Bound States Due to Resonance Scattering in Superconductor

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It is shown exactly that the bound state in the energy gap of superconductors is produced by the resonance scattering due to a single non-magnetic impurity.

In an appropriate renormalization procedure, we can show the growth of an impurity band in the case of impurities of finite concentration and a possibility for gapless superconductivity is indicated.

§ 1. Introduction

Since Abrikosov and Gorkov (A-G)\(^5\) discovered the so-called gapless superconductivity in the presence of magnetic impurities, it has been clarified that there are other types of mechanisms responsible for the gapless situation. These are summarized neatly by Maki\(^2\) in the following way:

a) Superconductors in a magnetic field,
b) Spin exchange field,
c) Magnetic impurities,
d) Type II superconductors in high field,
e) A metallic contact.

One can further classify these mechanisms into two categories; one has the bound state in the energy gap in its original situation and it grows to fill the gap, while the other has nothing to do with the bound states. A typical example of the former is the case of c) which A-G treated in the lowest Born approximation. Shiba\(^3\) has shown that the same situation occurs when the superconductor contains the impurity with classical spin.

In this paper we investigate another exactly soluble system which gives a bound state in the energy gap which grows to the impurity band as the concentration of the impurity increases. This new mechanism is caused by the resonance scattering\(^4\) due to localized impurities, though Shiba\(^3\) insists that there should not exist any bound state in this case. Actually, we investigate Anderson model in superconductor with \(U=0\) (\(U\) the Coulomb repulsion) and the effect of \(U\) is considered in the Appendix.

In § 2, a single impurity problem is solved exactly and it is shown that the bound state appears in the energy gap. The investigation of the case of finite concentration is given in § 3 where the growth of an impurity band is discussed and some detailed analysis is given in the final section.
§ 2. Single impurity problem

We consider the system which consists of conduction and localized electrons with mixing interaction in superconductor:

\[ H = \sum_{k \sigma} \epsilon_k C_{k \sigma} C_{k \sigma} + \sum_{k \tau} V_{k \sigma} (C_{k \sigma}^\dagger d_{\tau} + d_{\tau}^\dagger C_{k \sigma}) + E \sum_{\tau} n_{d \tau} - \Delta \sum_{k \tau} (C_{k \tau}^\dagger C_{-k \tau} + C_{-k \tau}^\dagger C_{k \tau}), \]  

(2.1)

where \( C_{k \sigma} (C_{k \sigma}^\dagger) \) and \( d_{\tau} (d_{\tau}^\dagger) \) are annihilation (creation) operators of a conduction electron and a localized electron, respectively. The average \( \Delta \) is the superconducting order parameter which is determined self-consistently by the following equation:

\[ \Delta = |\theta| \sum_{k \tau} \langle C_{k \tau}^\dagger C_{-k \tau} \rangle, \]  

(2.2)

where \( |\theta| \) is the strength of pairing interaction.

It is convenient to treat the problem in the Nambu space. We define in this space the double-time Green’s function:

\[ G_{k \kappa'}(\omega) = \begin{pmatrix} \langle C_{k \tau}^\dagger; C_{k \tau} \rangle & \langle C_{k \tau}^\dagger; C_{-k \tau'} \rangle \\ \langle C_{-k \tau}^\dagger; C_{k \tau'} \rangle & \langle C_{-k \tau}^\dagger; C_{-k \tau'} \rangle \end{pmatrix}. \]  

(2.3)

One can easily solve the equation of motion for the Green function, and obtain the following result (\( \tau_3 \) is the usual Pauli matrix):

\[ G_{k \kappa'}(\omega) = \frac{1}{2\pi} (G^0_{k \kappa'}(\omega) \delta_{k \kappa'} + G^0_{k \kappa'}(\omega) t(\omega) G^0_{k \kappa'}(\omega)), \]  

(2.4)

with

\[ G^0_{k \kappa'}(\omega) = (\omega - \epsilon_k \tau_3 + \Delta \tau_3)^{-1}, \]  

(2.5)

and

\[ t(\omega) = V_{k \kappa}^2 \tau_3 (\omega - E \tau_3 - V_{k \kappa}^2 \tau_3 F(\omega) \tau_3)^{-1} \tau_3, \]  

(2.6)

where

\[ F(\omega) = \sum_k G^0_{k \kappa}(\omega). \]  

(2.7)

For \( |\omega| < \Delta \), Eq. (2.7) is expressed as

\[ V_{k \kappa}^2 F(\omega) = -\Gamma \frac{\omega - \Delta \tau_3}{\sqrt{\Delta^2 - \omega^2}}, \]  

(2.8)

with

\[ \Gamma = \pi \rho V_{k \kappa}, \]  

(2.9)

where \( \rho \) is the density of states at the Fermi surface.

The position of the bound state is determined as the pole of \( t \)-matrix, Eq. (2.6), and therefore, is given by the following equation:
\[ \omega^2 \left( 1 + \frac{2\Gamma}{\sqrt{\Delta^2 - \omega^2}} \right) = E^2 + \Gamma^2. \quad (2.10) \]

It is easily seen that Eq. (2.10) has always two solutions irrespective of the value of \( E \) and \( \Gamma \). Thus, we can conclude that there always exists a bound state in the energy gap.

Next we calculate the change of the transition temperature \( T_c \) in the linear order of the concentration.

For the change of the transition temperature, we must treat the finite concentration of impurities, and average over the positions of impurities. In the linear order of concentration, however, we have only to multiply the \( t \)-matrix of the single impurity given by Eq. (2.6) by the concentration of impurities in the expression of the Green function, Eq. (2.4). Thus, we obtain the expression for \( T_c \) as

\[ \ln \frac{T_{c0}}{T_c} = c \frac{\Gamma}{\rho} Q, \quad (2.11) \]

where \( c \) is the concentration of impurities, and \( T_{c0} \) is the transition temperature of pure BCS superconductor. The function \( Q \) is defined as

\[ Q = T_c \sum_n \frac{1}{|\omega_n|} \left\{ \left( |\omega_n| + \Gamma \right)^2 + E_n^2 \right\}. \quad (2.12) \]

The corresponding expression was obtained for the Anderson model in the Hartree-Fock approximation in the limit of \( c \ll 1 \) and \( U \to 0 \).

\section*{§ 3. Finite concentration problem}

In this section we consider the effect of finite impurity concentration. For this purpose we employ the conventional approximation that the self-energy part \( \Sigma(\omega) \) is connected to the \( t \)-matrix by the following equation:

\[ \Sigma(\omega) = c \tilde{\tau}(\omega), \quad (3.1) \]

where

\[ \tilde{\tau}(\omega) = (\omega - E \tau_3 - V_{kk}^2 \sigma_3 \bar{F}(\omega) \tau_3)^{-1}, \quad (3.2) \]

with

\[ \bar{F}(\omega) = \sum_k \bar{G}_{kk}(\omega). \quad (3.3) \]

Here, \( \bar{G}_{kk}(\omega) \) contains \( \Sigma(\omega) \) and thus, we must determine \( \bar{G}_{kk}(\omega) \) and \( \Sigma(\omega) \) self-
consistently. In order to solve Eqs. (3.1) \sim (3.3), we put
\[ G_{kk'}(\omega) = (\omega - \epsilon_k \tau + \Delta \tau - \Sigma(\omega))^{-1} = (\omega - \epsilon_k \tau + \Delta \tau)^{-1}. \] (3.4)

Then we can easily obtain the self-consistent equation for \( \bar{\omega} \) and \( \bar{\Delta} \) as
\[
\bar{\omega} = \omega - c V_{k \sigma} \left( \omega + \frac{\bar{\omega} \Gamma}{\sqrt{\Delta^2 - \bar{\omega}^2}} \right) \left\{ \omega^2 + \frac{2 \Gamma \omega \bar{\omega}}{\sqrt{\Delta^2 - \bar{\omega}^2}} - (E^2 + \Gamma^2) \right\}^{-1},
\]
\[
\bar{\Delta} = \Delta - c V_{k \sigma} \frac{\bar{\Delta} \Gamma}{\sqrt{\Delta^2 - \bar{\omega}^2}} \left\{ \omega^2 + \frac{2 \Gamma \omega \bar{\omega}}{\sqrt{\Delta^2 - \bar{\omega}^2}} - (E^2 + \Gamma^2) \right\}^{-1}. \] (3.5)

If we introduce auxiliary parameters \( u = \bar{\omega} / \bar{\Delta} \) and \( v = \omega / \Delta \), then Eq. (3.5) reduces to
\[
v = u + \zeta \frac{v}{u^2 + 2 \Gamma (u^2 / \sqrt{1 - u^2}) - \xi^2}, \] (3.6)
where we have defined
\[
\zeta = \frac{1}{\Delta \cdot \tau} = \frac{c}{\bar{\Delta}} V_{k \sigma}, \quad \Gamma = \Gamma / \Delta \]
and
\[
\xi^2 = \left( \frac{E}{\Delta} \right)^2 + \left( \frac{\Gamma}{\Delta} \right)^2. \]
It is a difficult task to solve Eq. (3.6) analytically, but for the small concentration \( c \ll 1 \) or \( \zeta \ll 1 \), we can solve Eq. (3.6) iteratively; for the 0-th iteration we have
\[
v = u,
\]
and then for the first iteration, Eq. (3.6) reduces to
\[
v = u \left( 1 + \zeta \frac{1}{u^2 + 2 \Gamma (u^2 / \sqrt{1 - u^2}) - \xi^2} \right). \] (3.7)
In the following we use Eq. (3.7) in order to find the qualitative feature of the density of states. First we define a function of \( u \) as
\[
\phi(u) = u + \zeta \frac{u}{u^2 + 2 \Gamma (u^2 / \sqrt{1 - u^2}) - \xi^2}. \] (3.8)
The function \( \phi(u) \) has very similar behavior as that defined by Eq. (3.10) in Shiba's paper. We can plot qualitatively the variation of \( \phi(u) \) as represented in Figs. 2 and 3.

Using Figs. 2 and 3, it is easy to obtain the density of state \( N_\sigma(\omega) \) which is given by
and one can get the behavior of $N_s(\omega)$ as shown in Fig. 4.

When the concentration of impurities is further increased we must solve the self-consistent equation (3·6) more rigorously. For this purpose we have examined this equation numerically. The results of our calculation are represented in Figs. 5 and 6 for some typical cases.

Using these values one can obtain the density of states. But we reach essentially the same conclusion as illustrated in Fig. 4.

Here we give a brief discussion about the growth of impurity band. When
there is only one impurity, bound state appears in the gap; as the impurity concentration increases, bound state spreads out in the gap, and on the other hand the edge of the continuum moves toward the outside of the gap. In the case of rather large value of $\xi$ the impurity band touches the bottom of the continuum first, then it fills the rest of the gap as the impurity concentration increases and finally the gapless situation occurs. On the other hand in the case of small value of $\xi$ the impurity band touches at $\omega = 0$, then it fills the rest of the gap and finally the gapless situation occurs.

§ 4. Discussion and conclusion

Effect of resonance scattering on superconductivity has been investigated in some details. First, let us summarize the results obtained in the previous sections:

a) A single “non-magnetic” impurity causes the bound state in the energy gap in the absence of the Coulomb repulsion ($U=0$), irrespective of the values of the energy parameters in the system. Depression of the transition temperature caused by it is rather small.

b) In the case of finite impurity concentration, one can find the growth of impurity band in the energy gap and finally the gapless superconductivity sets in.

Conclusion a) has been reached exactly and we have found another mechanism responsible for the bound state in the energy gap; only exactly soluble model, hitherto known to us, is the classical spin system examined by Shiba.$^8$ When we proceed to generalize an impurity problem to finite concentration problem, one inevitably encounters a renormalization procedure due to randomly distributed many impurities. Then we have employed an appropriate method of renormalization and found the growth of impurity band in the energy gap. Though the relation between $v$ and $u$ (Eq. (3·6)) is very complicated in comparison with that of A-G theory$^3$ and of Shiba,$^9$ one can observe essentially the same growing process of the impurity band. The difference of the self-consistent equation will affect the shape of the band, but do not alter the process of the growth itself qualitatively. As one can see from Fig. 4, the original bound state grows with increasing value of $\zeta$ to form an impurity band and at last we encounter the gapless situation. The next problem one must inquire is the effect of the Coulomb repulsion, $U$, at the impurity site between opposite spin electrons; to take into account this effect within Hartree-Fock approximation is not so difficult and a single impurity case is investigated in the Appendix, where it is shown
that the presence of $U$ does not affect the essential feature of a single impurity problem so that we have the bound state in general cases.

In this way we have investigated the effects of resonance scattering on superconductivity and obtained the results which contradicts a general belief that there exist no bound states in the resonance model for superconductors.

Before concluding this paper, it should be noted that the low temperature properties of the magnetic impurity system reveal entirely the same physical behaviors as those discussed here and this system is discussed in a separate paper.

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Appendix

Effect of the Coulomb correlation is examined briefly in this appendix within Hartree-Fock approximation. In this case we treat the system given by

$$\hat{\mathcal{H}} = \mathcal{H} - \Delta_0 (d^+_r d^+_l + d^+_l d^+_r),$$

where $\mathcal{H}$ is the Hamiltonian represented by Eq. (2.1) and the average $\Delta_0$ is defined as

$$\Delta_0 = - U \langle d^+_r d^+_l \rangle,$$

which takes the negative value. Following the same procedure as in §2, we obtain the $t$-matrix:

$$t(\omega) = V_{k \sigma}^2 (\omega - E_{\sigma} \tau + \Delta_0 \tau - V_{k \sigma}^2 F(\omega) \tau)^{-1} \tau,$$

where $E_{\sigma}$ is of the form

$$E_{\sigma} = E + U \langle n_{\sigma} \rangle,$$

and the equation which determines the bound state is given by

$$\omega^2 \left( 1 + \frac{2 \Gamma}{\sqrt{\Delta^2 - \omega^2}} \right)^{-1} - 2 \Gamma \frac{\Delta_0 A}{\sqrt{\Delta^2 - \omega^2}} = E_{\sigma}^2 + \Gamma^2 + \Delta_0^2.$$

Examination on this equation reveals that there always exists a bound state in the energy gap.

Thus we have arrived at the same conclusion as that derived in §2.

References

6) K. Machida and F. Shibata, to be published.