A NEW METHOD IN THE THEORY OF SUPERCONDUCTIVITY. I

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The canonical transformation method previously developed by the author for the theory of superfluids is generalized in the present paper. By application of this method and the principle of compensation of "dangerous" diagrams, it is shown that a superconducting state is inherent in the Fröhlich model. Computation of the principal parameters of this state leads to formulas that confirm those of the theory of Bardeen, Cooper, and Shrieffer.

After the discovery of the isotopic effect, the idea became universal that the interaction between the electrons and the lattice must play a fundamental role in the phenomenon of superconductivity. A series of very interesting syntheses, which treat a system of electrons interacting with the phonon field have already been carried out. In the present paper, we shall show that, by further development of a method which we have put forward previously for the theory of superfluidity, it is possible to give a systematic theory of the superconducting state. In this case, in particular, the results of the theory of Bardeen, Cooper, and Shrieffer are confirmed.

For simplicity, we shall start out from the model proposed by Fröhlich, in which the Coulomb interaction is not introduced explicitly and the dynamic system is characterized by the Hamiltonian

\[ H_{0} = \sum_{k, s} E(k) a_{k}^{+} a_{k}s + \sum_{q} \omega(q) b_{q}^{+} b_{q} + \text{conjugate}, \]

where \( E(k) \) is the energy of the electron, \( \omega(q) \) is the energy of the phonon, \( g \) is the coupling constant, and \( V \) the volume.

As is now well known, ordinary perturbation theory in terms of powers of the coupling constant is inapplicable, since the electron-phonon interaction, in spite of its smallness, is seen to be very considerable when close to the Fermi surface. Therefore, we shall first carry out a certain canonical transformation, starting out from the following considerations.

First, we note that the matrix elements, corresponding to virtual creation of "particles" from the vacuum, are always associated with the energy denominators

\[ \epsilon(k_{1}) + \cdots + \epsilon(k_{2}) \pm \omega(q_{1}) + \cdots + \omega(q_{r})^{-1}, \]

in which \( \epsilon(k) \sim |E(k) - E_{F}| \) is the energy of the particle (electron \(- E(k) > E_{F}\) or hole \(- E(k) < E_{F}\)) which becomes small at the Fermi surface.

Such denominators are not generally "dangerous," and do not lead to singularities in integration over the momenta \( k_{1}, \ldots, k_{2}, q_{1}, \ldots, q_{r} \), except when we deal with a virtual process of the creation of a single pair, without phonons. Then, because of the conservation law, the particles of this pair will have oppositely directed momenta \( \pm k \), and the energy denominator \( \frac{1}{2} \epsilon(k) \) will become "dangerous" for integration. We note further that their spins will also be opposite.

Thus, in the choice of the canonical transformation, it must be kept in mind that it is necessary to guarantee the mutual compensation of the diagrams which lead to virtual creation from the vacuum of pairs of particles with opposite momenta and spins.

We now underscore the analogy with the situation holding in our theory of superfluids, namely, in the consideration of a non-ideal Bose gas, where virtual creation of a pair of particles (with mo-
menta ± k) from the condensate plays the same role. We then made use of a linear transformation of the Bose amplitudes, "mixing" $b_q$ with $b_{-q}$.

Generalizing this transformation, we now bring into consideration the case of new Fermi amplitudes $a_{k}$:

$$a_{k} = \frac{1}{2} \left[ a_{k} + a_{-k} \right],$$

where $u_k$, $v_k$ are real numbers, connected by the relation

$$u_k^2 + v_k^2 = 1.$$

It is not difficult to check that such a transformation preserves all the commutation properties of the Fermi operators and is therefore canonical.

We further note that it represents a generalization of the ordinary transformation, with the help of which the creation and annihilation operators of holes inside the Fermi surface and of electrons outside this surface are introduced. Actually, if we set

$$u_k = 1, v_k = 0 \text{ for } E(k) > E_F,$$

$$u_k = 0, v_k = 1 \text{ for } E(k) < E_F,$$

then we obtain

$$a_{k0} = a_k, \quad a_{k1} = a_{-k}, \quad a_{k2} = a_k^+, \quad a_{k3} = a_{-k}^+ \text{ for } E(k) > E_F,$$

$$a_{k0} = -a_k, \quad a_{k1} = a_k, \quad a_{k2} = a_k^+, \quad a_{k3} = a_{-k}^+ \text{ for } E(k) < E_F,$$

so that, for example, $a_{k0}$ will be an annihilation operator for an electron of momentum $k$ and spin $\frac{1}{2}$ outside the Fermi sphere, and will be an annihilation operator for a hole with momentum $-k$ and spin $-\frac{1}{2}$ inside.

In the general case, when $(u_k, v_k) \neq (0, 1)$, we have to deal with the superposition of a hole and an electron.

Generalizing to the consideration of the Fröhlich Hamiltonian, we note that it will be more advantageous to us not to restrict ourselves to the relation

$$\sum_{k, \pm} \alpha_{k\pm}^+ \alpha_{k\pm} = N_0,$$

where $N_0$ is the total number of electrons; we therefore make use of the ordinary procedure in such a situation and introduce a parameter $\lambda$ which plays the role of the chemical potential. Then, instead of $H_{F\rho}$, we have the Hamiltonian

$$H = H_{F\rho} - \lambda N.$$

We determine the parameter $\lambda$ in turn from the condition that in the state under examination

$$\bar{N} = N_0.$$

Transforming $H$ to the new Fermi amplitudes, we get

$$H = U + H_0 + H_{int}, \quad H_{int} = H_1 + H_2 + H_3,$$

where $U$ is the constant

$$U = 2\sum E(k) v_k^2 - 2\sum v_k^2,$$

and where

$$H_1 = \sum_{k, h} g \sqrt{\frac{\omega(q)}{2\nu}} \left( u_h v_{k-h} \delta_{k-h}^{+} + u_{-h} v_{k+h} \delta_{k+h}^{+} \right) + \text{conjugate},$$

$$H_2 = \sum_{k, h} g \sqrt{\frac{\omega(q)}{2\nu}} \left( u_h v_{k-h} \delta_{k-h}^{+} + u_{-h} v_{k+h} \delta_{k+h}^{+} \right) + \text{conjugate},$$

$$H_3 = \sum_{k} (E(k) - \lambda (u_k^2 - v_k^2)) a_k^+ a_{k1} + a_{k1} a_{k0},$$

$$H_0 = \sum_{k} (E(k) - \lambda (u_k^2 - v_k^2)) (a_{k0}^+ a_{k0} + a_{k1}^+ a_{k1}) + \sum \omega(q) b_q^+ b_q.$$

We introduce the filling number

$$\gamma_{k0} = a_{k0}^+ a_{k0}, \quad \gamma_{k1} = a_{k1}^+ a_{k1}$$

of new quasi-particles, which are generated by the operator $\alpha^+$. Then the "interaction-free vacuum," i.e., the state $\psi$ in which

$$H_0\psi = 0,$$

will evidently be

$$\psi = \prod_k \delta(\gamma_{k0}) \delta(\gamma_{k1})$$

with zero values of the numbers $\nu$.

We further note that $\lambda$ ought to be close to $E_F$, since $\lambda = E_F$ in the absence of interaction, and that consequently, the expression

$$\varepsilon(k) = (E(k) - \lambda)(u_k^2 - v_k^2)$$

ought to vanish on a surface close to the Fermi surface.

We now see that the virtual process of creation from the vacuum of a pair of quasi-particles $\nu_{k0}$ and $\nu_{k1}$ without phonons will be "dangerous" in the sense of the criterion given earlier, since the corresponding energy denominator will be

$$1 / 2\varepsilon(k).$$

The Hamiltonian $H_3$, which, being applied to a
vacuum, gives the diagram of Fig. 1, leads directly to such a process. This same process is also obtained, moreover, as a result of the combined action of $H_1$, $H_2$. Thus, for example, in the second order in the coupling constant $g$, we have the diagrams shown in Fig. 2a.

Expanding it, we finally obtain

$$\mathcal{E}(k) = E(k) - \frac{1}{2V} \sum_{k'} \frac{\omega(k-k')}{\omega(k-k') + \varepsilon(k) + \varepsilon(k')} \frac{\alpha_k^0 - \alpha_{k'}^0}{u_k v_k}, \quad (4)$$

where

$$\mathcal{E}(k) = E(k) - \lambda.$$ 

Staying within the limits of the approximation, we replace $E(k) = \{E(k) - \lambda\} (\alpha_k^0 - \alpha_{k'}^0)$ in the denominator of the right side by $\tilde{\varepsilon}(k) = \{E(k) - \lambda\} (\alpha_k^0 - \alpha_{k'}^0)$.

Then, setting $\tilde{\mathcal{E}}(k) = \lambda = \xi(k)$, we write down the equation in the form

$$\xi(k) = \mu = \xi(k),$$

we find from (6) where

$$\mu = \frac{1}{2(2\pi)^3} \sum_{k'} \frac{\omega(k-k')}{\omega(k-k') + \varepsilon(k) + \varepsilon(k')} \frac{\alpha_k^0 - \alpha_{k'}^0}{u_k v_k} d{k'}.$$ 

This equation obviously contains the trivial solution

$$\mu = 0, \quad (u, v) = (0, 1),$$

which corresponds to the "normal state." It possesses, however, an additional solution of another type which goes over into the trivial one at great distances from the Fermi surface.

Denoting

$$C(k) = 1 \frac{1}{(2\pi)^3} \int \frac{\omega(k-k')}{\omega(k-k') + \varepsilon(k) + \varepsilon(k')} \frac{\alpha_k^0 - \alpha_{k'}^0}{u_k v_k} d{k'},$$

we find from (6) where

$$\mu = \frac{1}{2} \left\{ 1 + \frac{\xi(k)}{V C^2(k) + \xi^2(k)} \right\};$$

$$\nu = \frac{1}{2} \left\{ 1 + \frac{\xi(k)}{V C^2(k) + \xi^2(k)} \right\}; \quad (7)$$

whence

$$\mu v = \frac{C(k)}{2V C^2(k) + \xi^2(k)}; \quad \varepsilon = \frac{\xi^2(k)}{V C^2(k) + \xi^2(k)}. $$

Thus, our equation reduces to the following form:

$$C(k) = 1 \frac{1}{(2\pi)^3} \int \frac{\omega(k-k')}{\omega(k-k') + \varepsilon(k) + \varepsilon(k')} \frac{\alpha_k^0 - \alpha_{k'}^0}{u_k v_k} d{k'}.$$ 

We note that this equation has a singular prop-
In view of the fact that the integral on the right side of (8) remains logarithmically divergent in the vicinity of the surface \( \xi(k) = 0 \) if we set \( C = 0 \).

In such a situation, it is not difficult to obtain an asymptotic form of the solution for small \( g \):

\[
C(k) = \frac{\omega}{2} \exp\left(-\frac{A}{g^2}\right),
\]

where

\[
p = g^2 \frac{1}{2 \omega^2} \left( \frac{k^2}{dE(k)dk} \right) ; \quad E(k) = \lambda,
\]

\[
\ln \omega = \frac{1}{2} \int \frac{d}{\omega^2} \left( \frac{k^2}{dE(k)dk} \right) \left[ \frac{\omega}{2} \frac{1}{(1-i)} \right] dt.
\]

Taking into account the additional condition (3) and the expressions (7), (9) for \( u, v \), it can be noted that

\[
k_0 = k_F.
\]

Furthermore, it is clear that the corrections to Eq. (5), obtained by replacing \( u_k, v_k \) in (5) by their "normal" values

\[
u_h = \theta_0(k) = \begin{cases} 1, & |k| > k_F \\ 0, & |k| < k_F \end{cases}
\]

\[
u_h = \theta_0(k) = \begin{cases} 1, & |k| > k_F \\ 0, & |k| < k_F \end{cases}
\]

will be exponentially small.

We can therefore replace \( \tilde{E}(k) \) by the corresponding formula for the normal state in Eqs. (10) without loss of accuracy, and integrate the factor

\[
\frac{1}{2 \pi^2} \left( \frac{k^2}{dE/dk} \right) = \frac{1}{V} \left( \frac{4\pi k^2}{dE} \right)
\]
as the relative density \( dn/dE \) of the number of electron levels in an infinitely narrow energy band close to the Fermi surface. Then

\[
p = g^2 dn/dE.
\]

We now proceed to the calculation of the energy of the ground state in the second approximation.

Of the entire \( H_{\text{int}} \), we shall now take into account only \( H_1 \). Consequently, we get for the eigenvalue of \( H \) in the ground state

\[
U = \langle C_V H_1 H_0^{-1} C_V \rangle = 2 \sum_k \left( E(k) - \lambda \right) \frac{\omega}{2} \sum_{k' \neq k} \frac{\omega(k' - k)}{\omega(k' - k) + \epsilon(k) + \epsilon(k')}.
\]

Then, substituting the expressions we have obtained for \( u_k, v_k \), we compute the difference \( \Delta E \) between the energy of the ground state and the energy of the normal state. We have

\[
\Delta E = -\frac{dn}{dE} \omega \exp\left(-\frac{2}{\rho}\right).
\]

It is interesting to observe that this result coincides with the result of Bardeen and his coworkers\(^3\). To see this we need only write the Bardeen parameters \( \omega, V \) in the following fashion:

\[
2\omega = \omega; \quad V = g^2.
\]

We now construct, in the given approximation, the formula for the energy of the elementary excitation. For this purpose, we choose an excited state

\[
C_1 = \sum_n C_n
\]
and apply perturbation theory to it in the usual fashion. We obtain the following expression for the energy of an elementary excitation with momentum \( k \):

\[
E_e(k) = \varepsilon(k) - C_1 H_{\text{int}} (H_0 - \varepsilon(k))^{-1} H_{\text{int}} C_1 > \epsilon_{\text{coup}},
\]

for which we find

\[
E_e(k) = \sum_k \left[ 1 - \frac{g^2}{V} \sum_{k'} \frac{\omega(k - k')}{\omega(k - k') + \epsilon(k')^2 - \epsilon^2(k)} \right]
\]

Here the first term, proportional to \( \tilde{E}(k) \) has no singular properties whatever and vanishes on the Fermi surface. The second term is equal to

\[
\frac{g^2}{2} \sum_{k'} u_{k'} v_{k'} \sum_k \frac{\omega(k - k')}{\omega(k - k') + \epsilon(k')^2 - \epsilon^2(k)} u_{k'} v_{k'} \epsilon(k).
\]

on the Fermi surface.

Thus the energies of the excited states are different from the energy of the ground state by the gap

\[
\Delta = \omega e^{-1/2}.
\]

We note that in the work of Bardeen and his co-
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workers, there is an expression of the type $2\bar{\omega} \times e^{-1/\rho}$ which is interpreted there as the energy necessary to break up a "pair."

We now consider the "ground current state," i.e., the state with the lowest energy among all the possible states with given momentum $p$.

We therefore need to find the eigenvalue of $H$ for the additional condition

$$\sum_{k,s} k a_{k,s}^+ a_{k,s} = p.$$  

Instead, making use of the usual method, we introduce (in addition to the scalar parameter $\lambda$) an additional vector parameter $u$ which plays the role of an average velocity, and choose the total Hamiltonian in the form

$$H = H_{F} - \lambda \sum_{k,s} a_{k,s}^+ a_{k,s} - \sum_{k,s} (\mathbf{u}k) a_{k,s}^+ a_{k,s} =$$

$$= \sum_{k,s} (E(k) - (\mathbf{u}k) - \lambda^2) a_{k,s}^+ a_{k,s} + \sum_{q} \omega(q) b_{q}^+ b_{q} + H_{int}. \quad (18)$$

The value of $u$ is determined from the condition

$$\sum_{k,s} k a_{k,s}^+ a_{k,s} = p.$$  

Since we are always dealing in our discussions only with a small region on the Fermi surface, we can for simplicity write the following

$$E(k) = \frac{k^2}{2m} + D; D = E_F - \frac{k^2}{2m},$$

and then, in the final equations, take

$$m = \left( \frac{dE/dk} {\hbar} \right)_{k - k_F}.$$  

Then

$$E(k) - (\mathbf{u}k) = E(k - mu) - \frac{1}{2} m u^2,$$

and therefore, making the following translation in the momentum space of $k$:

$$k \rightarrow k + um, a_{k,s} \rightarrow a_{k+mu,s}, \quad (19)$$

and putting

$$\lambda \rightarrow \lambda + mu^2/2,$$

then the Hamiltonian (18) takes the form (2) and the vector $u$ drops out. We again arrive at the case of a ground state with zero momentum. No new investigation is thus needed for the current state, but it will suffice only to make a transformation inverse to (19) in the formulas obtained earlier.

Thus, we can verify, for example, that the energy of the ground current state, with mean velocity $u$, differs from the energy of the ground state without current by an amount $Nmu^2/2$.

The excitations are separated from the energy of the ground current state by a gap

$$\Delta_u = \Delta - k_F u > \Delta - k_F |u|.$$  

Consequently, if

$$k_F |u| < \Delta,$$

the current state, although it possesses an energy greater than the non-current (so long as the action of the magnetic field is not taken into account), is shown to be stable relative to the excitations.

Thus, we see that our model contains the property of superconductivity.

Let us make a few other observations.

In our method of investigation, we must take the parameter $\rho$ to be small in order to make it possible to restrict ourselves to asymptotic approximations. However, as was shown by Tolmachev and Tiablikov (with the aid of a method which does not make use of any assumption on the smallness of $\rho$) the sound velocity becomes imaginary for $\rho > \frac{1}{2}$, i.e., the lattice becomes unstable. In cases in which the lattice is so rigid that the electron-phonon interaction has no essential effect on the energy of the phonon, the parameter $\rho$ must be small. Even for $\rho = \frac{1}{4}$, the value of $e^{-1/\rho}$ is $\frac{1}{55}$. This, in our opinion, explains the smallness of the value of the energy gap and therefore of the critical temperature.

We further note that if we explicitly add a term of Coulomb interaction to the Fröhlich Hamiltonian, then it will be necessary to carry out a summation of the diagrams of electron-holes of the Gelman-Bruckner type, in order to guarantee the phenomenon of screening.

By way of a preliminary estimate, we could first introduce into the Hamiltonian the Coulomb interaction in the screened form, and also treat it by means of perturbation theory. Then we would have obtained substantially the same formulas as earlier, but we would need to replace $g^2$ by

$$g^2 - \frac{1}{2} \int_{-1}^{1} \nu_{e}(k_F V^2(1-t)) dt,$$

where $\nu_{e}(k)$ is the Fourier transform of the screened function.

Thus it could be immediately established that the Coulomb interaction contradicts the phenomenon of superconductivity.

In conclusion I consider it my pleasant duty to thank D. N. Zubarev, V. V. Tolmachev, S. V. Tiab-
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:

\[ H_{el} = \sum_{\mathbf{k}, \mathbf{q}} \left( \frac{\hbar}{\omega} (E_k - \lambda) a_{\mathbf{k}, \sigma}^+ a_{\mathbf{k}, \sigma} + H_{ph} \right) \]

\[ H_{ph} = \sum_{\mathbf{q}} \hbar \omega_\mathbf{q} b_{\mathbf{q}}^+ b_{\mathbf{q}}; \]

\[ H_{int} = \frac{g^2}{V^2} \sum_{\mathbf{k}, \mathbf{k}', \mathbf{\sigma}} \hbar \omega (\mathbf{k} - \mathbf{k'}) (a_{\mathbf{k}, \sigma}^+ a_{\mathbf{k}', \sigma} b_{\mathbf{k}'}^* b_{\mathbf{k}-\mathbf{k}'}^*); \]

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

\[ \sum_{\mathbf{k}, \sigma} a_{\mathbf{k}, \sigma}^+ a_{\mathbf{k}, \sigma} = \bar{N}, \]

where \( \bar{N} \) 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-