[Journal of the Faculty of Science, Hokkaidô University, Japan, Ser. II, Vol. V, No. 4, 1959]

A Note of the Excited State at $T=0°K$ in the Superconducting State

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(Received Sept. 15, 1959)

A wave function of the excited state in the superconducting state slightly more general than what in BARDEEN-COOPER-SCHRIEFER's theory is adopted, and it is shown that in the case of weak interaction the minimum energy gap at $T=0°K$ comes out to be $2\epsilon_0$.

§ 1. Introduction

The energy gap at $T=0°K$ estimated from the experiments on specific heat, microwave transmission, etc.[1),2)] proves to be about $3kT_c$ for some superconductors, while BARDEEN-COOPER-SCHRIEFER's theory[3)] shows that it should be $3.5kT_c$. They claim that their result is in the quantitative agreement with experiments. However, the excited state wave function at 0°K assumed in B.C.S.-theory may not be so general; being appropriate only in the case where the $\boldsymbol{k}'$ and $\boldsymbol{k}''$ states each occupied by a single electron are related with each other by a special condition (expression (11) given below).

We consider a more general excited state in which any arbitrary $\boldsymbol{k}'$ and $\boldsymbol{k}''$ states are each occupied by a single excited electron. For convenience's sake, the method adopted by B.C.S.-theory of calculating the energy gap at 0°K will be briebly outlined in the following, the notations being the same as in their theory.

The wave function of the superconducting ground state and the reduced Hamiltonian are assumed to be

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

(Φ_0: vacuum state)

and

$$H_{\text{red}} = 2\sum_{k>k_F} \epsilon_k b_k^* b_k + 2\sum_{k<k_F} |\epsilon_k| b_k b_k^* - V\sum_{k,k'} b_k^* b_k \ , \qquad (2)$$

respectively.

When N pairs of electrons are considered in the ground state, h_k must satisfy the condition:

$$\sum_k h_k = N . \tag{3}$$

The expectation value of H_{red} of the ground state is

$$W_0 = 2\sum_{k>k_F} \epsilon_k h_k + 2\sum_{k<k_F} |\epsilon_k|(1-h_k) - V\sum_{k,k'} \left[h_k(1-h_k)h_{k'}(1-h_{k'})\right]^{\frac{1}{2}} , \tag{4}$$

in which h_k is to be determined from the variational equation

$$\frac{\partial W_0}{\partial h_k} = 0 , \tag{5}$$

the subsidiary condition (3) being taken into account.

The effective contribution to W_0 is only due to the electrons in the region $-\hbar\omega < \epsilon_k < \hbar\omega$, provided the Fermi-surface is taken as the origin of energy; and h_k in (4) naturally satisfies the condition (3), so far as the electrons above the Fermi-surface and the holes below it are concerned. From the equations (4) and (5), the following relation is obtained;

$$h_k = \frac{1}{2}\left[1 - \frac{\epsilon_k}{(\epsilon_k^2 + \epsilon_0^2)^{\frac{1}{2}}}\right] , \tag{6}$$

where

$$\epsilon_0 = V\sum_k \left[h_k(1-h_k)\right]^{\frac{1}{2}} = N(0)\, V\epsilon_0 \int_0^{\hbar\omega} \frac{d\epsilon}{(\epsilon^2 + \epsilon_0^2)^{\frac{1}{2}}} . \tag{7}$$

In the excited state, $-\boldsymbol{k}'\downarrow$ and $\boldsymbol{k}''\uparrow$ states are each occupied by one electron, while all the other states in $\boldsymbol{k}$-space are occupied by pairs with the same probability as the ground states. Thus, the wave function of the excited state takes the form

$$\Psi_{\text{exc}} = \prod_{\substack{k \\ (\neq k', k'')}} \left\{(1-h_k)^{\frac{1}{2}} + h_k^{\frac{1}{2}} b_k^*\right\} c^*_{-k'\downarrow} c^*_{k''\uparrow} \Phi_0 . \tag{8}$$

Since the number of electrons occupying the excited state must be the same as that in the ground state, the number of pairs in the excited state is $(N-1)$:

$$\sum_{\substack{k \\ (\neq k', k'')}} h_k = N-1 . \tag{9}$$

From the equations (3) and (9), it results that $h_{k'}$ and $h_{k''}$ satisfy the relation

$$h_{k'}+h_{k''}=1\ . \tag{10}$$

It is to be noticed that this relation holds, not for arbitrary $\boldsymbol{k}'$ and $\boldsymbol{k}''$ states, but only for those whose energies are of the same magnitude:

$$\epsilon_{k'}=-\epsilon_{k''}\ . \tag{11}$$

To get the minimum value of the energy difference between the ground and the excited one, $\epsilon_{k'}$ and $\epsilon_{k''}$ must be brought to zero under the state condition (11), and thus comes out to be the value of energy gap at 0°K

$$\underset{\epsilon_k\to 0}{\Delta W}=W_{\text{exc}}-W_0=2\epsilon_0\ . \tag{12}$$

So far is the result of B.C.S.-theory.

We now assume as the excited state at 0°K the state which corresponds to the breaking-up of the pairs in any two arbitrary states, $\boldsymbol{k}'$ and $\boldsymbol{k}''$, and of a portion of the pair in every other state in the ground state, such that the total sum of the broken-up portions amounts to one pair, and each of the $-\boldsymbol{k}'\downarrow$ and $\boldsymbol{k}''\uparrow$ states is occupied by a single electron.

That is to say, the excited state is none other than the state produced from the vacuum state by exciting a single electron into each of the $-\boldsymbol{k}'\downarrow$ and $\boldsymbol{k}''\uparrow$ states and distributing $2(N-1)$ electrons as pairs in the $\boldsymbol{k}$-space except $\boldsymbol{k}'$ and $\boldsymbol{k}''$ states.

§ 2. Energy gap at $T=0$°K

The wave function of the excited state and its expectation value of the reduced Hamiltonian (2) are respectively

$$\Psi_{\text{exc}}=\prod_{\substack{k\\(\neq k',k'')}}\left\{(1-p_kh_k)^{\frac{1}{2}}+(p_kh^k)^{\frac{1}{2}}b_k^*\right\}c^*_{-k'\downarrow}c^*_{k''\uparrow}\Phi_0\ , \tag{13}$$

and

$$W_{\text{exc}}=2\sum_{\substack{k>k_F\\(\neq k',k'')}}\epsilon_kp_kh_k+2\sum_{\substack{k<k_F\\(\neq k',k'')}}|\epsilon_k|(1-p_kh_k)+\epsilon_{k'}+\epsilon_{k''}$$
$$-V\sum_{\substack{l,l'\\(\neq k',k'')}}\left[p_lh_l(1-p_lh_l)p_{l'}h_{l'}(1-p_{l'}h_{l'})\right]^{\frac{1}{2}}, \tag{14}$$

where h_k has the same value as in the ground state, so that p_k is the

ratio of the probability with which the k state is occupied by pair in the excited state to that in the ground state. By minimizing W_{exc} with respect to p_k an integral equation for determining p_k is obtained for $k>k_F$;

$$2\epsilon_k h_k - V \sum_{\substack{l \\ (\neq k',k'')}} p_k^{-\frac{1}{2}}\left[h_k(1-p_k h_k)p_l h_l(1-p_l h_l)\right]^{\frac{1}{2}}$$

$$-V \sum_{\substack{l \\ (\neq k',k'')}} (1-p_k h_k)^{\frac{1}{2}}\left[p_k h_k\right]^{\frac{1}{2}} h_k\left[p_l h_l(1-p_l h_l)\right]^{\frac{1}{2}} = 0. \tag{15}$$

For $k<k_F$, in place of the first term in (15) we may use $-2|\epsilon_k|h_k$, which equals $2\epsilon_k h_k$. Therefore, (15) is realized for all k's. Putting

$$\eta = V \sum_{\substack{l \\ (\neq k',k'')}} \left[p_l h_l(1-p_l h_l)\right]^{\frac{1}{2}}, \tag{16}$$

we obtain from (15)

$$\eta = 2\epsilon_k(1-2p_k h_k)^{-1}\left[p_k h_k(1-p_k h_k)\right]^{\frac{1}{2}}, \tag{17}$$

and

$$p_k h_k = \frac{1}{2}\left\{1-\frac{\epsilon_{lK}}{(\epsilon_k^2+\eta^2)^{\frac{1}{2}}}\right\}. \tag{18}$$

By combining (17) and (18), we get

$$\eta = V \sum_{\substack{l \\ (\neq k',k'')}} \frac{\eta}{2(\epsilon_l^2+\eta^2)^{\frac{1}{2}}}. \tag{19}$$

or, replacing the summation by an integral,

$$\frac{1}{V} = N(0)\int_0^{\hbar\omega} \frac{d\epsilon}{(\epsilon^2+\eta^2)^{\frac{1}{2}}} - \frac{1}{2(\epsilon_{k'}^2+\eta^2)^{\frac{1}{2}}} - \frac{1}{2(\epsilon_{k''}^2+\eta^2)^{\frac{1}{2}}}. \tag{20}$$

Substitution of η satisfying equation (20) in (14) gives the minimum value of W_{exc}:

$$W_{\text{exc}} = 2\sum_{\substack{k>k_F \\ (\neq k',k'')}} \epsilon_k p_k h_k + 2\sum_{\substack{k<k_F \\ (\neq k',k'')}} |\epsilon|(1-p_k h_k) + |\epsilon_{k'}| + |\epsilon_{k''}| - \frac{\eta^2}{V}$$

$$= 2N(0)\int_0^{\hbar\omega} \epsilon\left\{1-\frac{\epsilon}{(\epsilon^2+\eta^2)^{\frac{1}{2}}}\right\}d\epsilon + \frac{\epsilon_{k'}^2}{(\epsilon_{k'}^2+\eta^2)^{\frac{1}{2}}} + \frac{\epsilon}{(\epsilon_{k''}^2+\eta^2)^{\frac{1}{2}}} - \frac{\eta^2}{V}. \tag{21}$$

In case the difference of distribution function between the excited state

and the ground state is small,

$$p_k = 1-\Delta_k \,, \tag{22}$$

where $|\Delta_k| \ll 1$.

From equation (16), we obtain in the first order approximation of Δ_k

$$\eta = \epsilon_0 - V\sum_k \frac{\Delta_k h_k(1-2h_k)}{2[h_k(1-h_k)]^{\frac{1}{2}}} - V\left\{\left[h_{k'}(1-h_{k'})\right]+\left[h_{k''}(1-h_{k''})\right]^{\frac{1}{2}}\right\}$$
$$+V\left\{\frac{\Delta_{k'}h_{k'}(1-2h_{k'})}{2[h_{k'}(1-h_{k'})]^{\frac{1}{2}}}+\frac{\Delta_{k''}h_{k''}(1-2h_{k''})}{2[h_{k''}(1-h_{k''})]^{\frac{1}{2}}}\right\}$$
$$= \epsilon_0 - \Delta\eta_1 - \Delta\eta_2(\boldsymbol{k}', \boldsymbol{k}''), \tag{23}$$

where

$$\Delta\eta_1 = V\sum_{\substack{k \\ (\neq k',k'')}} \frac{\Delta_k h_k(1-2h_k)}{2[h_k(1-h_k)]^{\frac{1}{2}}} \tag{24}$$

and

$$\Delta\eta_2 = V\left\{\left[h_{k'}(1-h_{k'})\right]^{\frac{1}{2}}+\left[h_{k''}(1-h_{k''})\right]^{\frac{1}{2}}\right\}$$
$$= \frac{V\epsilon_0}{2}\left\{\frac{1}{(\epsilon_{k'}^2+\epsilon_0^2)^{\frac{1}{2}}}+\frac{1}{(\epsilon_{k''}^2+\epsilon_0^2)^{\frac{1}{2}}}\right\}. \tag{25}$$

In equation (25), the values of $h_{k'}$ and $h_{k''}$ for the ground state (6) are used.

Combining (19), (23) and (25) with (9), we can get the equation for $\Delta\eta_2$, in the first order approximation of $\Delta\eta_1$ and $\Delta\eta_2$;

$$\Delta\eta_1\left[\frac{2N(0)\hbar\omega}{\epsilon_0^2}\left\{1+\left(\frac{\hbar\omega}{\epsilon_0}\right)^2\right\}^{\frac{1}{2}}-\frac{\epsilon_0}{(\epsilon_{k'}^2+\epsilon_0^2)^{\frac{3}{2}}}-\frac{\epsilon_0}{(\epsilon_{k''}^2+\epsilon_0^2)^{\frac{3}{2}}}\right]$$
$$=\left[\frac{1}{(\epsilon_{k'}^2+\epsilon_0^2)^{\frac{1}{2}}}+\frac{1}{(\epsilon_{k''}^2+\epsilon_0^2)^{\frac{1}{2}}}\right]\left[-\frac{N(0)V\hbar\omega}{\epsilon_0}\left\{1+\left(\frac{\hbar\omega}{\epsilon_0}\right)^2\right\}^{-\frac{1}{2}}\right.$$
$$\left.+1+\frac{V\epsilon_0^2}{2(\epsilon_{k'}^2+\epsilon_0^2)^{\frac{3}{2}}}+\frac{V\epsilon_0^2}{2(\epsilon_{k''}^2+\epsilon_0^2)^{\frac{3}{2}}}\right]. \tag{26}$$

Thus, $\Delta\eta_1$ which minimizes W_{exc} for the given $\boldsymbol{k}'$ and $\boldsymbol{k}''$ has been obtained on the condition that h_k has the same value as in the ground state.

From (21) and (23), the energy of the excited state becomes

$$W_{\text{exc}}=2N(0)\int_0^{\hbar\omega}\epsilon\left\{1-\frac{\epsilon}{(\epsilon^2+\epsilon_0^2)^{\frac{1}{2}}}\right\}d\epsilon-2N(0)\int_0^{\hbar\omega}\frac{\epsilon_0\epsilon^2(\Delta\eta_1+\Delta\eta_2)}{(\epsilon^2+\epsilon_0^2)^{\frac{1}{2}}}d\epsilon$$
$$+\frac{\epsilon_{k'}^2}{(\epsilon_{k'}^2+\epsilon_0^2)^{\frac{1}{2}}}+\frac{\epsilon_{k''}^2}{(\epsilon_{k''}^2+\epsilon_0^2)^{\frac{1}{2}}}+\epsilon_0(\Delta\eta_1+\Delta\eta_2)\left\{\frac{\epsilon_{k'}^2}{(\epsilon_{k'}^2+\epsilon_0^2)^{\frac{3}{2}}}\right.$$
$$\left.+\frac{\epsilon_{k''}^2}{(\epsilon_{k''}^2+\epsilon_0^2)^{\frac{3}{2}}}\right\}-\frac{\epsilon_0^2}{V}+\frac{2\epsilon_0}{V}(\Delta\eta_1+\Delta\eta_2). \tag{27}$$

With the aid of (6), W_0 can be expressed as

$$W_0=2N(0)\int_0^{\hbar\omega}\epsilon\left\{1-\frac{\epsilon}{(\epsilon^2+\epsilon_0^2)^{\frac{1}{2}}}\right\}d\epsilon-\frac{\epsilon_0^2}{V}. \tag{28}$$

Therefore, the energy gap at $T=0°$K comes out

$$\Delta W=W_{\text{exc}}-W_0=\frac{\epsilon_{k'}^2}{(\epsilon_{k'}^2+\epsilon_0^2)^{\frac{1}{2}}}+\frac{\epsilon_{k''}^2}{(\epsilon_{k''}^2+\epsilon_0^2)^{\frac{1}{2}}}$$
$$+\left[\frac{2\epsilon_0}{V}-2N(0)\epsilon_0\left(\frac{1}{N(0)V}-\frac{\hbar\omega}{\sqrt{\epsilon_0^2+(\hbar\omega_0^2)^2}}\right)\right.$$
$$\left.+\frac{\epsilon_{k'}^2\epsilon_0}{(\epsilon_{k'}^2+\epsilon_0^2)^{\frac{3}{2}}}+\frac{\epsilon_{k''}^2\epsilon_0}{(\epsilon_{k''}^2+\epsilon_0^2)^{\frac{3}{2}}}\right]$$
$$\times\left[\frac{V\epsilon_0}{2}\left\{\frac{1}{(\epsilon_{k'}^2+\epsilon_0^2)^{\frac{1}{2}}}+\frac{1}{(\epsilon_{k''}^2+\epsilon_0^2)^{\frac{1}{2}}}\right\}+\Delta\eta_1\right]. \tag{29}$$

Equation (29) shows that the minimum excitation energy is obtained, when $\epsilon_{k'}$ and $\epsilon_{k''}$ tends to zero.

Therefore $\Delta\eta_1$ and the minimum excitation energy become

$$\underset{\epsilon_k\to 0}{\Delta\eta_1}=\left[-\frac{N(0)V)\hbar\omega}{\left\{1+\left(\frac{\hbar\omega}{\epsilon_0}\right)^2\right\}^{\frac{1}{2}}}+\epsilon_0\right]\Big/\left[N(0)\hbar\omega\left\{1+\left(\frac{\hbar\omega}{\epsilon_0}\right)^2\right\}^{-\frac{1}{2}}-1\right], \tag{30}$$

and

$$\underset{k\to 0}{\Delta W}=\left[\frac{2\epsilon_0}{V}-2N(0)\epsilon_0\left\{\frac{1}{N(0)V}-\left(\frac{\hbar\omega}{\epsilon_0}\right)\left(1+\frac{\hbar^2\omega^2}{\epsilon_0^2}\right)^{-\frac{1}{2}}\right\}\right][V+\Delta\eta_1]. \tag{31}$$

In the case of weak interaction, we find that, by using a relation $\hbar\omega>\epsilon_0$,

$$\Delta\eta_1\cong(1-N(0)V)/N(0) \tag{32}$$

and $$\Delta W\cong 2_0\epsilon\ , \tag{33}$$

which is the same result as the B.C.S.-theoy.

References

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