A NEW METHOD IN THE THEORY OF SUPERCONDUCTIVITY. III

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Submitted to JETP editor October 17, 1957

J. Exptl. Theoret. Phys. (U.S.S.R.) 34, 73-79 (January, 1958)

The Hamiltonian of Bardeen is analyzed in this paper and the method of summation of the principal diagrams is applied. It is shown that the same results are obtain in this way as in Refs. 1 and 2.

RECENTLY great successes have been attained in the solution of problems of statistical physics by means of summation of the principal diagrams.

In the present paper we shall show that in the theory of superconductivity, we can also obtain (by this method) those results which were found in previous researches[1,2] with the aid of a canonical transformation and the principle of compensation of diagrams with "dangerous" energy denominators.

As has been shown by Tolmachev and Tiablikov,[2] we can consider the Hamiltonian of Bardeen in place of that of Fröhlich, since they both, up to a known degree, give equivalent results for the effect of electron-phonon interaction on the dynamics of electrons close to the Fermi surface. In our case the Bardeen Hamiltonian is considerably simpler.

Therefore, for a more graphic description and to establish the connection with the ideas of the work of Bardeen, Cooper, and Schrieffer,[3] we shall start out from the Hamiltonian of Bardeen:

$$H_B = \sum_{k,s} E(k)\, a^+_{ks} a_{ks} - \frac{I}{V} \sum_{(k_1 k_2, k_1', k_2')} a^+_{k_1,-1/2}\, a^+_{k_2,1/2}\, a_{k_2',1/2}\, a_{k_1',-1/2}\, \theta(k_1)\,\theta(k_2) \times \theta(k_1')\,\theta(k_2')\,\Delta(k_1+k_2-k_1'-k_2'),$$

where

$$\theta(k) = \begin{cases} 1, & E(k_F) - \omega < E(k) < E(k_F) + \omega \\ 0, & |E(k) - E(k_F)| > \omega \end{cases},$$

$$\Delta(k) = \begin{cases} 1, & k = 0, \\ 0, & k \neq 0 \end{cases}$$

and where $E(k)$ is the radially symmetric function representing the energy of an electron of momentum k; I and ω are the Bardeen parameters. In the Fröhlich model, we must set[2]

$$I = g^2, \quad \omega = \tilde{\omega}/2.$$

We shall take into account the value N of the total number of electrons by means of the chemical potential λ, for which purpose we add the term $-\lambda N$ to H_B. Then we obtain the Hamiltonian

$$H = H_0 + H_{\text{int}},$$

$$H_0 = \sum_{k,s} \{E(k) - \lambda\}\, a^+_{ks} a_{ks},$$

$$H_{\text{int}} = -\frac{I}{V} \sum_{(k_1, k_2, k_1', k_2')} a^+_{k_1,-1/2}\, a^+_{k_2,1/2}\, a_{k_2',1/2}\, a_{k_1',-1/2} \times \theta(k_1)\,\theta(k_2)\,\theta(k_1')\,\theta(k_2')\,\Delta(k_1+k_2-k_1'-k_2'),$$

for which we shall also consider the question of the summation of the principal diagrams.

Since the interaction is effective only in a small region of the Fermi sphere and only between particles (electrons or holes) with oppositely directed spins, we see that a very important role will be played by diagrams of the type shown in Fig. 1. These diagrams were constructed from an "irreducible complex" (see Fig. 2), consisting of a pair of particles with momenta $\pm k$ and spins $\pm \frac{1}{2}$.

FIG. 1

FIG. 2

To sum the diagrams, we make use of the method of approximate second quantization, i.e., we construct a simplified Hamiltonian, for which the diagrams will only be of that class which we desire to sum, and furthermore, with the same contribution which is made in the present Hamiltonian.*

Since the complexes of pairs of particles $(\pm k, \pm \frac{1}{2})$ are not broken up in the diagrams considered by us, it is natural to compare their quantum amplitudes b_k, b_k^+ with the commutation relations

$$[b_k, b_{k'}] = 0, \quad [b_k^+, b_{k'}^+] = 0, \quad [b_k^+, b_{k'}] = 0; \quad k \neq k'. \quad (2)$$

Furthermore, since there do not exist several pairs with the same value of k, we must have

$$b_k^2 = 0, \quad b_k^{+2} = 0, \quad b_k b_k^+ + b_k^+ b_k = 1. \quad (3)$$

We note further that the eigenenergy of the complex will be

$$2(E(k) - \lambda) b_k^+ b_k$$

and that the matrix element of the Hamiltonian (1) for the transition $k \to k'$ will be proportional to $-I/V$.

From these considerations, we obtain a simplified Hamiltonian of the form

$$H = H_0 + H_{\text{int}}, \quad H_0 = \sum_k 2(E(k) - \lambda) b_k^+ b_k,$$

$$H_{\text{int}} = -\frac{I}{V} \sum_{(k \neq k')} b_k^+ b_{k'} \theta(k) \theta(k'), \quad (4)$$

which contains the operators b_k, b_k^+ [with the commutation relations (2), (3)] which we shall call the Pauli operators.

Taking expressions of arbitrary order

$$H_{\text{int}} (H_0 - E)^{-1} H_{\text{int}} \ldots (H_0 - E)^{-1} H_{\text{int}},$$

it is now easy to verify directly that the sum of contributions from the diagrams of the type considered for the Hamiltonian (1) will be equal to the sum of contributions of all diagrams for the simplified Hamiltonian (4).

Thus, the problem of the summation of a special class of diagrams for the Hamiltonian (1) is shown to be equivalent to the problem of the model of the dynamical system that is characterized by the Hamiltonian (4).

*We emphasize that the new meaning of "summation" introduced here cannot be taken in the universally accepted sense. Strictly speaking, we do not sum here a series of terms of a given class, but we compare the Hamiltonian for which the expansion of perturbation theory exactly coincides with the given series. From the mathematical viewpoint, we are dealing here with concepts close to those of the theory of quasi-analytic functions.

We proceed to the construction of an asymptotically exact solution of this latter problem, neglecting only the quantities which vanish in the limit: $V \to \infty$.

We shall distinguish between pairs of electrons and pairs of holes, for which purpose we introduce the new Pauli operators, setting

$$\beta_k = b_k^+, \quad E(k) < \lambda,$$
$$\beta_k = b_k, \quad E(k) > \lambda.$$

We get

$$H = U + 2 \sum_k |E(k) - \lambda| \beta_k^+ \beta_k$$
$$- \frac{I}{V} \sum_{k \neq k'} \theta(k) \theta(k') \{\theta_G(k) \beta_k^+$$
$$+ \theta_F(k) \beta_k\} \{\theta_G(k') \beta_{k'} + \theta_F(k') \beta_{k'}^+\}, \quad (5)$$

where

$$\theta_F(k) = \begin{cases} 1, & E(k) < \lambda \\ 0, & E(k) > \lambda \end{cases}$$

$$U = 2 \sum_k \{E(k) - \lambda\} \theta_F(k), \quad \theta_G(k) + \theta_F(k) = 1.$$

Let us consider the wave function C for which all the filling factors

$$n_k = \beta_k^+ \beta_k$$

are equal to zero. Then

$$\beta_k C = 0.$$

We shall show that this wave function is an asymptotically exact eigenfunction of the Hamiltonian H, giving it the value U.

In fact, we have

$$H = H' + H'' + U,$$

$$H' = 2 \sum_k |E(k) - \lambda| \beta_k^+ \beta_k - \frac{I}{V} \sum_{k \neq k'} \theta(k) \theta(k') \{\theta_G(k) \beta_k^+$$
$$+ \theta_F(k) \beta_k\} \theta_G(k') \beta_{k'} - \frac{I}{V} \sum_{k \neq k'} \theta(k) \theta(k') \theta_F(k) \theta_F(k') \beta_{k'}^+ \beta_k,$$

$$H'' = -\frac{I}{V} \sum_{k \neq k'} \theta(k) \theta(k') \theta_G(k) \theta_F(k') \beta_k^+ \beta_{k'}^+.$$

But, obviously,

$$H'C = 0.$$

On the other hand,

$$\langle C^* \mid H''|^2 C\rangle = \langle C^* \overset{+}{H}{}'' H'' C\rangle =$$
$$= \frac{I^2}{V^2} \sum_{k \neq k'} \theta(k)\,\theta(k')\,\theta_G(k)\,\theta_F(k') < \text{const when } V \to \infty.$$

But, in the limit $V \to \infty$, H must be proportional to V, while $|\overline{H''}|^2$ as we have noted, remains finite. Therefore, in fact, C is an asymptotically exact eigenfunction of H, giving it the value U.

We have also

$$\overline{N} = \langle C^* N C\rangle = \sum_{E(k) < \lambda} 2.$$

Equating this expression to the total number of electrons in the Fermi sphere

$$\sum_{E(k) < E_F} 2,$$

we see that

$$\lambda = E_F = E(k_F).$$

We now analyze the problem of the stability of the state C. We consider first the case in which

$$I < 0. \tag{6}$$

We supplement the double sum in (5) with terms for which $k = k'$, terms that make no contribution in the transition to the limit $V \to \infty$. We then note that $H - U$ is essentially a positive form. The value U will consequently be a minimum and the state C will be stable from the same considerations.

The situation will be different in the case

$$I > 0. \tag{7}$$

We note that since all the filling facts $n_k = \beta_k^+ \beta_k$ in the state C will be equal to zero, we can, upon computation of the energy of the elementary excitations, consider the Pauli operators β, β^+ to be Bose in character.

There then remains only the diagonalization to quadratic form of the operators β, β^+ which represent $H - U$ of (5). This diagonalization can be achieved, for example, with the aid of a method set forth in our monograph.[4]

For the determination of the energy E of the elementary excitation, we get the following secular equation:

$$1 = \frac{I}{V} \sum_k \theta(k) \left\{ \frac{\theta_F(k)}{\varepsilon_k - E} + \frac{\theta_G(k)}{\varepsilon_k + E} \right\},$$
$$\varepsilon_k = 2\,|E(k) - E(k_F)|,$$

whence, upon simplifying, we get

$$1 = \frac{I}{V} \sum_{(E_F < E(k) < E_F + \omega)} \frac{2\varepsilon_k}{\varepsilon_k^2 - E^2},$$

or

$$1 = \frac{\rho}{2} \int_0^{\omega} k^2 \frac{dk}{dE} \frac{2z\,dz}{z^2 - E^2/4},$$

where

$$\rho = \frac{I}{2\pi^2} \left(k^2 \frac{dk}{dE} \right)_{k = k_F}. \tag{8}$$

As is seen, this equation, in the case (7) under consideration, always has a negative root for E^2. Consequently we obtain a purely imaginary value for the energy E:

$$E \sim \pm i 2\omega e^{-1/\rho}. \tag{9}$$

Thus the state C is found to be unstable.

In order to find the stable ground state with minimum energy, we introduce the new Pauli amplitudes β_k, β_k^+ in non-trivial fashion, as earlier, with the aid of the relations

$$\begin{aligned} \beta_k &= u_k v_k (2 b_k^+ b_k - 1) + u_k^2 b_k - v_k^2 b_k^+, \\ \beta_k^+ &= u_k v_k (2 b_k^+ b_k - 1) - v_k^2 b_k + u_k^2 b_k^+, \end{aligned} \tag{10}$$

where u_k and v_k are real numbers satisfying the relation

$$u_k^2 + v_k^2 = 1. \tag{11}$$

It is not difficult to note that the amplitudes (10) actually satisfy all the commutation relations of the Pauli operators.

Turning to the transformation (10), we find:

$$\begin{aligned} b_k &= u_k v_k (1 - 2\beta_k^+ \beta_k) + u_k^2 \beta - v_k^2 \beta_k^+, \\ b_k^+ &= u_k v_k (1 - 2\beta_k^+ \beta_k) - v_k^2 \beta_k + u_k^2 \beta_k^+, \\ b_k^+ b_k &= v_k^2 + (u_k^2 - v_k^2)\,\beta_k^+ \beta_k + u_k v_k (\beta_k + \beta_k^+). \end{aligned} \tag{12}$$

Substituting these expression in the Hamiltonian (4), we find:

$$H = U + \sum \Big\{ 2(E(k) - \lambda)\, u_k v_k$$
$$- \frac{I}{V} \theta(k) (u_k^2 - v_k^2) \sum_{k'} u_{k'} v_{k'} \theta(k') \Big\} (\beta_k + \beta_k^+)$$
$$+ \sum_k 2E_e(k)\, \beta_k^+ \beta_k - \frac{I}{V} \sum_{k_1 \neq k_2} \{ u_{k_1}^2 \beta_{k_1}^+ - v_{k_1}^2 \beta_{k_1} - 2u_{k_1} v_{k_1} \beta_{k_1}^+ \beta_{k_1} \}$$
$$\times \{ u_{k_2}^2 \beta_{k_2} - v_{k_2}^2 \beta_{k_2}^+ - 2u_{k_2} v_{k_2} \beta_{k_2}^+ \beta_{k_2} \}\, \theta(k_1)\, \theta(k_2),$$

where

$$U = \sum_k 2(E(k) - \lambda)\, v_k^2 - \frac{I}{V} \sum_{(k_1, k_2)} \theta(k_1)\, \theta(k_2)\, u_{k_1} v_{k_1} u_{k_2} v_{k_2};$$

$$E_e(k) = (E(k)-\lambda)(u_k^2 - v_k^2) + \theta(k)\, u_k v_k \frac{2I}{V} \sum_{k'} \theta(k')\, u_{k'} v_{k'}. \qquad (15)$$

We let the coefficients for $(\beta_k + \beta_k^+)$ in Eq. (13) vanish, and get

$$2(E(k)-\lambda)\, u_k v_k - \frac{I}{V}\, \theta(k)(u_k^2 - v_k^2) \sum_{k'} \theta(k')\, u_{k'} v_{k'} = 0, \qquad (16)$$

which was found in Ref. 2 with the help of the principle of compensation of dangerous diagrams.

Noting that $\lambda = E(k_F)$ (with the accuracy required here), we have, just as in Ref. 2:

$$u^2(k) = \frac{1}{2}\left\{1 + \frac{E(k) - E(k_F)}{\sqrt{(E(k) - E(k_F))^2 + \theta(k) C^2}}\right\},$$
$$v^2(k) = \frac{1}{2}\left\{1 + \frac{E(k_F) - E(k)}{\sqrt{(E(k) - E(k_F))^2 + \theta(k) C^2}}\right\},$$
$$C = 2\omega e^{-1/\rho},$$
$$E_e(k) = \sqrt{(E(k) - E(k_F))^2 + \theta(k) C^2}. \qquad (17)$$

The Hamiltonian (13) can now be written in the form

$$H = U + H_0 + H' + H''$$

where

$$H_0 = \sum_k 2E_e(k)\, \beta_k^+ \beta_k,$$
$$H' = -\frac{I}{V} \sum_{(k_1 \neq k_2)} \theta(k_1)\, \theta(k_2)\, \{u_{k_1}^2 \beta_{k_1}^+ - v_{k_1}^2 \beta_{k_1}\}\{u_{k_2}^2 \beta_{k_2} - v_{k_2}^2 \beta_{k_2}^+\}, \qquad (18)$$

$$H'' = \frac{2I}{V} \sum_{(k_1 \neq k_2)} \theta(k_1)\, \theta(k_2)\, \{u_{k_2}^2 \beta_{k_2} - v_{k_2}^2 \beta_{k_2}^+ - 2u_{k_2} v_{k_2} \beta_{k_2}^+ \beta_{k_2}\}\, u_{k_1} v_{k_1} \beta_{k_1}^+ \beta_{k_1}$$
$$+ \frac{2I}{V} \sum_{(k_1 \neq k_2)} \theta(k_1)\, \theta(k_2)\, \{u_{k_1}^2 \beta_{k_1}^+ - v_{k_1}^2 \beta_{k_1} - 2u_{k_1} v_{k_1} \beta_{k_1}^+ \beta_{k_1}\}\, u_{k_2} v_{k_2} \beta_{k_2}^+ \beta_{k_2}.$$

We select the wave function C for which all the filling factors

$$\nu_k = \beta_k^+ \beta_k$$

are zero. We shall show, as before, that, with accuracy to quantities which vanish in the limit $V \to \infty$, C is an eigenfunction of the Hamiltonian H, giving it a value U. We actually have

$$(H_0 + H'')\, C = 0$$

and

$$\langle C^* \,|\, H'\,|^2\, C\rangle = \frac{I^2}{V^2} \sum \theta(k_1)\, \theta(k_2)\, \{u_{k_1}^4 v_{k_2}^4 + u_{k_1}^2 v_{k_1}^2 u_{k_2}^2 v_{k_2}^2\}$$
$$< \text{const}, \quad V \to \infty.$$

We now proceed to the consideration of elementary excitations. Since all the filling factors ν_k in the state C are equal to zero, we can consider the Pauli operators to be Bose operators in the calculation of the energy of the elementary excitations. Therefore, in the equation for the Hamiltonian (18) we can limit ourselves to the quadratic form $H_0 + H'$.

Carrying out the diagonalization by the method described earlier,[4] we obtain a set of linear equations:

$$(E - 2E_e(k))\, \varphi_k = \frac{I\theta(k)}{V}\, u_k^2 \sum_{k'} \{u_{k'}^2 \varphi_{k'} - v_{k'}^2 \chi_{k'}\}\, \theta(k') - \frac{I\theta(k)}{V}\, v_k^2 \sum_{k'} \{u_{k'}^2 \chi_{k'} - v_{k'}^2 \varphi_{k'}\}\, \theta(k'),$$
$$-(E + 2E_e(k))\, \chi_k = u_k^2 \frac{I}{V}\, \theta(k) \sum_{k'} \{u_{k'}^2 \chi_{k'} - v_{k'}^2 \varphi_{k'}\}\, \theta(k') - \frac{I}{V}\, \theta(k)\, v_k^2 \sum_{k'} \{u_{k'}^2 \varphi_{k'} - v_{k'}^2 \chi_{k'}\}\, \theta(k') \qquad (19)$$

with the normalization condition

$$\sum_k \{|\varphi_k|^2 - |\chi_k|^2\} = 1. \qquad (20)$$

Then we obtain the secular equation:

$$\left\{1 + \frac{I}{V} \sum \left(\frac{u_k^4}{2E_e + E} + \frac{v_k^4}{2E_e - E}\right) \theta(k)\right\} \times \left\{1 + \frac{I}{V} \sum \left(\frac{v_k^4}{2E_e + E} + \frac{u_k^4}{2E_e - E}\right) \theta(k)\right\}$$
$$- \left\{\frac{I}{V} \sum \theta(k)\, u_k^2 v_k^2 \left(\frac{1}{2E_e + E} + \frac{1}{2E_e - E}\right)\right\}^2 = 0. \qquad (21)$$

It is easy to see that for

$$|E| < 2 \min E_e(k) = 2E_e(k_F)$$

this equation has no solution, since the subtrahend in Eq. (21) is then less than the minuend.

For

$$|E| > 2 \min E_e(k)$$

we have a continuous spectrum

$$E = \pm 2E_e(k) + O(1/V), \quad O(1/V) \to 0 \text{ when } V \to \infty.$$

As is seen from (19), the minus sign does not agree with the normalization condition (20).

Thus all the E are positive (this can be seen directly from the fact that the quadratic form under consideration is positive definite) and are separated from zero by the gap

$$E = 2E_e(k) \geqslant 2E_e(k_F) = 2C = 4\omega e^{-1/\rho}. \quad (22)$$

Here again we obtain the results of Bardeen as in the previous papers.[1,2]

Since we have confined ourselves only to diagrams consisting of pairs, we cannot decide directly from (22) that the excitation with energy $2E_e(k)$ [Eq. (22)] consists indeed of two excitations of the Fermi type, which was shown in Ref. 1.

As we see, the method of summation of diagrams is shown to be quite lucid and permits us to establish the connection with the ideas of the work of Bardeen, Cooper, and Schrieffer.

However, in our opinion, the method of canonical transformation is more flexible, allowing us easily to obtain the higher approximations. Moreover, it achieves various generalizations, for example, in the calculation of thermodynamic quantities.

In conclusion, I should thank D. N. Zubarev, V. V. Tolmachev, S. V. Tiablikov, and Iu. A. Tserkovnikov for their valued discussion.

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Translated by R. T. Beyer
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BREMSSTRAHLUNG OF PI MESONS AND PRODUCTION OF PI-MESON PAIRS BY GAMMA QUANTA IN COLLISION WITH NONSPHERICAL NUCLEI

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Submitted to JETP editor October 22, 1957

J. Exptl. Theoret. Phys. (U.S.S.R.) **34**, 80-86 (January, 1958)

The effective cross-sections are calculated for a number of radiative processes occurring in the interaction of high-energy π mesons with nonspherical nuclei. The nonspherical shape of the nuclei leads to a change of the angular distributions and the appearance in the cross-sections of factors that depend only on the geometrical shape of the nuclei.

In papers by Landau and Pomeranchuk,[1] Pomeranchuk,[2] and Vdovin[3] treatments have been given of the processes of bremsstrahlung in the interaction of π mesons with nuclei, production of π-meson pairs from nuclei by γ quanta, and production of nuclear stars by γ quanta, for very large π-meson energies E and γ-quantum energies ω ($E \gg \mu$; $\omega \gg \mu$, where μ is the mass of the π meson; we set $\hbar = c = 1$ throughout). A peculiarity of these processes at such energies is that very large distances from the nucleus ($r_{eff} \sim E/\mu^2 \gg R$) contribute to the matrix elements that give the probabilities of the processes, and one can use in the calculation the asymptotic form of the π-meson wave functions outside the region of their interaction with the nucleus. At large energies one can take these functions to be diffraction functions. The functions used in the papers mentioned are those of the diffraction by a black or a gray sphere.