PSEUDOMULTIPLICITY UNCERTAINTY IN SUPERCONDUCTIVITY THEORY

S. V. VONSOVSKIĬ and M. S. SVIRSKIĬ

Institute of Metal Physics, USSR Academy of Sciences; Chelyabinsk State Pedogogical Institute

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We consider the uncertainty in the population and the ensuring uncertainty of the pseudospin projections in a system described by a Bardeen-Cooper-Schrieffer (BCS) Hamiltonian. We show that the uncertainty of the population and of the energy gap associated with it is independent of the anomalous mean values. A method, based on allowance for the uncertainty of the total pseudospin with conservation of the total number of electrons in the system is considered. An exact solution is given for the case of one Cooper pair and two phase-space cells; this solution leads to an energy that does not depend on the sign of the parameter of the interelectron interaction and lies below the energy of the ground state calculated by the BCS method. It is shown that L. Cooper's problem admits of the existence of a gap between the ground state of the system and the continuum not only in the case of attraction but also in the case of sufficiently strong interelectron repulsion. Modifications of the trial wave function, which make it possible to include in the BCS method the case of interelectron repulsion, are considered. The role of large or small pseudospins is assessed in the case of interelectron attraction or repulsion.

1. INTRODUCTION

THE BCS method[1], the importance of which to the development of superconductivity theory is well known, is equivalent to the pseudomagnetic field approximation[2]. This method is connected with introduction of fictitious states and takes into account the possibility of superconductivity only in the case of interelectron attraction. Yet it is known from quantum theory of magnetism that a corresponding magnetic order can be obtained for any sign of the spin-interaction parameter. This gives grounds for expecting that in the case of the interelectron interaction described in the BCS theory by the parameter V, the corresponding ordering can occur at any sign of this parameter[1)]. We show in this article that the expected analogy between magnetism and superconductivity can indeed be established.

2. POPULATION UNCERTAINTY IN THE BCS THEORY

The BCS theory[1] starts from the Hamiltonian

$$H=\sum_{\sigma,\ k>k_F}\varepsilon_k n_{k\sigma}+\sum_{\sigma,\ k<k_F}|\varepsilon_k|(1-n_{k\sigma})-\sum_{k,\ k'}V_{kk'}b_{k'}^{*}b_k, \qquad (1)$$

where σ, k, and ϵ_k are the spin projection, wave vector, and kinetic energy of the conduction electron; k_F is the Fermi wave vector; $n_{k\sigma}$ is the operator of the number of electrons in the state (k, σ); b_k^* is the Cooper pair production operator; $V_{kk'}$ is the matrix element, assumed equal to zero when $|\epsilon_k| > \hbar\omega$ and equal to a constant V when $|\epsilon_k| < \hbar\omega$, where ω is the average phonon frequency. The approximation used in[1] for the ground-state wave function is

$$\Psi=\prod_k[(1-h_k)^{1/2}+h_k^{1/2}b_k^{*}]\Phi_0, \qquad (2)$$

where h_k is the probability that the pair fills the state $(k, \sigma; -k, -\sigma)$, and Φ_0 is the vacuum wave function.

[1)]The need for developing a method different from that of [1] in order to take into account both signs of V is noted in [3,4].

In the approximation (2), the mean value of the Hamiltonian (1) is

$$W=\sum_k|\varepsilon_k|(1-\sqrt{1-4(\bar{b}_k)^2})-V\sum_{k,\ k'}\bar{b}_{k'}\bar{b}_k. \qquad (3)$$

This expression has a minimum with respect to b_k if the following equality is satisfied:

$$\bar{b}_k=\varepsilon_0[2\sqrt{\varepsilon_k^2+\varepsilon_0^2}]^{-1},\quad \varepsilon_0=V\sum_{k'}\bar{b}_{k'}. \qquad (4)$$

From (3) and (4) follow the known results of the BCS theory[1]:

$$\varepsilon_0=\hbar\omega\left[\operatorname{sh}\left(\frac{1}{N_0V}\right)\right]^{-1},\quad W_0=-2N_0(\hbar\omega)^2[e^{2/N_0V}-1]^{-1},$$

where N_0 is the density of states at the Fermi surface.

It is easy to verify that the BCS variational problem was solved relative to the uncertainty of the population of the phase space, which is determined by the expression

$$\Delta n_{k\sigma}=\overline{((n_{k\sigma}-\bar{n}_{k\sigma})^2)}^{1/2}=[\bar{n}_{k\sigma}(1-\bar{n}_{k\sigma})]^{1/2}=\bar{b}_k, \qquad (5)$$

where it is recognized that $n_{k\sigma}^2 = n_{k\sigma}$ for Fermi particles and that according to (2) $\bar{b}_k = \sqrt{h_k(1-h_k)}$. It follows from (5) that in the BCS method the difference between $\Delta n_{k\sigma}$ and zero is due to the inequality

$$\bar{b}_k\neq 0, \qquad (6)$$

which follows from (4) and is usually regarded as the "gist of the BCS theory"[5]. We shall show that actually expression (5) does not hold, and that the existence of the uncertainty $\Delta n_{k\sigma}$ is not connected with satisfaction of (6).

The operators b_k and $N_\sigma = \sum_k n_{k\sigma}$ satisfy the commutation relation

$$b_kN_\sigma-N_\sigma b_k=b_k. \qquad (7)$$

On the other hand, the operator N_σ commutes with the Hamiltonian (1). It follows therefore from (7) that in the stationary state, in which N_σ has a negative value,

$$\delta_k = 0. \tag{8}$$

The discrepancy between (8) and (6) is a discrepancy between the BCS Hamiltonian and the BCS method. If we forego the approximation (2), then we can show that $\Delta n_{k\sigma}$ is different from zero if (8) is satisfied. To this end, we recognize that according to (2.26) we have from[1]

$$\Psi = h_{kN}^{1/2}\varphi_N(1_k) + (1-h_{kN})^{1/2}\varphi_N(0_k), \tag{9}$$

where the index N indicates that the number of electrons is fixed. From (9) it follows that

$$\Delta n_{k\sigma} = \sqrt{h_{kN}(1-h_{kN})}. \tag{10}$$

Since the eigenfunction of (1) is (9) and not $\varphi_N(1_k)$ and $\varphi_N(0_k)$ separately, it follows that $0 < h_{kN} < 1$. It follows in turn from (10) that $1/2 \geq \Delta n_{k\sigma} > 0$. On the other hand, owing to the orthogonality of $\varphi_N(1_k)$ and $\varphi_N(0_k)$, Eq. (9) leads to (8). Thus, the uncertainty of the population is independent of the introduction of nonzero anomalous mean values.

In the case of the Hamiltonian (1), the population uncertainty is connected with an energy gap for the excitations. Indeed, from the Schrödinger equation, in which (9) is an eigenfunction of (1), it follows that the energy of the system and h_{kN} are determined by the following equations:

$$E_\pm = 1/2(H_{11}+H_{00}) \pm \sqrt{\delta^2 + H_{10}^2}, \tag{11}$$

$$h_{kN,\pm}^{1/2} = \pm(1-h_{kN,\mp})^{1/2} = 2^{-1/2}H_{10}[H_{10}^2 + \delta^2 \pm \delta\sqrt{\delta^2+H_{10}^2}]^{-1/2},$$

where $H_{\alpha\beta} = \langle \varphi(\alpha k)|\, H \,|\varphi(\beta_k)\rangle$; α and β take on the values 0 and 1, and $\delta = (H_{11} - H_{00})/2$. It follows from (11) that the function (9) corresponds to an orthogonal wave function

$$\Psi = h_{kN}^{1/2}\varphi_N(0_k) - (1-h_{kN})^{1/2}\varphi_N(1_k), \tag{12}$$

and the energies of the states (9) and (12) are separated by a gap

$$\Delta E = E_+ - E_- = 2\sqrt{\delta^2 + H_{10}^2}. \tag{13}$$

Substituting h_{kN} from (11) in (10), we obtain a connection between the energy gap of pair excitation and $\Delta n_{k\sigma}$:

$$\Delta E \Delta n_{k\sigma} = |H_{10}| \tag{14}$$

In the approximation (2) it follows from (14). (5), and (4) that $\Delta E = 2\sqrt{\epsilon_k^2 + \epsilon_0^2} - V$, which coincides, accurate to within $-V$, with (2.54) of[1]. At a fixed number of particles, Eq. (14) establishes a connection between $\Delta n_{k\sigma}$ and the finite pair-excitation energy at a zero anomalous mean value (8). This allows us to state that an essential property of the microscopic theory of superconductivity is not the deviation of the anomalous mean values from zero, but the population uncertainty, accompanied by an energy gap for the excitations. In this respect, the superconductor differs from a normal metal, in which the smoothing of the Fermi steps as a result of interelectron interaction is not accompanied by the appearance of an energy gap in the quasiparticle spectrum. In the case of a uniform displacement of the conduction electron distribution, the superconductor is stable against excitations, provided that the product of the mean velocity by the Fermi momentum does not exceed the energy gap (see[6]).

3. UNCERTAINTY OF THE PSEUDOSPIN OF A SUPERCONDUCTOR

In the pseudospin method[2] the operators b_k and $n_{k\sigma}$ are expressed in terms of Pauli operators by the equations $b_k = \overline{s_k}$ and $n_{k\sigma} + n_{-k,-\sigma} = 1 - 2s_k^z$. Accordingly, we transform the Hamiltonian (1) into

$$H = 2\sum_{k>k_F}\varepsilon_k - 2\sum_k \varepsilon_k s_k^z - V\sum_{k\neq k'} s_{k'}^+ s_k^-. \tag{15}$$

The summation with respect to $k \neq k'$ corresponds to (23) of[2] and agrees with the remark made by BCS[1] that the diagonal terms of the interaction are the same in the normal and superconducting phases. Introducing the total pseudospin operator $S = \sum s_k$, we obtain from (15)

$$H = 1/2\sum_k V + 2\sum_{k>k_F}\varepsilon_k - 2\sum_k \varepsilon_k s_k^z - VS^2 + V(S_z)^2. \tag{16}$$

Under the conditions of[1], where the numbers of electrons and holes in the region $2\hbar\omega$ are equal, we have $S_Z = 0$ and therefore

$$H = 1/2\sum_k V + 2\sum_{k>k_F}\varepsilon_k - 2\sum_k \varepsilon_k s_k^z - VS^2. \tag{17}$$

The presence of the non-commuting operators s_k^z and S^2 in (17) shows that the superconductivity is connected with the uncertainty Δs_k^z. On the other hand, it follows from the definition of s_k^z that

$$\Delta n_{k\sigma} = \Delta s_k^z. \tag{18}$$

Consequently, the conclusions obtained above concerning $\Delta n_{k\sigma}$ hold also for the uncertainty of Δs_k^z.

It follows from (17) that the dependence of the Hamiltonian on s_k^z vanishes if different states correspond to the same kinetic energy. Such a case, which admits of an exact solution, was considered in[7]. However, this solution is limited to the case of strong coupling or to the interaction between nucleons belonging to a partly-filled shell.

To analyze the conditions under which superconductivity is realized, let us average (19) over a state with a definite value of S. According to Sec. 27 of[8], the operator s_k^z changes the value of S by ± 1 if the condition $S_Z = 0$ is satisfied. It therefore follows from (17) that in a state with definite S we have

$$W = 1/2\sum_k V + 2\sum_{k>k_F}\varepsilon_k - VS(S+1). \tag{19}$$

Regarding the state with definite S as a trial state, we can state that the minimum of (19) gives the upper limit of the superconductor ground-state energy. In the case of attraction ($V > 0$), the minimum of (19) is reached when $S_{max} = N_0\hbar\omega$, and its value is

$$W = N_0(\hbar\omega)^2(1 - N_0V), \tag{20}$$

and in the case of repulsion ($V < 0$) the minimum of (19) is reached at $S = 0$ and its value is

$$W = N_0\hbar\omega(\hbar\omega - |V|). \tag{21}$$

It follows therefore that in the case of attraction the starting point for the construction of the wave function should be the state with S_{max}, and in the case of repulsion the state with $S = 0$ (which in conjunction with

the condition $S_Z = 0$ corresponds to "pseudo-antiferromagnetism").

Since S^2 does not commute with s_k^z, the total pseudospin of the superconductor is likewise indeterminate. In this sense, (17) is analogous to the Hamiltonian considered in[9] in connection with the antiferromagnetism problem, where the terms containing the spins of individual sites lead to an indeterminate multiplicity of the spin system as a whole. The uncertainty of the pseudospin multiplicity takes place also in the normal state, in which $\Delta S^2 = \sqrt{N_e N_g}$ in the case of an unsmoothed Fermi step (N_e and N_g are the numbers of electrons and holes in the band). The presence in (17) of the term $-VS^2$, which is typical of superconductors, shows that the role of states with large S in the superposition of states with different S increases in the case of attraction ($V > 0$) and the role of states with small S increases in the case of repulsion ($V < 0$). This situation is illustrated below for the simplest case of one pair and two phase-space cells.

4. COOPER PAIR IN TWO PHASE-SPACE CELLS

In this problem, Eq. (17) takes the form

$$H = 2\varepsilon(1 + A_z) + V(1 - S^2), \tag{22}$$

where the antisymmetrical operator $A_Z = s_1^z + s_2^z$ transforms the singlet Ψ^s and the triplet Ψ_0^t into each other[10]. We therefore seek the solution in the form of the superposition

$$\Psi = \alpha\Psi^s + \beta\Psi_0^t, \quad \alpha^2 + \beta^2 = 1. \tag{23}$$

From (22) and (23) we obtain the energy spectrum

$$E_\pm = 2\varepsilon \pm \sqrt{(2\varepsilon)^2 + V^2} \tag{24}$$

and the coefficients

$$\alpha_\pm = \{1/2[1 \pm V/\sqrt{(2\varepsilon)^2 + V^2}]\}^{1/2}, \quad \beta_\pm = \pm\alpha_\mp. \tag{25}$$

According to (24) and (25), the energy of the excited state of the pair is separated from the energy of the ground state by a gap $\Delta E = 2\sqrt{(2\epsilon)^2 + V^2}$ (for single excitation, the gap is equal to $\sqrt{(2\epsilon)^2 + V^2}$, as can readily seen, and the uncertainty of the population is determined by the expression $\Delta n_{k\sigma} = |V| [2\sqrt{(2\epsilon)^2 + V^2}]^{-1}$. Both quantities are connected by the relation (14). In our problem, the ground-state energy E_- is negative and does not depend on the sign of V. In accord with Sec. 3, the sign of V influences the value of the psuedospin of the ground state, viz., when $V > 0$ (attraction) we get from (25) that $|\beta| > |\alpha|$ and Ψ^t with $S_{max} = 1$ predominates in (23), whereas for $V < 0$ (repulsion) we have $|\alpha| > |\beta|$ and Ψ^s with $S = 0$ predominates in (23).

The exact solution considered above can be obtained also by a variational method. Namely, it follows from (22) and (23) that

$$W = 2\varepsilon - 4\varepsilon\alpha\sqrt{1 - \alpha^2} - (1 - 2\alpha^2)V. \tag{26}$$

Minimizing (26) with respect to α, we obtain (25). From (25) and (26) follows expression (24) for E_-. Thus, the use of a trial wave function with a fixed number of particles enables us to obtain in this case the exact solution by a variational method.

Let us consider now, for comparison, the BCS variational method. This method yields, from (3) and (4),

$$\varepsilon_0 = \sqrt{(1/2V)^2 - \varepsilon^2}, \quad W_{0,\,BCS} = 2\varepsilon - 1/2V - 2\varepsilon^2/V. \tag{27}$$

A comparison with (24) shows that when $V > 2\epsilon$ the energy $W_{0,BCS}$ is negative, but is higher than the energy E_- from (24). In the BCS method we lose here the solution for the case $V < 0$ (repulsion), for when $V < 0$ it follows from (27) that $W_{0,BCS} > 0$.

To include the case of repulsion in the BSC method, we take in lieu of (2) the following trial function:

$$\Psi = [(1 - b_2)^{1/2} + b_2^{1/2} b_2^*][-(1 - b_1)^{1/2} + b_1^{1/2} b_1^*]\Phi_0. \tag{28}$$

We then get in place of (4)

$$b_2 = -b_1 = \varepsilon_0/2\sqrt{\varepsilon^2 + \varepsilon_0^2} = \varepsilon_0/|V|, \quad W_{0,\,BCS} = 2\varepsilon - 1/2|V| - 2\varepsilon^2/|V|. \tag{29}$$

Thus, modification of the type of trial wave function makes it possible to include in the BCS method the case of interelectron repulsion and to obtain, for $|V| > 2\epsilon$, a solution with an energy lying below the energy of the normal state, and with a pair-excitation energy gap equal to $2\sqrt{\epsilon^2 + \epsilon_0^2} = |V|$.

5. L. COOPER'S PROBLEM

The problem considered above is a particular case of K. Kuper's problem[11] for two groups of levels, when the state of one pair is connected by a constant matrix element with all the states of the other group. According to (3.24) of[11], the pair binding energy is likewise independent of the sign of V in this more general case. In the case of L. Cooper's problem[12] it is necessary to take into account the possibility of a transition between all the states inside a layer of thickness Δ. The equation for the pair energy has in this case the form

$$(2\varepsilon_k - E)a_k = V \sum_{k'(\neq k)} a_{k'}. \tag{30}$$

Unlike the usual expression (see[12]), the summation in the right-hand side of (3) is only over k' ($\neq k$). This corresponds to allowance for the equality of the diagonal interaction terms in the normal and superconducting states (see (15)). From (30) we get the equation

$$\frac{1}{V} = \sum_k \frac{1}{2\varepsilon_k - (E - V)}, \tag{31}$$

which differs from the usual equation in that E is replaced by $E - V$. In the case of two states only, Eq. (31) leads, with the indicated substitution, to the exact solution (24). In the case of a larger number of states lying inside Δ with a density g, it follows from (31) that

$$E = V - \Delta(e^{1/gV} - 1)^{-1}. \tag{32}$$

When $V > 0$, the binding energy is negative if

$$S_{max} = 1/2g\Delta > 1/2gV(e^{1/gV} - 1). \tag{33}$$

Since in Cooper's problem $S_Z = g\Delta/2 - 1$, it follows that S can assume only the values S_{max} and $S_{max} - 1$. Consequently, in the case of attraction the wave function is a superposition of states with sufficiently close S_{max} and $S_{max} - 1$, which agrees with Sec. 3.

When $V < 0$, the binding energy is negative if

$$S_{max} = {}^1/_2 g\Delta < {}^1/_2 g|V|(1 - e^{-1/g|V|}), \quad (34)$$

and consequently the total pseudospin is sufficiently small, which also agrees with Sec. 3. It follows from (34) that when $g|V| \ll 1$ the binding energy is negative if $|V| > \Delta$, so that pair production is convenient only in the case of sufficiently strong repulsion.

Thus, L. Cooper's problem, which is fundamental for the modern microscopic theory of superconductivity, admits of a state with negative pair-binding energy in the case of both attraction and sufficiently strong repulsion.

6. ENERGY OF A SYSTEM OF ELECTRON PAIRS

In the case of interelectron attraction, the BCS method leads to the results obtained in[1]. In order to include the case of repulsion in the BCS method, let us take, in analogy with (28), a trial wave function

$$\Psi = \prod_{k>k_F} [(1-h_k)^{1/2} + h_k^{1/2} b_k^*] \prod_{k<k_F} [-(1-h_k)^{1/2} + h_k^{1/2} b_k^*] \Phi_0. \quad (35)$$

The mean value of the Hamiltonian (1) has then the form

$$W = \sum_{k>k_F} 2\varepsilon_k h_k + \sum_{k<k_F} 2|\varepsilon_k|(1-h_k) + 2V \sum_k h_k(1-h_k). \quad (36)$$

Minimizing (36) with $V = -|V|$ with respect to h_k, we obtain

$$h_k = {}^1/_2(1 - 2\varepsilon_k/|V|), \quad W_0 = N_0\hbar\omega(\hbar\omega - |V|). \quad (37)$$

The expression for W_0 coincides with (21) and is negative for $|V| > \hbar\omega$. Just as in Sec. 4, the energy gap for the pair is $\Delta E_k = |V|$.

The trial function (35), like (2), does not take into account the constancy of the number of electrons. To take into account the conservation of the number of electrons, it is possible to use the pseudospin method, putting $S_Z = 0$. It should be borne in mind here that, in accord with Sec. 3, a major role is assumed in Ψ by states with either large or small S depending on the sign of V. Therefore the simplest approximation is one in which only one of the indicated states is enhanced. We take the trial wave function

$$\Psi = \alpha\Psi_n + \beta(\Psi_{S,0} - a\Psi_n)/\sqrt{1-a^2}, \quad (38)$$

where Ψ_n is the normal state, $\Psi_{S,0}$ the state with total pseudospin S and $S_Z = 0$, $a = \langle \Psi_{S,0} | \Psi_n \rangle$, and $\alpha^2 + \beta^2 = 1$. Minimizing the mean value (17) in the state (38) with respect to α, we obtain

$$W_0 = \frac{N^0(\hbar\omega)^2}{1-a^2} + \frac{1-2a^2}{1-a^2} V[N_0\hbar\omega - S(S+1)] + \frac{1}{2}[f_1 - \sqrt{f_1^2 + f_2^2}], \quad (39)$$

$$f_1 = -\frac{1}{1-a^2}\{N_0(\hbar\omega)^2 + (1-2a^2)V[N_0\hbar\omega - S(S+1)]\},$$

$$f_2 = \frac{2a}{\sqrt{1-a^2}} V[S(S+1) - N_0\hbar\omega]. \quad (40)$$

When $f_1 < 0$, the vanishing of f_2 leads to a normal-state energy $W_0 = 0$. When $f_2 \neq 0$ we have the inequality $W_0 < 0$ and (39) turns out to be lower than the normal-state energy. In the case of one pair and two phase-space cells, the solution (39) and (40) coincides with the exact solution of Sec. 4. In the strong-coupling limit ($N_0V \gg 1$), Eq. (39) leads in the case of attraction to the same result $W_0 = -N_0^2(\hbar\omega)^2 V$ as in the BCS theory[1]. In the case of repulsion, in the strong-coupling limit ($|V| \gg \hbar\omega$), Eq. (39) leads to the value $W_0 = -N_0\hbar\omega|V|$, which agrees with the result (37) obtained above by including repulsion in the BCS method.

The foregoing results are significant for both attraction and interelectron repulsion. In either case, independently of the introduction of the anomalous means values, which is equivalent to the introduction of fictitious states, the BCS Hamiltonian leads to relation (14) between the population uncertainty and the energy gap. The properties possessed by the system described by the BCS Hamiltonian in the case of attraction are present also in the case of sufficiently strong repulsion: in both cases it is possible to have an ordering of the conduction electrons that is more favored energywise than the normal state, and with an energy gap for the excitations. This makes it possible to re-examine the influence of the Coulomb, spin-wave, and other types of interelectron repulsion on the superconductivity.

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