

FORMATION OF BOUND STATES OF CONDUCTION-ELECTRON WITH LOCALIZED SPINS IN METALS

A. A. ABRIKOSOV

Institute of Theoretical Physics, U.S.S.R. Academy of Sciences

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A theory is developed which can be employed to study the electron bound states with localized spins of arbitrary magnitude. It is shown that no states with a total spin $S + 1/2$ are realized. The problem for states with $S - 1/2$ cannot be solved conclusively within the framework of the logarithmic approximation, since the amplitude of the state is proportional to an unknown constant which may even be zero. It is shown that if the amplitude is not zero the formation of bound states lowers the energy of the system.

1. INTRODUCTION

THE question of the possible occurrence of bound states of electrons with magnetic impurity atoms possessing localized spins has been under discussion in the literature since the publication of the paper by Nagaoka.^[1] This idea was suggested by the complex poles of the amplitude for scattering of electrons by magnetic atoms, observed by Suhl^[2] and the present author.^[3] These poles arise when account is taken of perturbation-theory terms of higher order in the exchange interaction. This singularity recalls the well known singularity in the amplitude of mutual scattering of electrons in a metal, which evidences the instability of the ordinary "normal" state and the phase transition into the superconducting state.

The many papers written on this topic do not make it possible, unfortunately, to answer the raised question. The papers in which the possibility of bound states is proved either use a variational procedure^[4] or else obtain, by means of very complicated calculations, several terms of an expansion in $J \ln(\epsilon_F/\xi)$ (where J is the exchange interaction and ξ the electron energy),^[5] which is not valid, since this parameter is not small. Nagaoka,^[1] who started these studies, used a method of simplifying complicated matrix elements, wherein it is very difficult to estimate the order of the discarded terms. In the paper of Takano and Ogawa,^[6] which is closest to ours, they did not take into account all the types of the F -functions, and therefore their result was incorrect (see below). Finally, most papers consider actually only an impurity spin $S = 1/2$, whereas the singularity of the scattering amplitude appears for any impurity spin.

On the other hand, Suhl and Wong,^[7] and also Mal'eev,^[8] have shown, when solving the equation obtained for the scattering amplitude by the Chew and Low method, that it is possible to obtain a scattering amplitude without a singularity by means of a correct analytic continuation with respect to the temperature, the coupling constant, or the electron energy. Nonetheless, this does not solve the problem of the bound states. First of all, the equation solved in^[7] and^[8], which is based on a definite assumption concerning the form of the intermediate states, while agreeing with the equa-

tion obtained in the more consistent theory^[3] in a logarithmic approximation, is not equally justified in higher approximations with respect to J . Second, although the singularity of the scattering amplitude is indeed a definite "hint" of the instability of the state, it cannot be stated that the possibility of constructing a nonsingular amplitude excludes such a possibility. Finally, one cannot exclude the possibility that the solution of Suhl and Wong actually corresponds to a bound state.^[1, 5]

In the present paper we make the next step necessary to clarify the question of bound states. In the technique developed by us earlier,^[3] the assumption concerning the bound state is manifest in the occurrence of four new "Green's functions," similar to F and F_+ in the Gor'kov method^[9] for superconductors. Solution of the equations for the corresponding "amplitudes" makes it possible in principle to solve completely the problem of the bound states. In the present paper we confine ourselves only to the logarithmic approximation (that is, to allowance for terms with the maximum degree of $\ln(\epsilon_F/\xi)$ at a specified degree of J). Unlike Yosida and Okiji,^[5] we take into account in this approximation all the necessary terms. It is then possible to show that no states with total spin $S + 1/2$ are produced, regardless of the sign of the exchange interaction. As to the states with total spins $S - 1/2$, if the exchange-interaction term has the antiferromagnetic sign, then, within the framework of the logarithmic approximation, the bound state can be produced, although this approximation is inadequate for a final answer to the question. The energy of such a state is considered.

2. FUNDAMENTAL EQUATIONS

We confine ourselves here to the study of one impurity center at the point $r = 0$. We shall use the field-theory technique for the spins,^[3] based on representing the spin operators in the form

$$\hat{S}_i = a_{\beta}^{\dagger} S_{\beta\beta'}^i a_{\beta}, \tag{1}$$

where a_{β} are Fermi operators, and $S_{\beta\beta'}^i$ are the matrices of the spin operators. The Hamiltonian of the interaction takes the form

$$H_{int} = -(J/N) \psi_{\alpha}^{\dagger}(0) a_{\beta}^{\dagger} a_{\beta'} \psi_{\alpha'}(0) \sigma_{\alpha\alpha'}^i S_{\beta\beta'}^i \tag{2}$$



FIG. 1

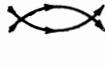


FIG. 2

($\sigma_{\alpha\alpha'}$ —Pauli matrices—electron spin, N —number of atoms of the basic metal per unit volume).

It was already mentioned in [3] that introduction of the spin pseudoparticles leads to the appearance of unphysical states. They were eliminated there by an artificial device. In the present paper, however, this will not be necessary. Indeed, we consider here only $T = 0$. Then we need only the mean values averaged over the ground state of the system. The function $\mathcal{G}^{(0)} = i \langle T(a_\beta(t)a_{\beta'}(t')) \rangle$ which is needed for the calculations should satisfy the equation

$$i\partial \mathcal{G}_{\beta\beta'}^{(0)}(t-t')/\partial t = \delta(t-t')\delta_{\beta\beta'},$$

which is merely the consequence of the commutation relation of the operators a_β . From this we get

$$\mathcal{G}_{\beta\beta'}^{(0)} = \omega^{-1} \delta_{\beta\beta'}. \quad (3)$$

All that depends on the choice of the state over which the averaging is carried out is the method of going around the pole at $\omega = 0$. But in all the subsequent calculations only the principal value of $\mathcal{G}^{(0)}$ will be significant. Incidentally, the ground state could be introduced by using a transition to the limit in an infinitesimally weak magnetic field.

In calculating the scattering amplitude in [3], logarithmic singularities appeared in the diagrams for the vertex part, shown in Fig. 1. We now use the analogy with superconductivity. In the latter sense, a logarithmic singularity occurred in the diagram shown in Fig. 2. This led to the assumption of occurrence of electron pairs. To describe these pairs, there were introduced in the Gor'kov method [9] two functions

$$F = \langle T(\psi(x)\psi(x')) \rangle, \quad F^+ = \langle T(\psi^+(x)\psi^+(x')) \rangle,$$

corresponding to pair annihilation and production. In the present case, the singularity arises in two types of diagrams, and not one. In view of this, we introduce four new F-functions:

$$F_{\alpha\beta}^{(1)}(x, t') = \langle T(\psi_\alpha(x)a_\beta(t')) \rangle, \quad F_{\alpha\beta}^{(2)}(x, t') = \langle T(\psi_\alpha^+(x)a_\beta^+(t')) \rangle, \quad (4)$$

$$F_{\alpha\beta}^{(3)}(x, t') = \langle T(\psi_\alpha(x)a_\beta^+(t')) \rangle, \quad F_{\alpha\beta}^{(4)}(x, t') = \langle T(\psi_\alpha^+(x)a_\beta(t')) \rangle.$$

In superconductivity theory one considers only that part of the interaction which leads to the occurrence or annihilation of bound states, and one "throws out" the part connected with the scattering. As applied to our problem, this would mean that it is necessary to go over from the Hamiltonian (2) to the expression

$$H_{int} = \Delta_{\alpha\beta}^{(2)} \psi_\alpha(0) a_\beta + \Delta_{\alpha\beta}^{(4)} \psi_\alpha^+(0) a_\beta^+ - \Delta_{\alpha\beta}^{(3)} \psi_\alpha(0) a_\beta^+ - \Delta_{\alpha\beta}^{(1)} \psi_\alpha^+(0) a_\beta. \quad (5)$$

where, for example,

$$\Delta_{\alpha\beta} = JN^{-1} \langle \psi_\alpha(0, t) a_\beta(t) \rangle \sigma_{\alpha, \alpha} S_{\beta, \beta}.$$

In this case, however, owing to the presence of two types of diverging elements (a and b in Fig. 1), the situation is somewhat more complicated, and part of the "scattering" effects must be taken into account. This question will be considered somewhat later. For the time being we note only that the result is equivalent to formula (5), except that each term must be trans-

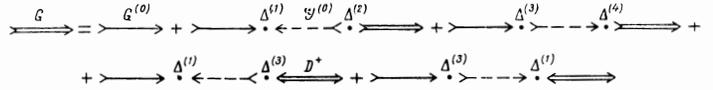


FIG. 3

formed in accordance with the principle

$$\Delta_{\alpha\beta}^{(2)} \psi_\alpha(0) a_\beta \rightarrow \Delta_{\alpha\beta}^{(2)}(t-t') \psi_\alpha(0, t) a_\beta(t')$$

and the averaging of all the $\Delta_{\alpha\beta}$ is more complicated.

We must now take into account the fact that the produced states have a total spin $I = S + 1/2$, or else $I = S - 1/2$. This is expressed by the following conditions:

$$\begin{aligned} I = S + 1/2 & \quad I = S - 1/2 \\ (\sigma S)_{\alpha\beta, \alpha, \beta} F_{\alpha, \beta}^{(1)} = S F_{\alpha\beta}^{(1)} & \quad (\sigma S)_{\alpha\beta, \alpha, \beta} F_{\alpha, \beta}^{(1)} = -(S+1) F_{\alpha\beta}^{(1)} \\ (\sigma S)_{\alpha, \beta, \alpha, \beta} F_{\alpha, \beta}^{(2)} = S F_{\alpha\beta}^{(2)} & \quad (\sigma S)_{\alpha, \beta, \alpha, \beta} F_{\alpha, \beta}^{(2)} = -(S+1) F_{\alpha\beta}^{(2)} \\ (\sigma S)_{\alpha\beta, \alpha, \beta} F_{\alpha, \beta}^{(3)} = -S F_{\alpha\beta}^{(3)} & \quad (\sigma S)_{\alpha\beta, \alpha, \beta} F_{\alpha, \beta}^{(3)} = (S+1) F_{\alpha\beta}^{(3)} \\ (\sigma S)_{\alpha, \beta, \alpha, \beta} F_{\alpha, \beta}^{(4)} = -S F_{\alpha\beta}^{(4)} & \quad (\sigma S)_{\alpha, \beta, \alpha, \beta} F_{\alpha, \beta}^{(4)} = (S+1) F_{\alpha\beta}^{(4)} \end{aligned} \quad (6)$$

The Hamiltonian (5) leads to an equation for the electron function $G(\mathbf{r}, \mathbf{r}', \omega)$, shown schematically in Fig. 3:

$$\begin{aligned} G_{\alpha\alpha'}(\mathbf{r}, \mathbf{r}', \omega) &= G^{(0)}(\omega, \mathbf{r} - \mathbf{r}') \delta_{\alpha\alpha'} \\ &+ G^{(0)}(\omega, \mathbf{r}) [\Delta_{\alpha\beta}^{(4)}(\omega) \Delta_{\alpha, \beta}^{(2)}(-\omega) \mathcal{G}^{(0)}(-\omega) \\ &- \Delta_{\alpha\beta}^{(3)}(\omega) \Delta_{\alpha, \beta}^{(4)}(-\omega) \mathcal{G}^{(0)}(\omega)] G_{\alpha, \alpha'}(\omega, 0, \mathbf{r}') \\ &+ G^{(0)}(\omega, \mathbf{r}) [\Delta_{\alpha\beta}^{(1)}(\omega) \Delta_{\alpha, \beta}^{(3)}(-\omega) \mathcal{G}^{(0)}(-\omega) \\ &- \Delta_{\alpha\beta}^{(2)}(\omega) \Delta_{\alpha, \beta}^{(1)}(-\omega) \mathcal{G}^{(0)}(\omega)] D_{\alpha, \alpha'}^+(\omega, 0, \mathbf{r}'), \end{aligned} \quad (7)$$

where $D_{\alpha\alpha'}^+ = i \langle T(\tilde{\psi}_\alpha^+ \tilde{\psi}_{\alpha'}^+) \rangle$ (by $\tilde{\psi}$ we mean the Heisenberg operators). The equation for $D_{\alpha\alpha'}^+$ can be obtained in similar fashion:

$$\begin{aligned} D_{\alpha\alpha'}^+(\omega, \mathbf{r}, \mathbf{r}') &= G^{(0)}(-\omega, \mathbf{r}) [\Delta_{\alpha\beta}^{(2)}(\omega) \Delta_{\alpha, \beta}^{(4)}(-\omega) \mathcal{G}^{(0)}(\omega) \\ &- \Delta_{\alpha\beta}^{(4)}(\omega) \Delta_{\alpha, \beta}^{(3)}(-\omega) \mathcal{G}^{(0)}(-\omega)] D_{\alpha, \alpha'}^+(\omega, 0, \mathbf{r}') \\ &+ G^{(0)}(-\omega, \mathbf{r}) [\Delta_{\alpha\beta}^{(3)}(\omega) \Delta_{\alpha, \beta}^{(1)}(-\omega) \mathcal{G}^{(0)}(\omega) \\ &- \Delta_{\alpha\beta}^{(1)}(\omega) \Delta_{\alpha, \beta}^{(2)}(-\omega) \mathcal{G}^{(0)}(-\omega)] G_{\alpha, \alpha'}(\omega, 0, \mathbf{r}'). \end{aligned} \quad (8)$$

With the aid of (7) and (8) we can find G and D^+ , by expressing them in terms of $G^{(0)}$ and $\Delta^{(1)}$. To this end it is necessary to put $\mathbf{r} = 0$, after which the equations will contain only $G(\omega, 0, \mathbf{r}')$ and $D^+(\omega, 0, \mathbf{r}')$. By finding them, we can obtain also the complete G and D^+ . With the aid of these functions we can determine the functions F . For example, for $F^{(2)}$ we have the diagram equations shown in Fig. 4. It corresponds to

$$\begin{aligned} F_{\alpha\beta}^{(2)}(\omega, \mathbf{r}, 0) &= -i G_{\alpha\alpha_1}(-\omega, \mathbf{r}, 0) \mathcal{G}^{(0)}(\omega) \Delta_{\alpha, \beta}^{(2)}(\omega) \\ &+ i D_{\alpha\alpha_1}^+(\omega, \mathbf{r}, 0) \mathcal{G}^{(0)}(\omega) \Delta_{\alpha, \beta}^{(3)}(\omega). \end{aligned} \quad (9a)$$

Analogously we have

$$F_{\alpha\beta}^{(4)}(\omega, \mathbf{r}, 0) = -i G_{\alpha\alpha_1}(\omega, \mathbf{r}, 0) \mathcal{G}^{(0)}(-\omega) \Delta_{\alpha, \beta}^{(1)}(\omega) \quad (9b)$$

$$+ i D_{\alpha\alpha_1}(\omega, \mathbf{r}, 0) \mathcal{G}^{(0)}(-\omega) \Delta_{\alpha, \beta}^{(4)}(\omega),$$

$$F_{\alpha\beta}^{(3)}(\omega, \mathbf{r}, 0) = -i G_{\alpha\alpha_1}(\omega, \mathbf{r}, 0) \mathcal{G}^{(0)}(\omega) \Delta_{\alpha, \beta}^{(3)}(\omega)$$

$$+ i D_{\alpha\alpha_1}(\omega, \mathbf{r}, 0) \mathcal{G}^{(0)}(\omega) \Delta_{\alpha, \beta}^{(2)}(\omega),$$

$$F_{\alpha\beta}^{(1)}(\omega, \mathbf{r}, 0) = -i G_{\alpha\alpha_1}(-\omega, \mathbf{r}, 0) \mathcal{G}^{(0)}(\omega) \Delta_{\alpha, \beta}^{(4)}(\omega)$$

$$+ i D_{\alpha\alpha_1}^+(\omega, \mathbf{r}, 0) \mathcal{G}^{(0)}(-\omega) \Delta_{\alpha, \beta}^{(1)}(\omega).$$

Here

$$D_{\alpha\alpha'}(x, x') = -i \langle T(\tilde{\psi}_\alpha(x) \tilde{\psi}_{\alpha'}(x')) \rangle.$$

The equation for this function is similar to (8):

$$\begin{aligned} D_{\alpha\alpha'}(\omega, \mathbf{r}, \mathbf{r}') = & G^{(0)}(\omega, \mathbf{r}) [\Delta_{\alpha\beta}^{(1)}(\omega) \Delta_{\alpha,\beta}(-\omega) \mathcal{G}^{(0)}(-\omega) \\ & - \Delta_{\alpha\beta}^{(3)}(\omega) \Delta_{\alpha,\beta}^{(4)}(-\omega) \mathcal{G}^{(0)}(\omega)] D_{\alpha,\alpha'}(\omega, 0, \mathbf{r}') \\ & + G^{(0)}(\omega, \mathbf{r}) [\Delta_{\alpha\beta}^{(1)}(\omega) \Delta_{\alpha,\beta}^{(3)}(-\omega) \mathcal{G}^{(0)}(-\omega) \\ & - \Delta_{\alpha\beta}^{(3)}(\omega) \Delta_{\alpha,\beta}^{(1)}(-\omega) \mathcal{G}^{(0)}(\omega)] G_{\alpha,\alpha'}^{(0)}(-\omega, 0, \mathbf{r}'). \end{aligned} \quad (10)$$

Finally, the complete function \mathcal{G} is expressed in terms of F^i (see Fig. 5):

$$\begin{aligned} \mathcal{G}_{\beta\beta'}(\omega) = & \mathcal{G}^{(0)}(\omega) \delta_{\beta\beta'} - i \mathcal{G}^{(0)}(\omega) \Delta_{\alpha\beta}^{(4)}(-\omega) F_{\alpha\beta}^{(3)}(\omega, 0, 0) \\ & + i \mathcal{G}^{(0)}(\omega) \Delta_{\alpha\beta}^{(1)}(-\omega) F_{\alpha\beta}^{(2)}(\omega, 0, 0). \end{aligned} \quad (11)$$

Thus, all the functions can in principle be expressed in terms of $G^{(0)}$, $\mathcal{G}^{(0)}$, and $\Delta^{(1)}$. It is necessary to add to this the equations defining the $\Delta^{(i)}$.

$$\overleftrightarrow{F^{(2)}} = \overleftrightarrow{\Delta^{(2)}} \cdot + \overleftrightarrow{\Delta^{(3)}} \cdot$$

FIG. 4

$$\overleftrightarrow{G} = \overleftrightarrow{\Delta^{(4)}} \cdot + \overleftrightarrow{F^{(3)}} \cdot + \overleftrightarrow{\Delta^{(1)}} \cdot$$

FIG. 5

3. SOLUTION OF THE EQUATIONS

We shall obtain all the quantities in the logarithmic approximation. To this end it is not necessary to solve all the equations written out above. We note simply the following circumstance. To find $\Delta^{(1)}$ we shall need $F^{(1)}(\omega, 0, 0)$. These quantities are expressed in terms of $G(\omega, 0, 0)$, $D^+(\omega, 0, 0)$, and $D(\omega, 0, 0)$. It follows from (7) that, accurate to corrections of order $\pi\Delta^2\alpha/\omega$ (where $\alpha = p_0 m/2\pi^2$) we have $G(\omega, 0, 0) = G^{(0)}(\omega, 0) = -i\pi\alpha \text{sign } \omega$, the quantities D^+ and D are of first order in $\pi\Delta^2\alpha/\omega$, $\mathcal{G}(\omega) \approx \mathcal{G}^{(0)}(\omega)$, and finally, in the expressions for the functions F we can discard the terms with D and D^+ , and replace G by $G^{(0)}$ in the first terms. We obtain here

$$\begin{aligned} F_{\alpha\beta}^{(1)}(\omega, 0, 0) & \approx \frac{\pi\alpha}{|\omega|} \Delta_{\alpha\beta}^{(1)}, & F_{\alpha\beta}^{(2)}(\omega, 0, 0) & = \frac{\pi\alpha}{|\omega|} \Delta_{\alpha\beta}^{(2)}, \\ F_{\alpha\beta}^{(3)}(\omega, 0, 0) & = -\frac{\pi\alpha}{|\omega|} \Delta_{\alpha\beta}^{(3)}, & F_{\alpha\beta}^{(4)}(\omega, 0, 0) & = -\frac{\pi\alpha}{|\omega|} \Delta_{\alpha\beta}^{(4)}. \end{aligned} \quad (12)$$

In the first approximation in J/N we get for $\Delta_{\alpha\beta}^{(1)}$

$$\begin{aligned} \Delta_{\alpha\beta, \pm}^{(1)} & = JN^{-1} \langle \psi_{\alpha_i}(0, t) a_{\beta_i}(t) \rangle \sigma_{\alpha\alpha_i}^i \delta_{\beta\beta_i}^i \\ & = \frac{J}{N} \int \frac{d\omega}{2\pi} F_{\alpha_i\beta_i}^{(1)}(\omega, 0, 0) \sigma_{\alpha\alpha_i}^i \delta_{\beta\beta_i}^i. \end{aligned}$$

It follows from (12) that this expression is essentially reduced to a logarithmic integral. The upper limit, as always, will be ε_F , and the lower will be of the order $\pi\alpha\Delta^2$. In other words, we need with logarithmic accuracy actually $|\omega| \gg \pi\alpha\Delta^2$, which fully justifies the expressions in (12). The expression given above for $\Delta^{(1)}$ corresponds to the diagram of Fig. 6a.

Let us consider now the diagram 6b. The new element contained in it yields a factor $JN^{-1} \ln(\varepsilon_F/\xi)$. The quantity can in no way be regarded as small. In this

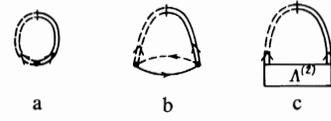


FIG. 6

lies the difference from the superconductivity case.

The situation with two singular logarithmic elements of the vertex part was considered in a recent paper by Bychkov, Gor'kov, and Dzyaloshinskiĭ,^[10] devoted to one-dimensional superconductivity. That paper contains a method of finding Δ , which we shall follow here. It is easy to see that, with logarithmic accuracy, it is necessary to replace the simple vertex $\gamma = JN^{-1}\sigma S$ in the expression for $\Delta^{(1)}$ in terms of $F^{(1)}$ by the sum $\gamma + \Lambda^{(2)}$, where $\Lambda^{(2)}$ is the aggregate of diagrams which can be cut apart by two antiparallel electron and spin fermion lines, but cannot be cut by similar two parallel lines (see^[13]). Thus, the total expression corresponds to diagram 6a, and to diagram 6c. This is an integral expression, which takes the form

$$\Delta_{\alpha\beta}^{(1)}(\omega) = \int \frac{d\omega_1}{2\pi} [\gamma + \Lambda^{(2)}(\omega + \omega_1)] F_{\alpha\beta}^{(1)}(\omega_1, 0, 0). \quad (13)$$

It is possible to write similarly equations for the other $\Delta^{(i)}$; the only difference is that in the expressions for for $\Delta^{(3)}$ and $\Delta^{(4)}$ the quantity $\Lambda^{(2)}$ is replaced by $\Lambda^{(1)}$ and, in addition, the sequence of the multiplication in the spin indices will be different in all the expressions (it is the same as in the left side of (6)).

In^[13] we derived expressions for $\Lambda^{(2)}$ and $\Lambda^{(1)}$ in terms of the total vertex Γ and the total vertex itself is

$$\Gamma(\xi) = \frac{\sigma S}{N/J + 2\alpha\xi}; \quad (14)$$

$$\Lambda_{\alpha\beta, \alpha\beta'}^{(1)}(\xi) = \alpha \int_0^\xi \Gamma_{\alpha\beta, \alpha\beta'}(\eta) \Gamma_{\alpha\beta, \alpha\beta'}(\eta) d\eta, \quad (15)$$

$$\Lambda_{\alpha\beta, \alpha\beta'}^{(2)}(\xi) = -\alpha \int_0^\xi \Gamma_{\alpha\beta', \alpha\beta}(\eta) \Gamma_{\alpha\beta, \alpha\beta'}(\eta) d\eta,$$

where $\xi = \ln(\varepsilon_F/|\omega|)$. Substituting (14) in (15), we get

$$\begin{aligned} \gamma + \Lambda^{(1)} & = \frac{(1 + \alpha\xi J/N)\sigma S + \alpha\xi J S(S+1)/N}{N/J + 2\alpha\xi}, \\ \gamma + \Lambda^{(2)} & = \frac{(1 + \alpha\xi J/N)\sigma S - \alpha\xi J S(S+1)/N}{N/J + 2\alpha\xi}. \end{aligned} \quad (16)$$

In the integral of (13) there are two regions: $|\omega_1| \gg |\omega|$, where the argument in $\Lambda^{(1)}$ and $\Lambda^{(2)}$ is equal to $\ln(\varepsilon_F/|\omega_1|)$ and $|\omega_1| \ll |\omega|$, where the argument in $\Lambda^{(1)}$ and $\Lambda^{(2)}$ is equal to $\ln(\varepsilon_F/|\omega|)$, that is, $\gamma + \Lambda^{(1)}$ can be taken outside the integral sign.

The result of multiplication of $\gamma + \Lambda^{(1)}$ by the corresponding F -function is determined by the formulas in (6). From them and from (12) it follows that the equations for all the $\Delta^{(i)}$ are the same for a given I . When $I = S + 1/2$ we have

$$\Delta(\xi) = \alpha \int_0^\xi \frac{S(1 - JN^{-1}S\alpha\eta)}{N/J + 2\alpha\eta} \Delta(\eta) d\eta + \alpha \frac{S(1 - JN^{-1}S\alpha\xi)}{N/J + 2\alpha\xi} \int_0^\xi \Delta(\eta) d\eta \quad (17a)$$

and when $I = S - 1/2$

$$\Delta(\xi) = -\alpha \int_0^\xi \frac{(S+1)[1 + JN^{-1}(S+1)\alpha\eta]}{N/J + 2\alpha\eta} \Delta(\eta) d\eta \quad (17b)$$

$$- \alpha \frac{(S+1)[1 + JN^{-1}(S+1)\alpha\xi]}{N/J + 2\alpha\xi} \int_{\xi_0}^{\omega} \Delta(\eta) d\eta,$$

where $\eta = \ln(\epsilon_F/|\omega_1|)$, and $\xi_0 = \ln(\epsilon_F/\pi\alpha\Delta^2)$ is the boundary of the logarithmic region. Inasmuch as Δ depends on the frequency, it is necessary to take in ξ_0 that value of the frequency, at which $\pi\alpha\Delta^2 \sim \omega$. We note that integration with respect to ω_1 in (13) includes two signs of ω_1 , which of necessity leads to the conclusion that $\Delta\omega = \Delta(-\omega)$ and to a doubling of the integrals. This was taken into account in (17).

To solve (17) it is convenient to go over to a new variable $z = N/J + 2\alpha\xi$. We then obtain

$$\Delta(z) = \frac{1}{4} \int_{N/J}^z \left(-\frac{J}{N} S^2 + \frac{S(S+2)}{u} \right) \Delta(u) du + \frac{1}{4} \left(-\frac{J}{N} S^2 + \frac{S(S+2)}{z} \right) \int_z^{\infty} \Delta(u) du \quad (18a)$$

for $I = S + 1/2$ and

$$\Delta(z) = \frac{1}{4} \int_{N/J}^z \left(-\frac{J}{N} (S+1)^2 + \frac{S^2-1}{u} \right) \Delta(u) du + \frac{1}{4} \left(-\frac{J}{N} (S+1)^2 + \frac{S^2-1}{z} \right) \int_z^{\infty} \Delta(u) du \quad (18b)$$

for $I = S - 1/2$.

Differentiating twice with respect to z , we obtain the differential equations

$$z^2\Delta'' + 2z\Delta' - \frac{S(S+2)}{z} \Delta = 0, \quad I = S + 1/2; \quad (19a)$$

$$z^2\Delta'' + 2z\Delta' - \frac{S^2-1}{4} \Delta = 0, \quad I = S - 1/2. \quad (19b)$$

It follows hence that

$$\Delta = Pz^{S/2} + Qz^{-(S/2+1)}, \quad I = S + 1/2; \quad (20a)$$

$$\Delta = Pz^{(S-1)/2} + Qz^{-(S+1)/2}, \quad I = S - 1/2. \quad (20b)$$

Actually, however, the differential equations (19) have more solutions than the initial equations (18). Substituting (20) in (18), we get the following conditions:

$$P = 0, \quad Qz_0^{-S/2} = 0, \quad I = S + 1/2; \quad (21a)$$

$$Q = 0, \quad Pz_0^{(S+1)/2} = 0, \quad I = S - 1/2. \quad (21b)$$

Inasmuch as $z_0 = N/J + 2\alpha\xi$, it follows from (21a) that we must have $Q = 0$, and consequently also $\Delta = 0$. In other words, no bound system with $I = S + 1/2$ can be produced. A similar conclusion for $S = 1/2$ was reached by Yosida,^[5] although, as already mentioned, his method, which contains an expansion in $JN^{-1} \ln(\epsilon_F/|\omega|)$, did not make it possible to draw a rigorous conclusion.

In the case $I = S - 1/2$ for $\Delta \neq 0$ it is necessary to have $z_0 = 0$, which is possible in principle if $J < 0$. Taking into account the logarithmic accuracy, we obtain from this

$$\pi\alpha\Delta_0^2 = C\epsilon_F e^{-N/2\alpha|J|}. \quad (22)$$

The constant C , which generally speaking is of the order of unity, is not determined in the logarithmic approximation. It can be different for different $\Delta^{(1)}$, but in principle it can also equal zero. In view of this, the only thing that can be stated is that the assumption $\Delta \neq 0$ in the case $J < 0$ and $I = S - 1/2$ does not contradict the equations in the logarithmic accuracy. Strictly

speaking, however, the question of the existence of the bound states still remains unclear.

We propose, however, that the constant $C \neq 0$, and consequently also $\Delta \neq 0$. How must we interpret formula (20b) in this case? The point is that formula (20b) determines Δ only in the region $|\omega| \gg \pi\alpha\Delta^2$. From (20b) we see that with decreasing ω (with increasing z) $\Delta(\omega)$ increases when $S = 1/2$, remains unchanged when $S = 1$, and decreases when $S \geq 3/2$. We cannot determine the exact behavior of Δ in the region $|\omega| \sim \pi\alpha\Delta^2$. From (22) we can conclude, apparently, that in this region Δ begins to change more rapidly than logarithmically, and tends to the constant value (22).

4. ENERGY OF THE BOUND STATE

In conclusion let us find the energy of the bound state for $I = S - 1/2$, $J < 0$. As usual (see^[11]) we have

$$\frac{\partial E}{\partial |J/N|} = \frac{\langle H_{int} \rangle}{|J/N|}$$

Substituting (2) in this equation, we again take only the terms corresponding to creation and annihilation of the bound states. Here, however, the simple vertex γ must be replaced by $\gamma + \Lambda^{(1)}$ in one type of pairing and by $\gamma + \Lambda^{(2)}$ in the other. As a result we get

$$\frac{\partial E}{\partial |J/N|} = \left| \frac{J}{N} \right| \int \frac{d\omega_1 d\omega_2}{(2\pi)^2} \{ F_{\alpha\beta}^{(1)}(\omega_1) F_{\alpha\beta}^{(2)}(\omega_2) [\gamma + \Lambda^{(2)}(\omega_2 + \omega_1)]_{\alpha\beta, \alpha, \beta} - F_{\alpha, \beta}^{(3)}(\omega_1) F_{\alpha, \beta}^{(4)}(\omega_2) [\gamma + \Lambda^{(1)}(\omega_1 - \omega_2)]_{\alpha\beta, \alpha, \beta} \}.$$

Using the expressions for $\Delta^{(2)}$ and $\Delta^{(4)}$ in terms of the corresponding F , similar to relation (16), and substituting (12), we get

$$\frac{\partial E}{\partial |J/N|} = \frac{\alpha}{|J/N|} \int_0^{\xi_0} [\Delta_{\alpha\beta}^{(1)}(\xi) \Delta_{\alpha\beta}^{(2)}(\xi) + \Delta_{\alpha\beta}^{(3)}(\xi) \Delta_{\alpha\beta}^{(4)}(\xi)] d\xi. \quad (23)$$

The quantities $\Delta^{(1)}$ are actually not fully independent. This is specially easy to see in the first order of perturbation theory, where, for example,

$$\Delta_{\alpha\beta, 1}^{(1)} = \frac{J}{N} \langle \psi_{\alpha, a\beta} \rangle \sigma_{\alpha\alpha}^i \sigma_{\beta\beta, 1}^i, \quad \Delta_{\alpha\beta, 1}^{(2)} = \frac{J}{N} \langle \psi_{\alpha, +a\beta, +} \rangle \sigma_{\alpha, \alpha}^i \sigma_{\beta, \beta}^i.$$

It is seen from these two formulas that $\Delta^{(1)} = (-\Delta^{(2)})^*$. It can be verified that the same connection is retained also in the higher orders, in any case at the assumed accuracy. The same is valid also with respect to $\Delta^{(3)}$ and $\Delta^{(4)}$. It follows therefore that formula (23) can be written in the form

$$\frac{\partial E}{\partial |J/N|} = -\frac{\alpha}{|J/N|} \sum_{\alpha\beta} \int_0^{\xi_0} \{ |\Delta_{\alpha\beta}^{(1)}(\xi)|^2 + |\Delta_{\alpha\beta}^{(3)}(\xi)|^2 \} d\xi. \quad (24)$$

The previously obtained expressions for $\Delta^{(1)}$ can be written in the form

$$\Delta_{\alpha\beta}^{(i)} = P_{\alpha\beta}^{(i)} \left(\left| \frac{N}{J} \right| - 2\alpha\xi \right)^{(S-1)/2}. \quad (25)$$

Let us substitute this in (24). We get

$$\frac{\partial E}{\partial |J/N|} = -\frac{1}{2S} \left| \frac{N}{J} \right|^{S+1} \sum_{\alpha\beta} [|P_{\alpha\beta}^{(1)}|^2 + |P_{\alpha\beta}^{(3)}|^2], \quad (26)$$

where we have used the condition that $N/J - 2\alpha\xi_0 = 0$.

It is seen already from this expression that the formation of bound complexes, if possible ($P^{(1)} \neq 0$), lowers the energy of the system. To obtain the energy in this case it is necessary to know the dependence of the coef-

ficients P on $|J/N|$. This can be done by using the following considerations. The next approximation beyond the logarithmic one should produce an addition to ζ on the order of unity in (25). The expression for $\Delta^{(1)}$ can in this case be already reduced to $\omega \sim \pi\alpha\Delta_0^2$. From this and from (22) we get

$$\pi\alpha\Delta_0^2 = \pi\alpha^2 C_1 P^2 = C_{\epsilon_F} \exp\left\{-\frac{1}{2\alpha} \left| \frac{N}{J} \right|\right\},$$

where C_1 and C are of the order of unity. Obtaining P from this, substituting in (26), and integrating we get

$$E = K_{\epsilon_F} \left(\frac{N}{\alpha|J|}\right)^{S-1} \exp\left\{-\frac{N}{2\alpha|J|}\right\} \quad (27)$$

where $K \sim 1$.

In conclusion, the author wishes to express his indebtedness to Professor K. Yosida for a valuable discussion of the physical aspects of the theory and to I. E. Dzyaloshinskiĭ for friendly criticism.

APPENDIX

We wish to note here certain details of the spin technique proposed in ^[3]. It is already stated there that the introduction of Fermi operators a_β for the spins, by the method

$$\hat{S}_i^z = a_{\beta}^{\dagger} S_{\beta\beta}^z a_{\beta}, \quad (A.1)$$

can be carried out in two different ways. In the case of a spin $S = 1/2$ we can use the fact that the operators give zero when acting on the unphysical states (0, 0) and (1, 1). We could therefore use the operators directly in the form (A.1), following which we could correct the normalization during the averaging. But if $S > 1/2$, this is no longer the case, and in ^[3] we artificially introduced an energy λ for each spin pseudoparticle. Acting on the state (0, 0, ..., 0), the operators \hat{S}_i^z gave 0, and the next states in terms of energy were the physical states with $N = 1$, that is, of the type (0, 0, ..., 0, 1, 0, ..., 0).

This procedure involves a certain inconvenience. The energy λ is an utterly unphysical quantity—it takes part in the sums over the frequencies. To eliminate this quantity it is necessary to go over to integration over real frequencies, which is not always convenient, and furthermore increases greatly the number of different terms. At the same time the spin $S = 1/2$ is an exceptional case. It is therefore interesting to note that it is possible to get along without λ also for $S = 1$.

The point is as follows. All the possible states corresponding to the operators a_β actually correspond to different total spins. For example, for spin $1/2$, the state (1, 1) and (0, 0) actually correspond to $S = 0$ and not $S = 1/2$. In the case of a larger spin we obtain a larger number of such irreducible sets. For example, for $S = 3/2$ there are only 16 states, of which (0, 0, 0, 0) and (1, 1, 1, 1) correspond to $S = 0$, the states (0, 1, 0, 0), (0, 0, 1, 0), (1, 0, 0, 0), and (0, 0, 0, 1) correspond to $S = 3/2$; out of the six states with two ones, five correspond to $S = 2$ and one to $S = 0$, and finally there are four states with three ones, which again correspond to $S = 3/2$. It is very important that the operators \hat{S}_i^z , first, always give zero when they act on states

corresponding to $S = 0$, and second, they do not change the total number of pseudoparticles.

Let us consider the state $S = 1$. The states (0, 0, 0) and (1, 1, 1) are ineffective. The states (1, 0, 0), (0, 1, 0), and (0, 0, 1), which correspond to $S = 1$, were assumed by us to be physical. But it is easy to see that the same properties possessed also by the states (1, 1, 0), (1, 0, 1), and (0, 1, 1). If we take the trace of some product of \hat{S}_i^z over all the states, then we obtain the sum of two traces, each over physical states, and they are therefore identical. It follows therefore that under suitable normalization we again obtain the correct mean value. It is easy to see that the norm is $4/3$.

As to the spin $S > 1$, we have already shown with $S = 3/2$ as an example that the complete set of states must include some which correspond to a spin larger than that which we are considering. Consequently, we cannot get along here without λ .

We now proceed to the second remark. We have already seen in ^[12] that in the presence of a field it is necessary to change the normalization of the mean values. The same pertains to all cases when the individual orientations are not equivalent. We can propose a slight modification, which automatically takes this fact into account. Namely, in lieu of the normalization $e^{\lambda/T}/(2S + 1)$ for each atom, which we used in ^[3], we must introduce the factor

$$[e^{-(H+N\lambda)/T}]^{-1}, \quad N = \sum_{\beta} a_{\beta}^{\dagger} a_{\beta},$$

where N is the total number of "particles," and the trace is taken over all the states. Indeed, acting on the states with $N = 0$, we get zero, when $\lambda \gg T$ the main contribution will be made by physical states, and in the case of equivalence of the orientations we get the previous result. It is easy to see, however, that even in the absence of isotropy the proposed method will yield precisely what is required. Thus, the recipe reduces to dividing any mean value by $(N)^n$, where n is the number of different atoms contained in the mean value.

Naturally, this pertains only to the technique with λ . If we assume a technique without λ with $S = 1/2$ or $S = 1$, then, in view of the small number of the states, it is easy to choose the appropriate normalization.

We note finally that in the technique with λ we can use Bose operators in absolutely the same manner as Fermi operators. Indeed, as already noted in ^[3], Bose a_β give correct commutation relations for \hat{S}_i^z . On the other hand, in the presence of λ we do not have to regard states with an occupation-number sum larger than unity.

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