Role of potential scattering in the Shiba-Rusinov theory of the magnetic impurities in superconductors

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The Shiba-Rusinov theory of magnetic impurities in a superconductor is investigated, with special attention paid to the role of the potential scattering term in the electron-impurity interaction. The meaning of Anderson's theorem in the Shiba-Rusinov theory is discussed.

I. INTRODUCTION

About 15 years ago Shiba[1] and Rusinov[2] independently gave a theory of a low concentration of uncorrelated magnetic impurities in a superconductor. The Shiba-Rusinov (SR) theory is a generalization of the well-known Abrikosov-Gor'kov[3] (AG) theory. In the AG model the interaction between a conduction electron and a magnetic impurity is assumed weak and the lowest-order Born approximation is used to treat the scattering. The results of the AG theory are known to be valid for the rare-earth (except cerium) impurities in superconductors. In the SR model the scattering is calculated exactly for a single impurity problem by treating the impurity spin classically. This theory shows not only the existence of bound states within the Bardeen-Cooper-Schrieffer (BCS) energy gap but also modifies the thermodynamic and the transport properties. Several properties of the superconducting alloy in the SR model have been calculated by Nagi and collaborators,[4] and Ginsberg and collaborators.[5] The results of the SR model apply to the transition-metal impurities in superconductors. Recently an extension of the SR theory to include strong electron-phonon coupling has been made by Schachinger.[6]

Now the interaction of a conduction electron of spin μ with a paramagnetic impurity atom of spin $\vec{S}$ is given by

$$U_{\mu\mu'}=V\delta_{\mu\mu'}-\tfrac{1}{2}J\vec{S}\cdot\vec{\sigma}_{\mu\mu'}\ , \tag{1.1}$$

where $\vec{\sigma}$ is the Pauli-spin matrix vector, and V and J, respectively, are the strengths of the potential interaction and the exchange interaction. In the AG theory the thermodynamic properties do not depend on V. This fact is sometimes called Anderson's theorem,[7] which can be stated in a more general form[8]: The thermodynamic properties of superconductors remain unchanged in the presence of a static external perturbation which does not break the time-reversal symmetry. On the other hand, in the SR theory the role of the potential scattering has not been clearly recognized in literature. One of the purposes of this paper is to clarify the roles of the two parts of the interaction potential in the scattering process. This is especially important, for example, in the discussion of the gap anisotropy problem, where the potential scattering plays an important role.

The results of Shiba[1] and Rusinov[2] are identical for $V=0$, but these differ when $V\neq 0$. For the T matrix, one may compare Eq. (4.2) of Ref. 1 with Eq. (11) of Ref. 2. Because of this reason, we restudy the T-matrix problem briefly. We follow the method outlined by Müller-Hartmann[9] to study the Kondo problem. Since the single classical spin problem is exactly solvable, one may use a more direct method. However, we prefer the procedure given in Ref. 9 because it has several advantages in the quantum case.

II. T MATRIX FOR A SINGLE IMPURITY

We use a 4×4 matrix Green's function (see Ref. 1 for notation)

$$G_{\vec{k}\vec{k}'}=\langle\langle A_{\vec{k}};A^\dagger_{\vec{k}'}\rangle\rangle_\omega\ , \tag{2.1}$$

where

$$A^\dagger_{\vec{k}}=(a^\dagger_{\vec{k}\uparrow},a^\dagger_{\vec{k}\downarrow},a_{-\vec{k}\uparrow},a_{-\vec{k}\downarrow}) \tag{2.2}$$

and $A_{\vec{k}}$ is its conjugate. Here $a^\dagger_{\vec{k}\mu}$ represents the creation operator for a conduction electron. The BCS Green's function is

$$G^0_{\vec{k}}=(\omega-\epsilon_{\vec{k}}\rho_3-\Delta\rho_2\sigma_2)^{-1}\ , \tag{2.3}$$

where $\epsilon_{\vec{k}}$ is the energy of the conduction electron measured from the Fermi level, σ_i and ρ_i $(i=1,2,3)$ are Pauli-spin matrices operating on ordinary spin states and the electron-hole spin states, and Δ is the superconducting order parameter

$$\Delta=\frac{\lambda}{N}\sum_{\vec{k}}\langle a_{-\vec{k}\downarrow}a_{\vec{k}\uparrow}\rangle\ , \tag{2.4}$$

with λ as the BCS interaction constant and N as the number of atomic cells.

We consider a single impurity for which interaction is given by Eq. (1.1). Following the procedure given in Ref. 9 and modifying it to the 4×4 notation, we obtain

$$G_{\vec{k}\vec{k}'}=G^0_{\vec{k}}\delta_{\vec{k}\vec{k}'}+G^0_{\vec{k}}TG^0_{\vec{k}'} \tag{2.5}$$

with the T matrix

$$T=\frac{V}{N}\rho_3(1-F_V\rho_3)^{-1}+\frac{J}{4N}(1-\rho_3F_V)^{-1}\hat{t}(1-F_V\rho_3)^{-1}\ . \tag{2.6}$$

We have used the notations

$$F_X=\frac{X}{N}\sum_{\vec{l}}G^0_{\vec{l}}=-\pi N(0)X\left[\frac{\omega+\Delta\rho_2\sigma_2}{(\Delta^2-\omega^2)^{1/2}}\right]\quad(X=V,J) \tag{2.7}$$

$$\hat{t}=\frac{J}{N}\sum_{\vec{1},\vec{1}'}T_{\vec{1}\vec{1}'} , \tag{2.8}$$

where $T_{\vec{k}\vec{k}'}$ is defined by

$$T_{\vec{k}\vec{k}'}=\langle\langle(\vec{S}\cdot\vec{\alpha})A_{\vec{k}};A^{\dagger}_{\vec{k}'}(\vec{S}\cdot\vec{\alpha})\rangle\rangle_{\omega} \tag{2.9}$$

with

$$\vec{\alpha}=\frac{1+\rho_3}{2}\vec{\sigma}+\frac{1-\rho_3}{2}\sigma_2\vec{\sigma}\sigma_2 , \tag{2.10}$$

and $N(0)$ is the density of single-particle states at the Fermi level in the normal metal. Here we have considered the Green's function as $[G_{\vec{k}\vec{k}'}(\vec{S})+G_{\vec{k}\vec{k}'}(-\vec{S})]/2$. This is justified in the absence of a magnetic field.

For a quantum spin the above equations are not closed, so that a decoupling procedure or other techniques are necessary to solve the problem. For a classical spin, however, we can solve the T matrix exactly. Introducing the unitary matrix[10]

$$M=\frac{1+\rho_3}{2}-\frac{1-\rho_3}{2}i\sigma_2 , \tag{2.11}$$

Eq. (2.9) is rewritten as

$$\begin{aligned}T_{\vec{k}\vec{k}'}&=(\vec{S}\cdot\vec{\alpha})G_{\vec{k}\vec{k}'}(\vec{S}\cdot\vec{\alpha})\\&=M(\vec{S}\cdot\vec{\sigma})M^{\dagger}G_{\vec{k}\vec{k}'}M(\vec{S}\cdot\vec{\sigma})M^{\dagger}\\&=M(\vec{S}\cdot\vec{\sigma})^2M^{\dagger}G_{\vec{k}\vec{k}'}\\&=S^2G_{\vec{k}\vec{k}'} ,\end{aligned} \tag{2.12}$$

where we have taken $\vec{S}$ as a classical vector and have also used the fact that $(\vec{S}\cdot\vec{\sigma})$ commutes with $M^{\dagger}G_{\vec{k}\vec{k}'}M$.

Inserting Eqs. (2.12) and (2.5) into Eq. (2.8) we find that $\hat{t}$ satisfies the following equation:

$$\hat{t}=S^2F_J(1-\rho_3F_V)^{-1}[1+\tfrac{1}{4}\hat{t}(1-F_V\rho_3)^{-1}F_J] \tag{2.13}$$

which can be readily solved. Substituting the solution of Eq. (2.13) into Eq. (2.6), we obtain

$$T=\frac{1}{N\pi N(0)}\frac{1}{D}\left[-\frac{\omega}{(\Delta^2-\omega^2)^{1/2}}t_1+\frac{\Delta}{(\Delta^2-\omega^2)^{1/2}}t_2\rho_2\sigma_2+t_3\rho_3\right] , \tag{2.14}$$

where

$$t_1=v^2(1+v^2)+j^2(1-2v^2)+j^4 , \tag{2.15a}$$

$$t_2=v^2(1+v^2)-j^2(1+2v^2)+j^4 , \tag{2.15b}$$

$$t_3=v(1+v^2-j^2) , \tag{2.15c}$$

$$D=(1+v^2)^2-2j^2\left[\frac{\Delta^2+\omega^2}{\Delta^2-\omega^2}+v^2\right]+j^4 , \tag{2.16}$$

with $j=(JS/2)\pi N(0)$, $v=V\pi N(0)$.

Using the notation

$$\tan\delta_0^{\pm}=v\pm j \tag{2.17}$$

where $\delta_0^{\pm}$ are the scattering phase shifts for an electron of spin $\pm\frac{1}{2}$, we can easily show that our T matrix is identical with the one given in Ref. 2. On the other hand, it is different from that of Ref. 1.

The position of the bound state within the BCS energy gap for the one-impurity problem is obtained from the poles of the T matrix given in Eq. (2.14). The energy of the two bound states, $\pm\omega_B$, is given by

$$\epsilon_0^2=\frac{(1+v^2-j^2)^2}{(1+v^2-j^2)^2+4j^2} , \tag{2.18}$$

where

$$\epsilon_0=\omega_B/\Delta . \tag{2.19}$$

One may note that $|\epsilon_0|\leq 1$. When $v=0$, Eq. (2.18) reduces to

$$\epsilon_{00}^2=\left[\frac{1-j^2}{1+j^2}\right]^2 . \tag{2.20}$$

However, ϵ_0 depends on v generally. It is worthwhile to note that Eq. (2.18) can be written in the form

$$\epsilon_0^2=\left[\frac{1-j_{\text{eff}}^2}{1+j_{\text{eff}}^2}\right]^2 \tag{2.21}$$

with

$$j_{\text{eff}}^2=\frac{1}{2j^2}\{(1+v^2-j^2)^2+2j^2\pm(1+v^2-j^2)[(1+v^2-j^2)^2+4j^2]^{1/2}\} . \tag{2.22}$$

The double signs in Eq. (2.22) come from the fact that Eq. (2.21) is symmetric between j_{eff}^2 and $1/j_{\text{eff}}^2$.

III. FINITE CONCENTRATION PROBLEM AND ANDERSON THEOREM

Now let the concentration of magnetic impurities in the superconductor be finite. We assume that the impurities are randomly distributed and their concentration n_i is low enough so that the impurity-impurity interaction is negligible. Since our discussion is essentially the same as Ref. 2, we quote merely the results. The Green's function averaged over the positions and the spin directions of the impurities is written as

$$\bar{G}_{\vec{k}}=(\tilde{\omega}-\tilde{\epsilon}_{\vec{k}}\rho_3-\tilde{\Delta}\rho_2\sigma_2)^{-1} . \tag{3.1}$$

The quantities $\tilde{\omega}$, $\tilde{\Delta}$, and $\tilde{\epsilon}_{\vec{k}}$ satisfy the equations

$$\tilde{\omega}=\omega+\Gamma_1\frac{U(1-U^2)^{1/2}}{(\epsilon_0^2-U^2)} , \tag{3.2}$$

$$\tilde{\Delta}=\Delta+\Gamma_2\frac{(1-U^2)^{1/2}}{(\epsilon_0^2-U^2)} , \tag{3.3}$$

$$\tilde{\epsilon}_{\vec{k}}=\epsilon_{\vec{k}}+\Gamma_3\frac{(1-U^2)}{(\epsilon_0^2-U^2)} , \tag{3.4}$$

where we have used

$$U=\tilde{\omega}/\tilde{\Delta} \tag{3.5}$$

and

$$\Gamma_m = \bar{n}_i \frac{t_m}{(1+v^2-j^2)^2+4j^2} \quad (m=1,2,3) \tag{3.6}$$

with

$$\bar{n}_i = \frac{n_i}{\pi N(0)} . \tag{3.7}$$

For isotropic superconductors, thermal and transport properties are obtainable from the knowledge of the function U. An equation for U can be written from Eqs. (3.2) and (3.3), and is

$$\frac{\omega}{\Delta} = U \left[1 - \frac{\alpha(1-U^2)^{1/2}}{\epsilon_0^2 - U^2} \right] , \tag{3.8}$$

where

$$\alpha = (\Gamma_1 - \Gamma_2)/\Delta . \tag{3.9}$$

It may be noted that $(\Gamma_1 - \Gamma_2)$ can be expressed in a simple scaled form

$$\Gamma_1 - \Gamma_2 = \bar{n}_i f(\epsilon_0) \tag{3.10}$$

with

$$f(\epsilon_0) = \tfrac{1}{2}(1-\epsilon_0^2) . \tag{3.11}$$

In the presence of potential scattering, the energy of bound states is a function of both j and v [see Eq. (2.18)], so that all the properties do depend on v in the SR theory. However, the dependence on v is only through ϵ_0 [see Eq. (3.10)]. This fact may be considered as the extended Anderson theorem in the SR theory.

In some cases, such as superconductors with energy-gap anisotropy, the term $\Gamma_1 + \Gamma_2$ also plays a part. Contrary to $\Gamma_1 - \Gamma_2$, the quantity $\Gamma_1 + \Gamma_2$ cannot be written in a scaled form like Eq. (3.10). The only exception is when $v=0$. However, this is a consequence of the fact that there is only one parameter j in this case.

IV. SUMMARY AND DISCUSSION

We have studied the paramagnetic impurities in a superconductor treating the impurity spin classically. A special attention has been given to the role of the potential scattering term V of Eq. (1.1). In order to clarify the difference between the results of Shiba[1] and Rusinov[2] for $V \neq 0$, we have restudied the T matrix for the scattering from a single impurity. Our T matrix and, therefore, all the properties which follow from it are shown to be identical to Ref. 2. Although we have only considered the s-wave scattering in this paper, the other partial waves can be easily included in our analysis.

In the SR theory the potential scattering term V appears in the U equation, Eq. (3.8). This is contrary to the AG theory in which the V dependence is completely canceled out. The essential feature of the role of the potential scattering in the SR theory is that the dependences on V and J can be expressed in terms of one parameter ϵ_0, the bound-state energy. Equation (3.10) is the mathematical expression for this statement. In isotropic superconductors, one cannot obtain the information on V and J separately. All we can get is ϵ_0 [Eq. (2.18)] or, in other words, j_{eff} [Eq. (2.22)].

When there is an anisotropy in the energy gap, the potential scattering V plays a role even in the AG theory. Therefore, it is of great interest to investigate the impurity effect on anisotropic superconductors. This problem is studied in the following paper.

Note added in proof. Very recently, Professor H. Shiba informed us that he had noticed the error in Eq. (4.2) of Ref. 1. His corrected T matrix agrees with our Eq. (2.14). We thank Professor Shiba for his letter.

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[1] H. Shiba, Prog. Theor. Phys. 40, 435 (1968).

[2] A. I. Rusinov Zh. Eksp. Teor. Fiz. 56, 2047 (1969) [Sov. Phys.—JETP 29, 1101 (1969)].

[3] A. A. Abrikosov and L. P. Gor'kov, Zh. Eksp. Teor. Fiz. 39, 1781 (1960) [Sov. Phys.—JETP 12, 1243 (1961)].

[4] A. N. Chaba and A. D. S. Nagi, Can. J. Phys. 50, 1736 (1972); B. Leon and A. D. S. Nagi, J. Phys. F 5, 1533 (1975); S. C. Lo and A. D. S. Nagi, Phys. Rev. B 9, 2090 (1974); B. Sihota and A. D. S. Nagi, J. Low Temp. Phys. 43, 217 (1981); 51, 347 (1983).

[5] D. M. Ginsberg, Phys. Rev. B 20, 960 (1979); A. B. Kunz and D. M. Ginsberg, *ibid.* 22, 3165 (1980); T. R. Lemberger, D. M. Ginsberg, and G. Rickayzen, *ibid.* 18, 6057 (1978); 22, 4527 (1980).

[6] E. Schachinger, Z. Phys. B 47, 217 (1982).

[7] P. W. Anderson, J. Phys. Chem. Solids 11, 26 (1959).

[8] K. Maki, in *Superconductivity,* edited by R. D. Parks (Dekker, New York, 1969), Vol. 2, pp. 1035–1105.

[9] E. Müller-Hartmann, in *Magnetism,* edited by H. Suhl (Academic, New York, 1973), Vol. 5, pp. 353–382.

[10] L. P. Gor'kov and A. I. Rusinov, Zh. Eksp. Teor. Fiz. 46, 1363 (1964) [Sov. Phys.—JETP 19, 922 (1964)].