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Abstract

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THE METHOD OF THE GENERALIZED SELF-CONSISTENT FIELD AND COLLECTIVE EXCITATIONS IN THE THEORY OF SUPERCONDUCTIVITY

(Presented by Academician N. N. Bogolyubov, January 12, 1963)

The first versions of the microscopic theory of superconductivity took into account the simplest s -interaction in the form of a rectangular well near the Fermi surface. Within the framework of this approximation, a spectrum of elementary excitations separated by a gap from the ground state was obtained. As was first shown by N. N. Bogolyubov, in this case, alongside elementary excitations, there also exist collective excitations in superconducting systems, which in the case of a neutral system have the character of longitudinal quasiacoustic waves, turning, when the Coulomb interaction is included, into ordinary plasma excitations ^(1,2). Subsequently, collective excitations were investigated for a two-particle interaction expanded in spherical harmonics ^(3,4). In this case the above-mentioned results were confirmed for the s -interaction. For higher harmonics, under the condition that the corresponding interaction constant is negative, collective excitations possessing a momentum equal to the momentum of the interaction producing them were found.

In the present paper collective excitations are considered on the basis of the equations obtained by N. N. Bogolyubov in the approximation of the generalized self-consistent field ⁽²⁾. Let us consider these equations:

$$E\vartheta_q(p) = [\Omega(p-q) + \Omega(p)]\vartheta_q(p) + \frac{1}{V} \sum \vartheta_q(p') [J_q(p, p')a_q(p)a_q(p') + G_q(p, p')b_q(p)b_q(p')]; \quad (1)$$

$$E\theta_q(p) = [\Omega(p-q) + \Omega(p)]\theta_q(p) + \frac{1}{V} \sum \theta_q(p') [J'_q(p, p')d_q(p)d_q(p') + I_q(p, p')c_q(p)c_q(p')], \quad (2)$$

where

$$a_q(p) = u_p u_{p-q} - v_p v_{p-q}, \quad b_q(p) = u_p v_{p-q} + u_{p-q} v_p,$$

$$c_q(p) = u_p v_{p-q} - u_{p-q} v_p, \quad d_q(p) = u_p u_{p-q} + v_p v_{p-q},$$

$$J_q(p, p') = J(p, -p + q; -p' + q, p'),$$

$$I(p, p') = J(p, p' - q; p', p - q) + J(p, p' - q; p - q, p')$$

$$-J(p, -p'; -p' + q, p - q),$$

$$G_q(p, p') = J(p, p' - q; p', p - q) - J(p, p' - q; p - q, p')$$

$$+J(p, -p'; -p' + q, p - q),$$

$$u_p = \left[\frac{1}{2} \left(1 + \frac{\xi}{\Omega} \right) \right]^{1/2}, \quad v_p = \left[\frac{1}{2} \left(1 - \frac{\xi}{\Omega} \right) \right]^{1/2},$$

ξ is the particle energy measured from the Fermi surface, $\Omega = \sqrt{\xi^2 + c^2}$, and c is the gap in the spectrum of elementary excitations. Let us note that the kernels J and I are regular, while the singularities in equations (1) and (2) that appear in the presence of the Coulomb interaction are associated with the kernel G . Indeed, in the radially symmetric case $G_q(p, p') \rightarrow 2J(q) - J(p - p')$, and, since $J(p - p')$ is regular, the singularity in the kernel G_q as $q \rightarrow 0$ is associated with the Coulomb interaction $J(q) = 4\pi e^2/q^2$.

Let us consider equations (1) and (2) for an interaction of the form

$$\sum_{l=0}^{\infty} J_l(p, p') \sum_{m=-l}^l Y_{lm}(\vartheta, \varphi)^* Y_{lm}(\theta, \Phi), \quad (3)$$

where ϑ, φ and θ, Φ are the angles of the vectors p', p , respectively, in the coordinate system in which the vector q is directed along the z -axis. We shall assume $J_l(p, p') = J_l$

constant and different from zero for $-\omega \ll \xi \ll \omega$. An interaction of the form (3) makes it possible to algebraize the integral equations (1) and (2). Separating out the Coulomb interaction in (1), let us introduce new variables

$$X_{LM}(q) = \frac{1}{V} \sum_{p'} \vartheta_q(p') J_L Y_{LM}(\vartheta, \varphi)^* d_q(p'),$$

$$Z_{LM}(q) = \frac{1}{V} \sum_{p'} \vartheta_q(p') J_L Y_{LM}(\vartheta, \varphi)^* c_q(p'),$$

$$W_{LM}(q) = \frac{1}{V} \sum_{p'} \vartheta_q(p') J_L Y_{LM}(\vartheta, \varphi)^* a_q(p')$$

$$U_{LM}(q) = \frac{1}{V} \sum_{p'} \vartheta_q(p') J_L Y_{LM}(\vartheta, \varphi)^* b_q(p').$$

In the variables X, Z, W, U , instead of equations (1) and (2) we obtain the following four algebraic equations

$$X_{LM}(q) = J_L \sum_{l=0}^{\infty} \sum_{m=-l}^l \int [X_{lm}(q) P_{[d^2]} - Z_{lm}(q) P_{[cd]} + W_{lm}(q) P_{Ead} - U_{lm}(q) P_{Ebd}] Y_{lm}(\theta, \Phi) Y_{LM}(\theta, \Phi)^* d\omega + 2J_{LK}$$

$$Z_{LM}(q) = J_L \sum_{l=0}^{\infty} \sum_{m=-l}^l \int [X_{lm}(q) P_{[cd]} - Z_{lm}(q) P_{[c^2]} + W_{lm}(q) P_{Eac} - U_{lm}(q) P_{Ebc}] Y_{lm}(\theta, \Phi) Y_{LM}(\theta, \Phi)^* d\omega + 2J_{LK}$$

$$W_{LM}(q) = J_L \sum_{l=0}^{\infty} \sum_{m=-l}^l \int [X_{lm}(q) P_{Ead} - Z_{lm}(q) P_{Eac} + W_{lm}(q) P_{[a^2]} - U_{lm}(q) P_{[ab]}] Y_{lm}(\theta, \Phi) Y_{LM}(\theta, \Phi)^* d\omega + 2J_{LK}$$

$$U_{LM}(q) = J_L \sum_{l=0}^{\infty} \sum_{m=-l}^l \int [X_{lm}(q) P_{Ebd} - Z_{lm}(q) P_{Ebc} + W_{lm}(q) P_{[ab]} - U_{lm}(q) P_{[b^2]}] Y_{lm}(\theta, \Phi) Y_{LM}(\theta, \Phi)^* d\omega + 2J_{LK}$$

where

$$P_{\dots} = \frac{1}{8\pi^3} \int \frac{\dots}{\{E^2 - [\Omega(p-q) + \Omega(p)]^2\}} p^2 dp,$$

$$K(q) = J(q) \frac{1}{V} \sum \vartheta_q(p') b_p(p') = J(q) \frac{\sqrt{4\pi} U_{00}}{J_0},$$

and the $[\]$ in the subscript of P denotes $\Omega(p-q) + \Omega(p)$.

From equations (4)–(7) it is easy to see that the Coulomb interaction disappears for $M \neq 0$, since the quantities $P \dots$ can depend only on the angle θ . For the same reason the quantities X, Z, W, U enter equations (4)–(7) with the same M . In the case $L \neq 0$ we have, generally speaking, a system of coupled algebraic equations for X, Z, W, U with different L . Especially simple is the case $q = 0$. Then the quantities P contain no angular dependence, and equations (4)–(7) connect the quantities X, Z, W, U with the same L . Since $c_0 = 0$, it follows that $Z_{00} = 0$, and equation (5) identically becomes zero. Thus, one can obtain the following system of three equations:

$$X_{LM} = J_L P_{2\Omega}^0 X_{LM} - J_L P_{Ec/\Omega}^0 U_{LM} + J_L P_{E\xi/\Omega}^0 W_{LM} + 2J_L P_{Ec/\Omega}^0 K(0) \delta_{L0} \delta_{M0}; \quad (8)$$

$$U_{LM} = J_L P_{Ec/\Omega}^0 X_{LM} - J_L P_{2c^2/\Omega}^0 U_{LM} + J_L P_{2\xi c/\Omega}^0 W_{LM} + 2J_L P_{2c^2/\Omega}^0 K(0) \delta_{L0} \delta_{M0}; \quad (9)$$

$$W_{LM} = J_L P_{E\xi/\Omega}^0 X_{LM} - J_L P_{2\xi c/\Omega}^0 U_{LM} + J_L P_{2\xi^2/\Omega}^0 W_{LM} + 2J_L P_{2\xi c/\Omega}^0 K(0) \delta_{L1} \delta_{M0}, \quad (10)$$

where the zero index on the quantity P indicates that they are taken for $q = 0$. Since $P_{E\xi/\Omega}^0 = P_{C\xi/\Omega}^0 = 0$, equation (10) separates from (8) and (9). The case $L = 0$ can be considered on the basis of equations (1) and (2), as in ⁽²⁾. In the case $L \neq 0$, the terms containing the Coulomb interaction drop out of equations (8)–(10). Thus, the energy of the collective excitations for the case $L \neq 0, q = 0$, is determined from the conditions

$$(1 - J_L P_{2\Omega}^0)(1 + J_L P_{2c^2/\Omega}^0) + (J_L P_{Ec/\Omega}^0)^2 = 0; \quad (11)$$

$$1 - J_L P_{2\xi^2/\Omega}^0 = 0. \quad (12)$$

In the case $\nu = E/2\zeta \ll 1$, conditions (11) and (12) take the form

$$\left(\frac{1}{g_L} + \frac{\arcsin \nu}{\sqrt{1-\nu^2}} \right) \left(\frac{1}{g_L} - \frac{1}{g_0} - \frac{\nu \arcsin \nu}{\sqrt{1-\nu^2}} \right) + \frac{(\arcsin \nu)^2}{1-\nu^2} = 0; \quad (13)$$

$$\frac{1}{\nu} \sqrt{1-\nu^2} \arcsin \nu = \frac{1}{g_0} - \frac{1}{g_L}. \quad (14)$$

Equation (13) leads to the existence of collective excitations also for $g_L < 0$, i.e., to the existence, along with collective excitations of the particle–particle

type, of excitations of the particle–hole type. Equation (14) has no real roots for $g_0 > g_L$.

In the cases of small q , the quantities $P \dots$ can be expanded in powers of $|q|$; in doing so, terms independent of θ and depending on $\cos \theta$ and $\cos^2 \theta$ are separated. Expressing $\cos \theta$ and $\cos^2 \theta$ in terms of spherical functions and denoting by the indices 0, 1, 2 the corresponding dependence of the quantity $P \dots$ on $|q|$, from equations (4)–(7) we obtain

$$\begin{aligned}
 X_{LM} = J_L \Bigg\{ & \left(P_{\Gamma|d^2}^0 + \frac{1}{3} P_{\Gamma|d^2}^2 \right) X_{LM} - \left(P_{Ebd}^0 + \frac{1}{3} P_{Ebd}^2 \right) U_{LM} \\
 & + 2\sqrt{4\pi} K(q) \left[\left(P_{Ebd}^0 + \frac{1}{3} P_{Ebd}^2 \right) \delta_{L0} \delta_{M0} + \frac{2}{3\sqrt{5}} P_{Ebd}^2 \delta_{L2} \delta_{M0} \right] \\
 & + \sum_{lm} \sum_{j=|l-2|}^{l+2} \frac{2}{3} \sqrt{\frac{2l+1}{2j+1}} (l2m0|jm)(l200|j0) \left(P_{\Gamma|d^2}^2 X_{lm} - P_{Ebd}^2 U_{lm} \right) \delta_{jL} \delta_{mM} \\
 & + \sum_{lm} \sum_{j=|l-1|}^{l+1} \sqrt{\frac{2l+1}{2j+1}} (l1m0|jm)(l100|j0) \left(P_{Ead}^1 W_{lm} - P_{\Gamma|cd}^1 Z_{lm} \right) \delta_{jL} \delta_{mM} \Bigg\}; \quad (15)
 \end{aligned}$$

$$\begin{aligned}
 Z_{LM} = J_L \Bigg\{ & -\frac{1}{3} P_{\Gamma|c^2}^2 Z_{LM} + \frac{1}{3} P_{Eac}^2 W_{LM} + 2\sqrt{\frac{4\pi}{3}} P_{Ebc}^1 K(q) \delta_{L1} \delta_{M0} \\
 & + \sum_{lm} \sum_{j=|l-2|}^{l+2} \frac{2}{3} \sqrt{\frac{2l+1}{2j+1}} (l2m0|jm)(l200|j0) \left(P_{Eac}^2 W_{lm} - P_{\Gamma|c^2}^2 Z_{lm} \right) \delta_{jL} \delta_{mM} \\
 & + \sum_{lm} \sum_{j=|l-1|}^{l+1} \sqrt{\frac{2l+1}{2j+1}} (l1m0|jm)(l100|j0) \left(P_{\Gamma|cd}^1 X_{lm} - P_{Ebc}^1 U_{lm} \right) \delta_{jL} \delta_{mM} \Bigg\}; \quad (16)
 \end{aligned}$$

$$\begin{aligned}
 W_{LM} = J_L \Bigg\{ & \left(P_{\Gamma|a^2}^0 + \frac{1}{3} P_{\Gamma|a^2}^2 \right) W_{LM} - \frac{1}{3} P_{Eac}^2 Z_{LM} \\
 & + 2\sqrt{\frac{4\pi}{3}} P_{\Gamma|ab}^1 K(q) \delta_{L1} \delta_{M0} \\
 & + \sum_{lm} \sum_{j=|l-2|}^{l+2} \frac{2}{3} \sum \sqrt{\frac{2l+1}{2j+1}} (l2m0|jm)(l200|j0) \left(P_{\Gamma|a^2}^2 W_{lm} - P_{Eac}^2 Z_{lm} \right) \delta_{jL} \delta_{mM} \\
 & + \sum_{lm} \sum_{j=|l-1|}^{l+1} \sqrt{\frac{2l+1}{2j+1}} (l1m0|jm)(l100|j0) \left(P_{Ead}^1 X_{lm} - P_{\Gamma|ab}^1 U_{lm} \right) \delta_{jM} \delta_{mM} \Bigg\}; \quad (17)
 \end{aligned}$$

$$\begin{aligned}
U_{LM} = J_L \left\{ \left(P_{Ebd}^0 + \frac{1}{3} P_{Ebd}^2 \right) X_{LM} - \left(P_{\Gamma|b^2}^0 + \frac{1}{3} P_{\Gamma|b^2}^2 \right) U_{LM} \right. \\
\left. + 2\sqrt{4\pi} K(q) \left[\left(P_{\Gamma|b^2}^0 + \frac{1}{3} P_{\Gamma|b^2}^2 \right) \delta_{L0} \delta_{M0} + \frac{2}{3\sqrt{5}} P_{\Gamma|bd}^2 \delta_{L2} \delta_{M0} \right] + \right. \\
\left. + \sum_{lm} \sum_{j=|l-2|}^{l+2} \frac{2}{3} \sqrt{\frac{2l+1}{2j+1}} (l2m0|jm)(l200|j0)(P_{Ebd}^2 X_{lm} - P_{\Gamma|b^2}^2 U_{lm}) \delta_{jL} \delta_{mM} + \sum_{lm} \sum_{j=|l-1|}^{l-1} \sqrt{\frac{2l+1}{2j+1}} (l1m0|jm)(l100|j0) \right\}
\end{aligned}$$

Let us consider the case in which, in the expansion of the potential (3), only the s - and p -spherical harmonics are nonzero. Then from equations (15)–(18) it follows that the $X_{1,\pm 1}$, $U_{1,\pm 1}$ and $Z_{1,\pm 1}$, $W_{1,\pm 1}$ excitations split pairwise. Their energies are determined, respectively, from the conditions

$$\left[J_1 \left(P_{\square d^2}^0 + \frac{1}{5} P_{\square d^2}^2 \right) - 1 \right] \left[J_1 \left(P_{\square b^2}^0 + \frac{1}{5} P_{\square b^2}^2 \right) + 1 \right] = J_1^2 \left(P_{Ebd}^0 + \frac{1}{5} P_{Ebd}^2 \right)^2; \quad (19)$$

$$\left(1 + \frac{1}{5} P_{\square c^2}^2 J_1 \right) \left[\left(P_{\square d^2}^0 + \frac{1}{5} P_{\square d^2}^2 \right) J_1 - 1 \right] = \frac{1}{25} J_1^2 (P_{Eac}^2)^2. \quad (20)$$

Since the calculation is carried out to accuracy up to $|q|^2$, the right-hand side of (20) may be neglected. In this case equation (20) splits into two conditions, one of which coincides with the equation obtained in (3) for unphysical excitations. It is not difficult to see that the result of (3) for real excitations can be obtained as one of the conditions following from (19) if its right-hand side is incorrectly neglected in the calculation presented.

In the case $L = 1$, $M = 0$, the modes of type $1, 0$; $0, 0$ turn out to be coupled. In this case the X_{10} , U_{10} , Z_{00} , W_{00} excitations split off from the X_{00} , U_{00} , Z_{10} , W_{10} modes; moreover, for the first excitations the Coulomb interaction drops out. We give the condition determining the energies of the excitations X_{10} , U_{10} , Z_{00} , W_{00} :

$$\begin{vmatrix}
J_1 \left(P_{\square d^2}^0 + \frac{3}{5} P_{\square d^2}^2 \right) - 1 & - \left(P_{Ebd}^0 + \frac{3}{5} P_{Ebd}^2 \right) J_1 & - \frac{1}{\sqrt{3}} J_0 P_{\square cd}^1 & - \frac{1}{\sqrt{3}} J_0 P_{Ead}^1 \\
- J_1 \left(P_{Ebd}^0 + \frac{3}{5} P_{Ebd}^2 \right) & J_1 \left(P_{\square b^2}^0 + \frac{3}{5} P_{\square b^2}^2 \right) + 1 & - \frac{1}{\sqrt{3}} P_{Ebc}^1 J_0 & \frac{1}{\sqrt{3}} J_0 P_{\square ab}^1 \\
\frac{1}{\sqrt{3}} J_1 P_{Ead}^1 & - \frac{1}{\sqrt{3}} J_1 P_{\square cd}^1 & - \frac{1}{3} J_0 P_{Eac}^2 & 1 + \frac{1}{3} J_0 P_{\square c^2}^2 \\
- \frac{1}{\sqrt{3}} J_1 P_{\square ab}^1 & \frac{1}{\sqrt{3}} J_1 P_{Ebc}^1 & 1 - J_0 \left(P_{\square a^2}^0 + \frac{1}{3} P_{\square a^2}^2 \right) & \frac{1}{3} J_0 P_{Eac}^2
\end{vmatrix} = 0. \quad (21)$$

The result of (3) for 1,0-excitations corresponds to

$$1 = J_1 \left(P_{[]d^2}^0 + \frac{3}{5} P_{[]d^2}^2 \right).$$

The equations for X_{00} , U_{00} , Z_{10} , W_{10} may be used to determine the excitations with $L = 0$, using the definition of $K(q)$ through U_{00} .

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