sigma_1}^+ a_{k_1 \sigma_1}; a_{k\sigma}^+ \rangle \rangle.
\end{aligned}$$

(the arguments t, t' on the right-hand side of the equations have been omitted), where $A_q = (\omega_q/2V)^{1/2}g$; g is the coupling constant with the phonon field; $T_k = k^2/2m - \mu$; μ is the chemical potential.

The system (2a)–(2), in addition to the original Green functions, also contains higher-order Green functions containing four operators. We split the latter by pairing operators belonging to the same instant of time (cf. (2,3)):

$$\begin{aligned}
\langle \langle a_{k-q-q_1,\sigma_1} (b_{q_1} + b_{-q_1}^+) b_q; a_{k\sigma}^+ \rangle \rangle &= \nu_q \langle \langle a_{k\sigma}; a_{k\sigma}^+ \rangle \rangle \delta_{q+q_1}, \\
\langle \langle a_{k-q-q_1,\sigma} (b_{q_1} + b_{-q_1}^+) b_{-q}^+; a_{k\sigma}^+ \rangle \rangle &= (1 + \nu_q) \langle \langle a_{k\sigma}; a_{k\sigma}^+ \rangle \rangle \delta_{q+q_1}, \\
\langle \langle a_{k-q,\sigma} a_{k_1-q,\sigma_1}^+ a_{k_1 \sigma_1}; a_{k\sigma}^+ \rangle \rangle &= (1 - n_{k-q}) \langle \langle a_{k\sigma}; a_{k\sigma}^+ \rangle \rangle \delta_{k-k_1}^{\sigma-\sigma_1} \\
&- \langle a_{k-q,\sigma} a_{-k+q,-\sigma} \rangle \langle \langle a_{-k,-\sigma}^+; a_{k\sigma}^+ \rangle \rangle \delta_{k+k_1}^{\sigma+\sigma_1},
\end{aligned} \quad (3)$$

$$\nu_q = \langle b_q^+ b_q \rangle, \quad n_k = \langle a_{k\sigma}^+ a_{k\sigma} \rangle.$$

We also take into account pairings of the operators $a_{k\sigma}$ and $a_{-k,-\sigma}$, bearing in mind, in accordance with the method of the $u-v$ transformation (4), that an asymptotically small term has been added to the original Hamiltonian, which does not conserve the number of particles and which, in the final results, we shall let tend to zero (cf. the third formula in (3) with the splitting of Green's functions in Grin's paper (5)). For the Fourier components of Grin's functions we obtain:

$$\begin{aligned}
(E - T_k) \langle \langle a_{k\sigma} | a_{k\sigma}^+ \rangle \rangle &= \frac{1}{2\pi} + \sum_q A_q \langle \langle a_{k-q,\sigma} b_q | a_{k\sigma}^+ \rangle \rangle + \sum_q A_q \langle \langle a_{k-q,\sigma} b_{-q}^+ | a_{k\sigma}^+ \rangle \rangle, \\
\langle \langle a_{k-q,\sigma} b_q | a_{k\sigma}^+ \rangle \rangle &= \frac{A_q}{E - T_{k-q} - \omega_q} \{ (\nu_q + 1 - n_{k-q}) \langle \langle a_{k\sigma} | a_{k\sigma}^+ \rangle \rangle - \\
&- \langle a_{k-q,\sigma} a_{-k+q,-\sigma} \rangle \langle \langle a_{-k,-\sigma}^+ | a_{k\sigma}^+ \rangle \rangle \}, \quad (4)
\end{aligned}$$

$$\begin{aligned}
\langle\langle a_{k-q,\sigma} b_{-q}^+ | a_{k\sigma}^+ \rangle\rangle &= \frac{A_q}{E - T_{k-q} + \omega_q} \{(\nu_q + n_{k-q}) \langle\langle a_{k\sigma} | a_{k\sigma}^+ \rangle\rangle + \\
&\quad + \langle a_{k-q,\sigma} a_{-k+q,-\sigma} \rangle \langle\langle a_{-k,-\sigma}^+ | a_{k\sigma}^+ \rangle\rangle\}; \\
(E + T_k) \langle\langle a_{-k,-\sigma}^+ | a_{k\sigma}^+ \rangle\rangle &= - \sum_q A_q \langle\langle a_{-k+q,-\sigma}^+ b_q | a_{k\sigma}^+ \rangle\rangle - \\
&\quad - \sum_q A_q \langle\langle a_{-k+q,-\sigma}^+ b_{-q}^+ | a_{k\sigma}^+ \rangle\rangle, \\
\langle\langle a_{-k+q,-\sigma}^+ b_q | a_{k\sigma}^+ \rangle\rangle &= \frac{-A_q}{E + T_{k-q} - \omega_q} \{(\nu_q + n_{k-q}) \langle\langle a_{-k,-\sigma}^+ | a_{k\sigma}^+ \rangle\rangle - \\
&\quad - \langle a_{-k+q,-\sigma} a_{k-q,\sigma} \rangle \langle\langle a_{k\sigma} | a_{k\sigma}^+ \rangle\rangle\}, \tag{5}
\end{aligned}$$

$$\begin{aligned}
\langle\langle a_{-k+q,-\sigma}^+ b_{-q}^+ | a_{k\sigma}^+ \rangle\rangle &= \frac{-A_q}{E + T_{k-q} + \omega_q} \{(1 + \nu_q - n_{k-q}) \langle\langle a_{-k,-\sigma}^+ | a_{k\sigma}^+ \rangle\rangle + \\
&\quad + \langle a_{-k+q,-\sigma} a_{k-q,\sigma} \rangle \langle\langle a_{k\sigma} | a_{k\sigma}^+ \rangle\rangle\}.
\end{aligned}$$

Eliminating from equations (4), (5) the Green' s functions that contain Bose operators, we obtain for the Green' s functions

$$G_k(E) = \langle\langle a_{k\sigma} | a_{k\sigma}^+ \rangle\rangle, \quad \Gamma_{k\sigma}(E) = \langle\langle a_{-k,-\sigma}^+ | a_{k\sigma}^+ \rangle\rangle \tag{6}$$

the system of equations

$$\begin{aligned}
\{E - T_k - \mathfrak{M}_k(E)\} G_k(E) + \mathfrak{E}_{k\sigma}(E) \Gamma_{k\sigma}(E) &= \frac{1}{2\pi}, \\
\{E + T_k + \mathfrak{M}_k(-E)\} \Gamma_{k\sigma}(E) + \mathfrak{E}_{k\sigma}(-E) G_{k\sigma}(E) &= 0, \tag{7'}
\end{aligned}$$

where the following notation has been introduced:

$$\mathfrak{M}_k(E) = \sum_q A_q^2 \left[\frac{1 + \nu_q - n_{k-q}}{E - T_{k-q} - \omega_q} + \frac{\nu_q + n_{k-q}}{E - T_{k-q} + \omega_q} \right], \tag{8}$$

$$\mathfrak{E}_{k\sigma}(E) = \sum_q A_q^2 \langle a_{k-q,\sigma} a_{-k+q,-\sigma} \rangle \left[\frac{1}{E - T_{k-q} - \omega_q} - \frac{1}{E - T_{k-q} + \omega_q} \right].$$

The quantity $\mathfrak{M}_k(E)$ has the meaning of a “mass operator”; the quantity $\mathfrak{E}_{k\sigma}(E)$ determines, as we shall see below, the energy gap in the spectrum of elementary excitations.

Solving the system (7), we obtain for the Green’ s functions

$$G_k(E) = \frac{1}{2\pi} \frac{E + T_k + \mathfrak{M}_k(-E)}{\left\{ E - \frac{\mathfrak{M}_k(E) - \mathfrak{M}_k(-E)}{2} \right\}^2 - \left\{ T_k + \frac{\mathfrak{M}_k(E) + \mathfrak{M}_k(-E)}{2} \right\}^2 - \mathfrak{E}_{k\sigma}(E)\mathfrak{E}_{k\sigma}(-E)},$$

$$\Gamma_{k\sigma}(E) = -\frac{1}{2\pi} \frac{\mathfrak{E}_{k\sigma}(-E)}{\left\{ E - \frac{\mathfrak{M}_k(E) - \mathfrak{M}_k(-E)}{2} \right\}^2 - \left\{ T_k + \frac{\mathfrak{M}_k(E) + \mathfrak{M}_k(-E)}{2} \right\}^2 - \mathfrak{E}_{k\sigma}(E)\mathfrak{E}_{k\sigma}(-E)}. \quad (9)$$

Knowing the Green’ s functions, one can calculate the spectral intensities of the time correlation functions $J_k(\omega)$, $J_{k\sigma}(\omega)$ by means of the relations

$$G_k(\omega + i\varepsilon) - G_k(\omega - i\varepsilon) = \frac{1}{i} J_k(\omega) (e^{\beta\omega} + 1),$$

$$\Gamma_{k\sigma}(\omega + i\varepsilon) - \Gamma_{k\sigma}(\omega - i\varepsilon) = \frac{1}{i} J_{k\sigma}(\omega) (e^{\beta\omega} + 1), \quad (10)$$

where

$$\langle a_{k\sigma}^+(t') a_{k\sigma}(t) \rangle = \int_{-\infty}^{\infty} J_k(\omega) e^{-i\omega(t-t')} d\omega,$$

$$\langle a_{k\sigma}^+(t') a_{-k,-\sigma}^+(t) \rangle = \int_{-\infty}^{\infty} J_{k\sigma}(\omega) e^{-i\omega(t-t')} d\omega, \quad (11)$$

whence, putting $t = t'$, we find the distribution functions $n_k = \langle a_{k\sigma}^+ a_{k\sigma} \rangle$, $\langle a_{k\sigma}^+ a_{-k,-\sigma}^+ \rangle$.

In formulas (9), E is a complex quantity. Near the real axis $E = \omega \pm i\varepsilon$ we have

$$\mathfrak{M}_k(\omega \pm i\varepsilon) = M_k(\omega) \mp i\gamma_k(\omega), \quad \mathfrak{E}_{k\sigma}(\omega \pm i\varepsilon) = C_{k\sigma}(\omega) \mp i\delta_{k\sigma}(\omega), \quad (12)$$

where

$$M_k(\omega) = P \sum_q A_q^2 \left[\frac{1 + \nu_q - n_{k-q}}{\omega - T_{k-q} - \omega_q} + \frac{\nu_q + n_{k-q}}{\omega - T_{k-q} + \omega_q} \right],$$

$$C_{k\sigma}(\omega) = P \sum_q A_q^2 \langle a_{k-q, \sigma} a_{-k+q, -\sigma} \rangle \left[\frac{1}{\omega - T_{k-q} - \omega_q} - \frac{1}{\omega - T_{k-q} + \omega_q} \right], \quad (13)$$

$$\gamma_k(\omega) = \pi \sum_q A_q^2 [(1 + \nu_q - n_{k-q})\delta(\omega - T_{k-q} - \omega_q) + (\nu_q + n_{k-q})\delta(\omega - T_{k-q} + \omega_q)],$$

$$\delta_{k\sigma}(\omega) = \pi \sum_q A_q^2 \langle a_{k-q, \sigma} a_{-k+q, -\sigma} \rangle [\delta(\omega - T_{k-q} - \omega_q) - \delta(\omega - T_{k-q} + \omega_q)].$$

(Here P denotes the integral in the sense of the principal value.)

For $\gamma_k \rightarrow 0$, $\delta_{k\sigma} \rightarrow 0$, the spectral intensities are delta-like. If the damping is finite but small, then near $\omega = \Omega_k^\pm$ they have a sharp maximum. We shall assume that the functions $M_k(\omega)$, $C_{k\sigma}(\omega)$ vary slowly near this maximum and set them equal to constants. We shall, moreover, neglect the damping. Then the Green's functions (9) acquire poles at the points $\omega = \Omega_k^\pm$:

$$\Omega_k^\pm = \frac{M_k^+ - M_k^-}{2} \pm \sqrt{\left\{ T_k + \frac{M_k^+ + M_k^-}{2} \right\}^2 + C_{k\sigma}^+ C_{k\sigma}^-};$$

$$M_k^\pm = M_k(\pm\Omega_k^\pm), \quad C_{k\sigma}^\pm = C_{k\sigma}(\pm\Omega_k^\pm). \quad (14)$$

Noting that $M_k^+ - M_k^- = \eta_k \Omega_k^\pm$, where the quantity η_k is very small ($\eta_k \ll 1$), one may neglect η_k . Then for the energy of the elementary excitations we obtain

$$\Omega_k = \sqrt{\xi_k^2 + C_{k\sigma}^+ C_{k\sigma}^-}, \quad \Omega_k^\pm = \pm\Omega_k, \quad \xi_k = T_k + M_k, \quad M_k = M_k(0) \simeq M_k^+ \simeq M_k^-. \quad (15)$$

(It can be shown that for the exact mass operators $M_k(\omega) = M_k(-\omega)$, and also $C_{k\sigma}(\omega) = C_{k\sigma}(-\omega)$.)

For the spectral intensities $\mathcal{Y}_k(\omega)$, $J_{k\sigma}(\omega)$ and the corresponding distribution functions, with the aid of (10), (11) we find

$$y_k(\omega) = \frac{(e^{\beta\omega} + 1)^{-1}}{2\Omega_k} \{(\Omega_k + \xi_k)\delta(\omega - \Omega_k) - (\Omega_k - \xi_k)\delta(\omega + \Omega_k)\},$$

$$J_{k\sigma}(\omega) = -\frac{(e^{\beta\omega} + 1)^{-1}}{2\Omega_k} \{C_{k\sigma}^-\delta(\omega - \Omega_k) - C_{k\sigma}^+\delta(\omega + \Omega_k)\},$$
(16)

$$n_k = \frac{1}{2} \left(1 - \frac{\xi_k}{\Omega_k} \operatorname{th} \frac{\Omega_k}{2\theta} \right), \quad \langle a_{k\sigma}^+ a_{-k,-\sigma}^+ \rangle = -\frac{1}{2\Omega_k} \left\{ \frac{C_{k\sigma}^-}{e^{\beta\Omega_k} + 1} - \frac{C_{k\sigma}^+}{e^{-\beta\Omega_k} + 1} \right\}.$$

For the functions $C_{k\sigma}^\pm$ we obtain the integral equation

$$C_{k\sigma}^\pm = \frac{g^2}{2V} \sum_{q(k'=k-q)} \frac{\omega_q^2}{\omega_q^2 - (\pm\Omega_{k'} - T_{k'})^2} \frac{1}{\Omega_{k'}} \left\{ \frac{C_{k'\sigma}^-}{e^{\beta\Omega_{k'}} + 1} - \frac{C_{k'\sigma}^+}{e^{\beta\Omega_{k'}} + 1} \right\},$$
(17)

whose solution $C_{k\sigma}^+ \cong C_{k\sigma}^- = C_k(-1)^{\sigma-1/2}$ is easily obtained by the method set forth in paper ⁶.

The mean interaction energy is found from the first equation of system (4), whence the exact relation follows

$$\int_{-\infty}^{\infty} (\omega - T_k) y_k(\omega) d\omega = \sum_q A_q \langle a_{k\sigma}^+ a_{k-q,\sigma} (b_q + b_{-q}^+) \rangle.$$
(18)

Substituting here $y_k(\omega)$ from (16), we obtain the mean interaction energy

$$\langle H_{\text{int}} \rangle = \sum_{k\sigma} M_k n_k - \sum_{k,\sigma} \frac{C_k^2}{2\Omega_k} \operatorname{th} \frac{\Omega_k}{2\theta}.$$
(19)

The thermodynamic potential is obtained by integrating (19) with respect to the interaction constant. For example, at zero temperature, for the difference between the energies of the normal ($C_k = 0$) and superconducting ($C_k \neq 0$) states we obtain

$$E_n - E_{\text{s.p.}} = V \left(\frac{dn}{dE} \right) 2\tilde{\omega} \int_0^{1/2} e^{2/\varepsilon^2 \rho} \frac{d\varepsilon}{\varepsilon^2 \rho} \cong V \left(\frac{dn}{dE} \right) \tilde{\omega}^2 \frac{1}{2} e^{-2/\rho},$$

$$\tilde{\omega} = \bar{\omega} \exp \left\{ - \int_0^\infty \ln 2x \frac{d}{dx} \varphi^2(x) dx \right\}; \quad \bar{\omega} = \frac{1}{2} \omega_q|_{q=k_0},$$
(20)

$$\varphi(x) = \frac{g^2}{I} \int_0^{q_0/k_0} \frac{u^2 du}{2u + x}, \quad \varphi(0) = 1, \quad x = \frac{\xi}{\omega}, \quad \rho = I \left(\frac{dn}{dE} \right).$$

Here (dn/dE) is the density of states at the Fermi surface; q_0 is the maximum Debye momentum; k_0 is the limiting momentum of the electrons at the Fermi surface. Formula (20) coincides with that obtained in paper ⁴ (cf. ⁷).

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Note: Figure translations are in progress. See original paper for figures.

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