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*A NEW METHOD IN THE THEORY OF SUPERCONDUCTIVITY. II**

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The equivalence of the Bardeen Hamiltonian and the Fröhlich Hamiltonian is established in the adiabatic approximation. The energy of the ground state and of elementary excitations are calculated by means of a canonical transformation.

In Ref. 1, Bogoliubov has shown that the property of superconductivity is possessed by a model of an electron gas in which the mutual interaction of the electrons is neglected but their interaction with the phonon field is taken into account. These results were established with the help of the Fröhlich Hamiltonian for the description of the system:[2]

$$H = H_{\text{el}} + H_{\text{int}} + H_{\text{ph}}; \tag{1}$$

$$H_{\text{el}} = \sum_{(k,\,\sigma)} (E(k) - \lambda)\, a^{+}_{k,\sigma}\, a_{k,\,\sigma};\quad H_{\text{ph}} = \sum_{(q)} \hbar\omega(q)\, b_q^{+} b_q; \tag{2}$$

$$H^{\text{Fr}}_{\text{int}} = \frac{g}{V\sqrt{2V}} \sum_{(k,\,k',\,\sigma)} \hbar\omega(k-k')(a^{+}_{k',\sigma}\, a_{k,\sigma}\, b_{k-k'} + a^{+}_{k,\sigma}\, a_{k',\sigma}\, b^{+}_{k'-k}), \tag{3}$$

where E(k) is the energy of the electron; $\hbar\omega(q)$ the energy of the phonon; k, q are the wave vectors, σ the spin variable ($\sigma = \pm \frac{1}{2}$); V the volume of the system; g the coupling constant; and λ the chemical potential. The creation and annihilation operators of electrons (a^{+}, a) and phonons (b^{+}, b) satisfy the usual commutation relations, and λ is defined by the condition

$$\sum_{k,\,\sigma} \overline{a^{+}_{k,\sigma}\, a_{k,\sigma}} = \overline{N},$$

where $\overline{N}$ is the given number of electrons.

The results of Bardeen[3] were obtained with the use of a certain equivalent Hamiltonian of the electron-electron interaction in place of the Hamiltonian (3), under not completely clear assumptions as to the suitability of the formation of electron pairs on the Fermi surface. Below, we shall show the equivalence of the Hamiltonians of Bardeen and Fröhlich, and shall establish the property of superconductivity for the Hamiltonian of Bardeen thus obtained. In the calculation, we shall make use of the method of Bogoliubov.[1]

The characteristic feature of electron-phonon interaction [Eq. (3)] is the fact that it is effective only in a thin layer at the Fermi surface, and falls off rapidly with increasing distance from it. Therefore, the principal contributions to all effects will be made by electron transitions at the Fermi surface. In this case the energy of the electron tran-

*The first paper of this series[1] will be denoted by I.

sitions can be regarded as small in comparison with the energy of the phonons $\hbar\omega$, and we have typical adiabatic coupling, wherein the frequencies of one subsystem (the electrons) are regarded as small in comparison with the frequencies of the other subsystem (phonons). We note further that $H_{int} \approx \sqrt{\hbar\omega}$ and consider H_{int} to be of first order of smallness, while H_{el} is of second order of smallness. For convenience in the intermediate calculations, we introduce the small parameter ϵ. We shall set ϵ equal to unity in the final results. Under these assumptions, the Hamiltonian of the system (1) can be written in the form:

$$H = \varepsilon^2 H_{ph} + \varepsilon H_{int} + H_{el}. \qquad (4)$$

We make use further of the operator form of pertrubation theory.[4] For this purpose we denote by P the projection operator,* which projects the eigenfunctions C of the operator H on the subspace of eigenfunctions of the operator H_{ph}, while we denote by C_0 the eigenfunctions of this subspace ($C_0 = PC$). In this case the problem of finding the eigenfunctions and eigenvalues of the equation

$$(H - E)C = 0 \qquad (5)$$

reduces to the solution of the equation with a certain "deformed" operator. With accuracy up to terms in ϵ^2 inclusively (to which we also limit ourselves below) this equation has the form:

$$(E - E_0)C_0 = P\{\varepsilon H_{int} + \varepsilon^2 H_{el} - \varepsilon^2 (H_{int} - PH_{int}P)$$
$$(H_0 - E_0)^{-1} \times (H_{int} - PH_{int}P)\} PC_0, \qquad (6)$$

where E_0 is the eigenvalue of the operator H_{ph}.

We first consider the case of a phonon vacuum and set $E_0 = 0$. We also note that $PH_{el}P = H_{el}P$, since H_{el} does not act on the phonon variables and that $PH_{int}P = 0$, since H_{int} is linear in the operators b and b^+. Thus the third term in the curly brackets of (6) takes the form

$$PH_{int}(H_0 - E_0)^{-1} H_{int}P$$
$$= \frac{g^2}{2V} \sum_{\substack{k_1, k_2, k_1', k_2', \sigma_1, \sigma_2 \\ k_1 - k_1' = k_2' - k_2 \neq 0}} a^+_{k_1', \sigma_1} a_{k_1, \sigma_1} a^+_{k_2', \sigma_2} a_{k_2, \sigma_2}. \qquad (7)$$

In this expression it is easy to see that only the terms with $\sigma_1 \neq \sigma_2$ are different from zero. Putting the creation operators on the left and the annihilation operators on the right and adding the quadratic form in a^+a (isolated by this process) to the kinetic energy operator, we write down Eq. (6) in the following form

$$EC_0 = (H_0 + H^B_{int}) C_0, \qquad (8)$$

where

$$H_0 = \sum_{(k, \sigma)} \varepsilon(k) a^+_{k,\sigma} a_{k,\sigma}\ ;\ \varepsilon(k) = E(k) - \frac{g^2}{2V} \sum_{(k_1)} 1 - \lambda; \qquad (9)$$

$$H^B_{int} = \frac{g^2}{V} \sum_{\substack{k_1, k_2, k_1', k_2' \\ k_1 - k_1' = k_2' - k_2 \neq 0}} a^+_{k_1', 1/2} a^+_{k_2', -1/2} a_{k_1, 1/2} a_{k_2, -1/2} \qquad (10)$$

(here and below, the formal small parameter ϵ is set equal to unity). The second component in $\epsilon(k)$ takes into account the usual correction to the chemical potential.

The interaction term H^B_{int} in Eq. (10) coincides with the corresponding expression used in the work of Bardeen, Cooper, and Schrieffer. In our derivation of Eq. (8), we have considered the energy of electron transitions to be small in comparison with the energy of the phonons $\hbar\omega$, which is valid only for transitions in a spherical shell near the Fermi surface. The breadth of this layer will evidently be of the order of some effective frequency $\hbar\tilde{\omega}$. Use of the original Hamiltonian of Fröhlich H_{int} of Eq. (3) leads to a similar result, as was shown by Bogoliubov in I.

Application of perturbation theory to the operators (8) — (10) leads to a logarithmic divergence at large distances from the Fermi surface. The reason for this appearance lies in the fact that in the derivation of (8) in the adiabatic approximation the energy of electron transitions was considered to be small in comparison with the energy of the phonons. However, the latter is only valid near the Fermi surface in a certain spherical shell of thickness of the order of the "effective phonon energy" $\hbar\tilde{\omega}$.

In the more accurate variant of the research of Bogoliubov, it is seen that the principal contribution in all quantities is given by effects which take place in this layer.

In correspondence with these considerations, we introduce a cutoff parameter into Eqs. (8) — (10) and consider the equation in the spherical shell $k_F \pm \Delta$ where k_F is the Fermi wave vector which is determined from the condition $\epsilon(k) = 0$. In view of the logarithmic singularity, the quantities ought to be only slightly sensitive to the choice of the cutoff parameter Δ.

We note that the corresponding equation in the work of Bardeen, Cooper, and Schrieffer is understood in precisely this sense.

*The operator P is defined in the following manner: $PC = \varphi_0(\varphi_0 C)$, where φ_0 is the eigenfunction of the operator H_{ph}; the parentheses denote scalar multiplication.

We carry out a canonical transformation[1] on the operators

$$a_{k,\,1/2} = u_k\alpha_{k,\,1} + v_k\alpha^+_{-k,\,0};\quad a_{k,\,-1/2} = u_k\alpha_{k,\,0} - v_k\alpha^+_{-k,\,1};$$
$$a^+_{k,\,1/2} = u_k\alpha^+_{k,\,1} + v_k\alpha_{-k,\,0};\quad a^+_{k,\,-1/2} = u_k\alpha^+_{k,\,0} - v_k\alpha_{-k,\,1}; \qquad (11)$$

$$u_k^2 + v_k^2 = 1;\quad (u_{-k} = u_k;\ v_{-k} = v_k), \qquad (12)$$

where α, α^+ are new Fermi operators; u_k, v_k are the coefficients of the transformation, which will be defined below.

In the new variables, the Hamiltonian of Eq. (8) can be written in the form

$$H = \varepsilon_0 + H_0 + H_1 + H_2, \qquad (13)$$

where

$$\varepsilon_0 = 2\sum_{(k)}\varepsilon(k)\,v_k^2; \qquad (14)$$

$$H_0 = \sum\varepsilon(k)\,(u_k^2 - v_k^2)\,(\alpha^+_{k,\,1}\alpha_{k,\,1} + \alpha^+_{k,0}\,\alpha_{k,0}); \qquad (15)$$

$$H_1 = 2\sum\varepsilon(k)\,u_kv_k\,(\alpha^+_{k,\,1}\alpha^+_{-k,\,0} + \alpha_{-k,\,0}\alpha_{k,\,1}); \qquad (16)$$

$$H_2 = \frac{g^2}{V}\sum(u_{k_1}u_{k_2}\alpha^+_{k_1,\,1}\alpha^+_{k_2,\,0} - v_{k_1}v_{k_2}\alpha_{-k_1,\,0}\alpha_{-k_2,\,1}$$
$$-u_{k_1}v_{k_2}\alpha^+_{k_1,\,1}\alpha_{-k_2,1} + v_{k_1}u_{k_2}\alpha_{-k_1,\,0}\alpha^+_{k_2,\,0})$$
$$(u_{k_1}u_{k_2}\alpha_{k_1,\,1}\alpha_{k_2,\,0} - v_{k_1}v_{k_2}\alpha^+_{-k_1,\,0}\alpha^+_{-k_2,\,1}$$
$$- u_{k_1}v_{k_2}\alpha_{k_1,\,1}\alpha^+_{-k_2,\,1} + v_{k_1}u_{k_2}\alpha^+_{-k_1,\,0}\alpha_{k_2,\,0}). \qquad (17)$$

We shall further regard H_0 as the operator of zeroth approximation and H_1, H_2 as perturbations.

It was shown in I that, in line with perturbation theory, there will be dangerous terms corresponding to the creation of two particles; it is shown there that this is connected with the presence of logarithmic singularities on the Fermi surface.

The situation is very much the same for the Hamiltonian (13). To remove the difficulties with divergence in first order in g^2, we sum over all diagrams leading from the vacuum to the two-particle states, and so choose the functions u_k, v_k that they compensate one another. One such diagram is in the Hamiltonian H_1:

$$2\sum\varepsilon(k)\,u_kv_k\alpha^+_{k,\,1}\alpha^+_{-k,\,0}$$

and two in the Hamiltonian H_2:

$$\frac{g^2}{V}\sum_{\substack{k_1,\,k_2,\,k_1',\,k_2'\\ k_1-k_1'=k_2'-k_2\neq 0}}(-v_{k_1'}u_{k_2'}v_{k_1}v_{k_2}\delta_{-k_1',\,k_2'}\alpha^+_{k_1,\,0}\alpha^+_{-k_2,\,1}$$
$$-u_{k_2'}u_{k_1'}u_{k_1}v_{k_2}\alpha^+_{k_1',\,1}\alpha^+_{k_2',\,0}\delta_{k_1,\,-k_2})$$
$$= -\frac{g^2}{V}\sum_{(k_1)}u_{k_1}v_{k_1}\sum_{(k)}(u_k^2 - v_k^2)\,\alpha^+_{k,\,1}\alpha^+_{-k,\,0}.$$

The vanishing of the coefficients of $\alpha^+_{k,1}\alpha^+_{-k,0}$ leads to a system of equations for the functions u_k, v_k:

$$2\varepsilon(k)\,u_kv_k = (u_k^2 - v_k^2)\,\frac{g^2}{V}\sum_{(k_1)}u_{k_1}v_{k_1}. \qquad (18)$$

We note, furthermore, that the set (18) has a trivial solution $u_kv_k = 0$ and hence

$$u_k^2 = \begin{cases}0, & |k|<k_F,\\ 1, & |k|>k_F;\end{cases}\quad v_k^2 = \begin{cases}1, & |k|<k_F,\\ 0, & |k|>k_F.\end{cases} \qquad (19)$$

This solution, as is seen from what follows, corresponds to the normal (non-superconducting) state of the system.

In order to find the nontrivial solution, we introduce the notation:

$$C = (g^2/V)\sum u_kv_k. \qquad (20)$$

Then, making use of the normalization condition (12) for the functions u_k and v_k, it is not difficult to solve the set (18) relative to u_k^2 and v_k^2:

$$u_k^2 = \frac{1}{2}\left\{1 + \frac{\varepsilon(k)}{V\,C^2 + \varepsilon^2(k)}\right\};$$

$$v_k^2 = \frac{1}{2}\left\{1 - \frac{\varepsilon(k)}{V\,C^2 + \varepsilon^2(k)}\right\}. \qquad (21)$$

Substituting the results found for u_kv_k in (20), we get an equation for the constant C:

$$1 = (g^2/2V)\sum_{(k)}[C^2 + \varepsilon^2(k)]^{-1/2}. \qquad (22)$$

Transforming from sums to integrals in (22), and taking it into consideration that the range of integration in k lies in the interval $(k_F - \Delta,\ k_F + \Delta)$, we can obtain for C the following asymptotic solution:

$$C = 2\tilde{\Delta}e^{-1/\rho};\quad \rho = 2g^2k_F^2/(2\pi)^2\varepsilon'(k_F);\quad \tilde{\Delta} = \varepsilon'(k_F)\,\Delta. \qquad (23)$$

We now compute the energy of the elementary excitations in first approximation in g^2:

$$\Omega(k,\,1) = \varepsilon(k)\,(u_k^2 - v_k^2) + 2u_kv_k\,\frac{g^2}{V}\sum_{(k_1)}u_{k_1}v_{k_1},$$

or, utilizing Eqs. (20) and (21)*

$$\Omega(k,\,\gamma) = \sqrt{C^2 + \varepsilon^2(k)}, \qquad (24)$$

where the constant C is determined by Eq. (23).

For the normal state, obviously,

*Equation (24) was obtained by Bardeen, Cooper and Schrieffer, as pointed out in the paper of Bernardes.[5]

$$\Omega(k, \gamma) = \varepsilon(k). \tag{25}$$

We see from (24) that, in contrast to the normal state, the energy of the elementary excitations differs from the ground state by the gap

$$\Delta\Omega = C. \tag{26}$$

Just as in I, we can consider the current state, i.e., the state with the total momentum of the system different from zero. In this case we can show that for sufficiently small velocities u, the value of the gap falls off proportional to u.

Proceeding to the computation of the addition to the energy of the ground state, we note that the contribution in it amounts to only one term. As a result, we obtain

$$\Delta\varepsilon_0 = -\frac{g^2}{V}\left(\sum_{(k)} u_k v_k\right)^2 = -\frac{V}{g^2} C^2 \tag{27}$$

(for the normal state, $C = 0$ and $\Delta\epsilon_0 = 0$).

We now show that the superconducting state is energetically more advantageous than the normal. Making use of Eqs. (14), (27), and (31), we obtain for the difference of the lowest energy levels of the superconducting and normal states

$$\Delta E = \varepsilon_0 + \Delta\varepsilon_0 - \sum \varepsilon(k)\left\{1 - \frac{\varepsilon(k)}{|\varepsilon(k)|}\right\} = \\ = \sum\left\{|\varepsilon(k)| - \frac{\varepsilon^2(k)}{V C^2 + \varepsilon^2(k)}\right\} - \frac{V}{g^2} C^2. \tag{28}$$

Hence, with the same degree of accuracy as in the asymptotic solution for C, we finally obtain

$$\Delta E = -V \frac{k_F^2 (2\tilde{\Delta})^2}{(2\pi)^2 \varepsilon'(k_F)} e^{-2/\rho}. \tag{29}$$

We can interpret the quantity

$$\frac{2k_F^2}{(2\pi)^2 \varepsilon'(k_F)} = \frac{1}{V}\left\{\frac{V}{(2\pi)^3}\frac{4\pi k^2 dk}{dE}\right\}_{k=k_F}$$

as the relative density of electron levels, dn/dE. Then (29) is rewritten in the following form:

$$\frac{1}{V}\Delta E = -\frac{dn}{dE}\frac{(2\tilde{\Delta})}{2} e^{-2/\rho}; \quad \rho = g^2 \frac{dn}{dE}. \tag{30}$$

Identifying the thickness of the layer $2\tilde{\Delta}$ with the quantity $\tilde{\omega}$ from Eq. (14) of I, we obtain agreement with all the results obtained by Bogoliubov with the use of the Hamiltonian of Fröhlich. If we carry out the substitutions $\tilde{\Delta} \to \omega$, $g^2 \to V$, $dn/dE = N$ in (30), then clear agreement of the results is obtained with the results of Bardeen et al.[3] The minimum energy necessary to break up the pair calculated in Ref. 4 is evidently equal to twice the energy of the gap in the spectrum of elementary excitations (26). In the same way, complete correspondence is obtained between the Hamiltonians of Fröhlich and Bardeen and the results obtained with their help.

It should be pointed out that Eqs. (26) and (30) are only slightly sensitive to change in the form of the interaction assumed by us. Thus, if we replace the constant g^2 by the quantity $g^2(k_1 - k_2)$, concentrated about the Fermi surface, then Eqs. (26), (30) would be preserved with this one difference, that g^2 would be replaced by the mean value of $g^2(k_1 - k_2)$, and $\tilde{\Delta}$ would be replaced by some mean width $\tilde{\Delta}(k_1 - k_2)$. On the other hand, the Bose part of the spectrum can depend on the detailed form of the function $g(k_1 - k_2)$. We intend to consider this dependence in a subsequent paper.

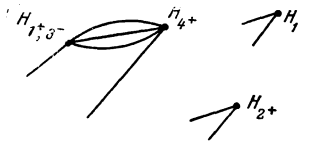

FIG. 1

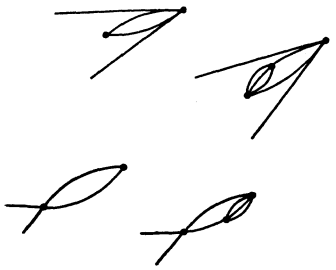

FIG. 2

The results worked out above were obtained in first order perturbation theory. It is not difficult to establish the fact that the compensation of diagrams in second order (g^4) does not change the results. Actually, there are terms in the perturbation operator H_2 [Eq. (17)] which describe, in their effect on the vacuum, the creation of four particles — H_{4+}, the creation of a single particle and the annihilation of three particles — $H_{1+,3-}$ etc. In second order perturbation theory, the contribution to the diagrams with two particles as a result give terms of the form

$$H_{1+,3-}(H_0 - E_0)^{-1} H_{4+}, \tag{31}$$

which are drawn in Fig. 1.

We now require that they be compensated in the sum with the diagrams obtained from H_1 and H_2 in first order, pictured in this same figure.

We note that the diagrams of the form shown in Fig. 2 are compensated automatically in this case by virtue of the compensation rule.

The operators H_{4+} and $H_{1+,3-}$ have the form

$$H_{4^+} = -\frac{g^2}{V} \sum_{\substack{k_1, k_2\ k_1', k_2' \\ k_1 - k_1' = k_2' - k_2' \neq 0}} u_{k_1'} u_{k_2'} v_{k_1} v_{k_2} \alpha^+_{k_1 1} \alpha^+_{k_2' 0} \alpha^+_{-k_1 0} \alpha^+_{-k_2 0}; \quad (32)$$

$$H_{1^+, 3^-}$$

$$= -\frac{g^2}{V} \sum_{\substack{k_1, k_2, k_1', k_2' \\ k_1 - k_1' = k_2' - k_2 \neq 0}} (v_{k_1'} v_{k_2'} u_{k_1} v_{k_2} - u_{k_1'} u_{k_2'} v_{k_1} u_{k_2}) \times \alpha^+_{-k_2 1} \alpha_{-k_2' 1} \alpha_{k_1 1} \alpha_{-k_1' 0}$$

$$-\frac{g^2}{V} \sum_{\substack{k_1, k_2, k_1', k_2' \\ k_1 - k_1' = k_2' - k_2 \neq 0}} (v_{k_1'} v_{k_2'} v_{k_1} u_{k_2} - u_{k_1'} u_{k_2'} u_{k_1} v_{k_2}) \times \alpha^+_{-k_1 0} \alpha_{-k_1' 0} \alpha_{-k_2' 1} \alpha_{k_2 0}. \quad (33)$$

Since the second term is obtained from the first by the substitution it is evident that it only doubles the effect of first term.

As a result, we obtain for u_k, v_k the following set of equations:

$$2 \left\{ \varepsilon(k) - \left(\frac{g^2}{V}\right)^2 \sum_{\substack{k_1, k_2, k_3 \\ k_2 - k_1 + k_3 = k}} \frac{\{u^2_{k_1} v^2_{k_2} - (u_{k_1} v_{k_1})(u_{k_2} v_{k_2})\}(u^2_{k_3} - v^2_{k_3})}{\varepsilon(k) + \varepsilon(k_1) + \varepsilon(k_2) + \varepsilon(k_3)} \right\}$$

$$= (u_k^2 - v_k^2) \left\{ \frac{g^2}{V} \sum_{(k_1)} u_{k_1} v_{k_1} + \left(\frac{g^2}{V}\right)^2 \sum_{\substack{k_1, k_2, k_3 \\ k_2 - k_1 + k_3 = k}} \frac{(u_{k_1} v_{k_1})\{(u_{k_2} v_{k_2})(u_{k_3} v_{k_3}) - u^2_{k_2} v^2_{k_3}\}}{\varepsilon(k) + \varepsilon(k_1) + \varepsilon(k_2) + \varepsilon(k_3)} \right\}. \quad (34)$$

In view of the fact that the additional terms of fourth order in g contain products of uv with the same index, which give an exponentially small contribution, then, as one can see, they do not change the asymptotic solution found earlier. We further note that terms of fourth order were considered for the model Hamiltonian (10), which is itself obtained with accuracy to terms of order g^2. Therefore, if we attempt to obtain the exact corrections from terms of order g^4, it is necessary first to improve the model Hamiltonian (10), extending the method of projection up to terms of fourth order.

In conclusion, the authors take the opportunity to express their gratitude to N. N. Bogoliubov, as well as to D. N. Zubarev and Iu. A. Tserkovnikov for discussion of the work.

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