

## Self-Consistent Treatment of Kondo's Effect in Dilute Alloys\*

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We investigate how conduction electrons in dilute alloys are affected by the exchange interaction with localized spins of impurities. It is shown that, if the interaction is antiferromagnetic, the perturbational treatment breaks down below a critical temperature, and that near the Fermi surface there appears a quasi-bound state between the conduction-electron spin and the localized spin. Because of the appearance of this quasibound state, the resistivity increases with decreasing temperature, but has a finite value at  $T=0$ . There is no logarithmic term in the resistivity at low temperatures, in contrast to Kondo's theory of the resistance minimum. There also appears an anomaly in the specific heat at low temperatures.

### 1. INTRODUCTION

MANY authors<sup>1</sup> have investigated how conduction electrons are affected by the exchange interaction with localized spins of impurities, i.e., by the so-called  $s$ - $d$  exchange interaction in connection with various properties of dilute alloys such as Cu-Mn alloy. Recently Kondo<sup>2</sup> explained the phenomenon of the resistance minimum in dilute alloys by this interaction. Calculating the transition probability of conduction electrons to the third order of the interaction, he showed that the transition probability has a logarithmic anomaly at the Fermi surface, and that in the resistivity there appears a term proportional to  $\ln T$ . According to Kondo, the resistance has a minimum at low temperature if the interaction is negative (antiferromagnetic). The theory is in good agreement with experiments.

From the theoretical point of view, however, there remains an essential difficulty in Kondo's theory; the lifetime of conduction electrons obtained by perturbation diverges at the Fermi surface in the third order [see Eq. (17) of Ref. 2], and, as will be shown later, even becomes negative if higher order terms are taken into account. This means that the perturbational treatment breaks down there, and that the unperturbed state of conduction electrons becomes unstable.

The situation seems to be quite similar to the case of superconductivity,<sup>3</sup> in which the perturbational treatment breaks down at the transition temperature. From the similarity between the two cases it is reasonable to expect that, in the case of dilute alloys, there appears some correlated state, or a kind of bound state, between localized spin and conduction-electron spin at low temperatures corresponding to the Cooper pair. In the theory of superconductivity, we solve the problem in a self-consistent way, taking into account the correlation between electrons. Similarly in solving our problem of dilute alloys we have to take into account the correlation

between localized spin and conduction-electron spin. Naturally there is also an essential difference between these two cases, i.e., in our problem one of the interacting particles is localized at the impurity site, and so the interaction does not conserve momentum. Therefore, some results, for example the energy spectrum of conduction electrons, are expected to be quite different from those in the case of superconductivity.

In this paper we shall investigate, by a method similar to the theory of superconductivity, how the conduction-electron states are modified by the  $s$ - $d$  exchange interaction, by taking a very simplified model for dilute alloys. In Sec. 2, the problem is formulated and some approximations are introduced. It is shown, in Sec. 3, that the usual perturbational treatment breaks down at low temperatures if the interaction is antiferromagnetic. In Sec. 4 the problem is solved in a self-consistent way for the case of antiferromagnetic interaction, and it is found that at low temperatures there appears a quasi-bound state between the localized spin and the conduction-electron spin. In Sec. 5 the resistivity and the specific heat of dilute alloys at low temperatures are calculated using the results obtained in Sec. 4. Some discussions are given in the last section.

### 2. FORMULATION AND APPROXIMATION

Let us consider a system of conduction electrons and an impurity on which a magnetic moment is localized. The so-called  $s$ - $d$  exchange interaction acts between the conduction electrons and the localized moment. The Hamiltonian of the system is given by

$$H = \sum_{\mathbf{k}\sigma} \epsilon_{\mathbf{k}} C_{\mathbf{k}\sigma}^\dagger C_{\mathbf{k}\sigma} - \frac{J}{2N} \sum_{\mathbf{k}\mathbf{k}'} \{ (C_{\mathbf{k}\uparrow}^\dagger C_{\mathbf{k}'\uparrow} - C_{\mathbf{k}\downarrow}^\dagger C_{\mathbf{k}'\downarrow}) \times S_z + C_{\mathbf{k}\uparrow}^\dagger C_{\mathbf{k}'\downarrow} S_- + C_{\mathbf{k}\downarrow}^\dagger C_{\mathbf{k}'\uparrow} S_+ \}, \quad (2.1)$$

where  $C_{\mathbf{k}\sigma}^\dagger$  and  $C_{\mathbf{k}\sigma}$  are the usual creation and annihilation operators of the conduction electron with wave vector  $\mathbf{k}$  and spin  $\sigma$ ,  $\epsilon_{\mathbf{k}}$  is its one-electron energy,  $S_z$  and  $S_\pm$  are the components of the spin operator associated with the impurity.  $N$  is the total number of atoms in the crystal and  $J$  is the strength of the exchange interaction which is assumed to be independent of  $k$  and  $k'$ . In the

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<sup>1</sup> For example, K. Yosida, Phys. Rev. **106**, 893 (1957).

<sup>2</sup> J. Kondo, Progr. Theoret. Phys. (Kyoto) **32**, 37 (1964).

<sup>3</sup> J. Bardeen, L. N. Cooper, and J. R. Schrieffer, Phys. Rev. **108**, 1175 (1957).

following calculations, we assume that  $J$  is small so that  $|J|\rho/N \ll 1$ ,  $\rho$  being the density of state of the conduction electrons at the Fermi surface, and we consider the case  $S = \frac{1}{2}$  for simplicity.

To investigate the effect of this exchange interaction on conduction electrons, we use the method of the retarded double-time Green's function,<sup>4</sup> which is defined by

$$\langle A|B \rangle_t = -i \langle [A(t), B(0)]_+ \rangle \quad \text{for } t > 0, \\ = 0 \quad \text{for } t < 0; \quad (2.2)$$

where  $\langle \rangle$  denotes the statistical average,  $A$  and  $B$  being operators. Its Fourier transform is given by

$$\langle A|B \rangle_\omega = \frac{1}{2\pi} \lim_{\eta \rightarrow 0^+} \int_{-\infty}^{\infty} \langle A|B \rangle_t e^{i\omega t - \eta t} dt. \quad (2.3)$$

In the following we suppress the suffix  $\omega$  of the Fourier transforms for simplicity. Using  $\langle A|B \rangle$ , we can obtain the average  $\langle BA \rangle$  by the formula

$$\langle BA \rangle = \int_{-\infty}^{\infty} \{-2 \operatorname{Im} \langle A|B \rangle\} f(\omega) d\omega, \quad (2.4)$$

with

$$f(\omega) = 1/(e^{\omega/T} + 1). \quad (2.5)$$

Here we took  $\hbar = 1$  and Boltzmann constant  $k_B = 1$ .

Introducing

$$G_{kk'}(\omega) = \langle C_{k'\uparrow} | C_{k\uparrow}^\dagger \rangle \quad (2.6)$$

$$\Gamma_{kk'}(\omega) = \langle C_{k'\uparrow} S_z + C_{k'\downarrow} S_- | C_{k\uparrow}^\dagger \rangle, \quad (2.7)$$

we set up the equations of motion to be satisfied by these functions in the usual way.<sup>4</sup> We have

$$(\omega - \xi_{k'}) G_{kk'}(\omega) + (J/2N) \sum_1 \Gamma_{k1}(\omega) = (1/2\pi) \delta_{kk'}, \quad (2.8)$$

$$(\omega - \xi_{k'}) \langle C_{k'\uparrow} S_z | C_{k\uparrow}^\dagger \rangle + (J/2N) \sum_1 \{ \langle C_{1\uparrow} S_z^2 | C_{k\uparrow}^\dagger \rangle + \frac{1}{2} \langle C_{1\downarrow} S_- | C_{k\uparrow}^\dagger \rangle \} \\ + (J/2N) \sum_{11'} \{ - \langle C_{k'\uparrow} C_{1\uparrow}^\dagger C_{1'\downarrow} S_- | C_{k\uparrow}^\dagger \rangle + \langle C_{k'\uparrow} C_{1\downarrow}^\dagger C_{1'\uparrow} S_+ | C_{k\uparrow}^\dagger \rangle \} = (1/2\pi) \langle S_z \rangle \delta_{kk'}, \quad (2.9)$$

$$(\omega - \xi_{k'}) \langle C_{k'\downarrow} S_- | C_{k\uparrow}^\dagger \rangle + (J/2N) \sum_1 \{ \frac{3}{4} \langle C_{1\uparrow} | C_{k\uparrow}^\dagger \rangle - \langle C_{1\uparrow} S_z^2 | C_{k\uparrow}^\dagger \rangle + \frac{1}{2} \langle C_{1\downarrow} S_- | C_{k\uparrow}^\dagger \rangle + \langle C_{1\uparrow} S_z | C_{k\uparrow}^\dagger \rangle \} \\ + (J/2N) \sum_{11'} \{ \langle C_{k'\downarrow} C_{1\uparrow}^\dagger C_{1'\uparrow} S_- | C_{k\uparrow}^\dagger \rangle - \langle C_{k'\downarrow} C_{1\downarrow}^\dagger C_{1'\downarrow} S_- | C_{k\uparrow}^\dagger \rangle - 2 \langle C_{k'\downarrow} C_{1\downarrow}^\dagger C_{1'\uparrow} S_z | C_{k\uparrow}^\dagger \rangle \} = 0, \quad (2.10)$$

where  $\xi_k = \epsilon_k - \epsilon_F$ , with  $\epsilon_F$  denoting the Fermi energy, and use has been made of the following relations which are valid for  $S = \frac{1}{2}$ :

$$S_\pm S_z = \mp \frac{1}{2} S_\pm, \quad S_z S_\pm = \pm \frac{1}{2} S_\pm, \quad S_+ S_- = \frac{3}{4} + S_z - S_z^2. \quad (2.11)$$

To solve Eqs. (2.9)–(2.11), we must approximate higher order Green's functions appearing in Eqs. (2.10) and (2.11). We shall take an approximation in which some combination of operators is replaced by its average value. In doing so, we should notice that only the average of such combinations that conserve the total spin does not vanish. For example  $\langle C_{k\uparrow}^\dagger C_{k'\uparrow} S_+ \rangle$  should vanish, but  $\langle C_{k\uparrow}^\dagger C_{k'\uparrow} S_z \rangle$  should not. Thus we put

$$\langle C_{k'\uparrow} C_{1\uparrow}^\dagger C_{1'\downarrow} S_- | C_{k\uparrow}^\dagger \rangle = \langle C_{k'\uparrow} C_{1\uparrow}^\dagger \rangle \langle C_{1'\downarrow} S_- | C_{k\uparrow}^\dagger \rangle + \langle C_{1\uparrow}^\dagger C_{1'\downarrow} S_- \rangle \langle C_{k'\uparrow} | C_{k\uparrow}^\dagger \rangle, \quad (2.12a)$$

$$\langle C_{k'\uparrow} C_{1\downarrow}^\dagger C_{1'\uparrow} S_+ | C_{k\uparrow}^\dagger \rangle = \langle C_{1\downarrow}^\dagger C_{1'\uparrow} S_+ \rangle \langle C_{k'\uparrow} | C_{k\uparrow}^\dagger \rangle - \langle C_{1\downarrow}^\dagger C_{k'\uparrow} S_+ \rangle \langle C_{1'\uparrow} | C_{k\uparrow}^\dagger \rangle, \quad (2.12b)$$

$$\langle C_{k'\downarrow} C_{1\uparrow}^\dagger C_{1'\uparrow} S_z | C_{k\uparrow}^\dagger \rangle = \langle C_{k'\downarrow} C_{1\uparrow}^\dagger \rangle \langle C_{1'\uparrow} S_z | C_{k\uparrow}^\dagger \rangle - \langle C_{1\uparrow}^\dagger C_{k'\downarrow} S_z \rangle \langle C_{1'\uparrow} | C_{k\uparrow}^\dagger \rangle, \quad (2.12c)$$

$$\langle C_{k'\downarrow} C_{1\downarrow}^\dagger C_{1'\downarrow} S_- | C_{k\uparrow}^\dagger \rangle = \langle C_{1\downarrow}^\dagger C_{1'\downarrow} S_- \rangle \langle C_{k'\downarrow} | C_{k\uparrow}^\dagger \rangle + \langle C_{k'\downarrow} C_{1\downarrow}^\dagger \rangle \langle C_{1'\downarrow} S_- | C_{k\uparrow}^\dagger \rangle. \quad (2.12d)$$

This approximation is quite similar to the approximation used by Zubarev<sup>5</sup> in his treatment of superconductivity by the use of the double-time Green's function, which gives the Bardeen-Cooper-Schrieffer (BCS) results. The approximation is reasonable and seems to be the simplest way to take into account the correlation between the conduction electrons and the localized spin in the calculation. The averaged quantities of the type  $\langle C^\dagger C S \rangle$ , which are closely related to the correlated spin polarization of the conduction electrons around the impurity, play an important role in our treatment.

Now it is easy to see that the average values appearing in Eqs. (2.12) are connected with each other by the following relations which come from the symmetry of the system:

$$\langle C_{1\uparrow}^\dagger C_{1'\uparrow} \rangle = \langle C_{1\downarrow}^\dagger C_{1'\downarrow} \rangle, \\ \langle C_{1\uparrow}^\dagger C_{1'\downarrow} S_- \rangle = \langle C_{1\downarrow}^\dagger C_{1'\uparrow} S_+ \rangle = 2 \langle C_{1\uparrow}^\dagger C_{1'\uparrow} S_z \rangle \\ = -2 \langle C_{1\downarrow}^\dagger C_{1'\downarrow} S_z \rangle. \quad (2.13)$$

Further, we have  $\langle S_z \rangle = 0$ .<sup>6</sup>

By the use of the approximation (2.12) and the relation (2.13), the equation of motion for  $\Gamma_{kk'}(\omega)$  can be ob-

<sup>4</sup> D. N. Zubarev, Usp. Fiz. Nauk **71**, 71 (1960) [English transl.: Soviet Phys.—Uspekhi **3**, 320 (1960)].

<sup>5</sup> See Sec. 6 of Ref. 4.

<sup>6</sup> It must be remarked here again that  $\langle \rangle$  means the statistical average, and not the expectation value at one of the degenerate ground states. Therefore, even if there exists a localized spin,  $\langle S_z \rangle$  should vanish while  $\langle S_z^2 \rangle$  should not.

tained from Eqs. (2.9) and (2.10) as

$$(\omega - \xi_{k'})\Gamma_{kk'}(\omega) + \frac{J}{N}(n_{k'} - \frac{1}{2})\sum_1 \Gamma_{k1}(\omega) + \frac{J}{2N}(\frac{3}{4} - m_{k'})\sum_1 G_{k1}(\omega) = 0, \quad (2.14)$$

where

$$n_{k'} = \sum_1 \langle C_{1\uparrow}^\dagger C_{k'\uparrow} \rangle, \quad (2.15)$$

$$m_{k'} = 3 \sum_1 \langle C_{1\uparrow}^\dagger C_{k'\downarrow} S_- \rangle. \quad (2.16)$$

Equations (2.8) and (2.14) are to be compared with Eq. (6.14) of Ref. 4.

Now that we have obtained a set of simultaneous equations for  $G_{kk'}(\omega)$  and  $\Gamma_{kk'}(\omega)$ , i.e., Eqs. (2.8) and (2.14), it is easy to solve them, and the solutions are found to be

$$G_{kk'}(\omega) = \frac{1}{2\pi} \left\{ \frac{\delta_{kk'}}{\omega - \xi_k} - \frac{J^2}{4N} \frac{1}{(\omega - \xi_k)(\omega - \xi_{k'})} \times \frac{\Gamma(\omega)}{1 + JG(\omega) + \frac{1}{4}J^2F(\omega)\Gamma(\omega)} \right\}, \quad (2.17)$$

$$\Gamma_{kk'}(\omega) = \frac{1}{2\pi} \frac{J}{2N} \frac{1}{(\omega - \xi_k)(\omega - \xi_{k'})} \times \frac{(m_{k'} - \frac{3}{4})[1 + JG(\omega)] - (n_{k'} - \frac{1}{2})J\Gamma(\omega)}{1 + JG(\omega) + \frac{1}{4}J^2F(\omega)\Gamma(\omega)}, \quad (2.18)$$

where

$$F(\omega) = \frac{1}{N} \sum_{\mathbf{k}} \frac{1}{\omega - \xi_{\mathbf{k}}}, \quad (2.19)$$

$$G(\omega) = \frac{1}{N} \sum_{\mathbf{k}} \frac{n_{\mathbf{k}} - \frac{1}{2}}{\omega - \xi_{\mathbf{k}}}, \quad (2.20)$$

$$\Gamma(\omega) = \frac{1}{N} \sum_{\mathbf{k}} \frac{m_{\mathbf{k}} - \frac{3}{4}}{\omega - \xi_{\mathbf{k}}}; \quad (2.21)$$

or, introducing

$$G_{\mathbf{k}}(\omega) = \sum_{k'} G_{k'\mathbf{k}}(\omega), \quad (2.22)$$

$$\Gamma_{\mathbf{k}}(\omega) = \sum_{k'} \Gamma_{k'\mathbf{k}}(\omega), \quad (2.23)$$

we have

$$G_{\mathbf{k}}(\omega) = \frac{1}{2\pi} \frac{1}{\omega - \xi_{\mathbf{k}}} \frac{1 + JG(\omega)}{1 + JG(\omega) + \frac{1}{4}J^2F(\omega)\Gamma(\omega)} \quad (2.24)$$

$$\Gamma_{\mathbf{k}}(\omega) = \frac{1}{4\pi} \frac{JF(\omega)}{\omega - \xi_{\mathbf{k}}} \frac{(m_{\mathbf{k}} - \frac{3}{4})[1 + JG(\omega)] - (n_{\mathbf{k}} - \frac{1}{2})J\Gamma(\omega)}{1 + JG(\omega) + \frac{1}{4}J^2F(\omega)\Gamma(\omega)}. \quad (2.25)$$

By the use of Eq. (2.4),  $n_{\mathbf{k}}$  and  $m_{\mathbf{k}}$  are obtained from

$$n_{\mathbf{k}} = \int_{-\infty}^{\infty} \{-2 \operatorname{Im} G_{\mathbf{k}}(\omega)\} f(\omega) d\omega, \quad (2.26)$$

$$m_{\mathbf{k}} = \int_{-\infty}^{\infty} \{-4 \operatorname{Im} \Gamma_{\mathbf{k}}(\omega)\} f(\omega) d\omega. \quad (2.27)$$

Now Eqs. (2.24)–(2.27) form a set of simultaneous equations which is to be solved in a self-consistent way.

### 3. PERTURBATIONAL TREATMENT: SOLUTION AT HIGH TEMPERATURES

Before looking for self-consistent solutions of the equations obtained in the last section, we shall try to solve them perturbationally. Then we can replace  $n_{\mathbf{k}}$  and  $m_{\mathbf{k}}$  by their zeroth-order quantities with respect to  $J$ , because they appear only in higher order terms. Therefore we put

$$m_{\mathbf{k}} = 0, \quad n_{\mathbf{k}} = f_{\mathbf{k}} \equiv f(\xi_{\mathbf{k}}) \quad (3.1)$$

in Eq. (2.17), and obtain

$$G_{kk'}(\omega) = \frac{1}{2\pi} \left\{ \frac{\delta_{kk'}}{\omega - \xi_k} + \frac{3J^2}{16N} \times \frac{1}{(\omega - \xi_k)(\omega - \xi_{k'})} \frac{F(\omega)}{1 + JG^0(\omega)} \right\}; \quad (3.2)$$

and, in particular, we have

$$\frac{1}{2\pi} G_{kk}(\omega)^{-1} = \omega - \xi_k - \frac{3J^2}{16N} \frac{F(\omega)}{1 + JG^0(\omega)}, \quad (3.3)$$

where

$$G^0(\omega) = \frac{1}{N} \sum_{\mathbf{k}} \frac{f_{\mathbf{k}} - \frac{1}{2}}{\omega - \xi_{\mathbf{k}}} \quad (3.4)$$

and higher order terms were neglected in the denominator.

In the following discussion it is assumed for simplicity that the real part of  $F(\omega)$  can be neglected, and that its imaginary part is independent of  $\omega$ ; that is  $F(\omega)$  is replaced by a pure imaginary constant as

$$F(\omega) = -i\pi\rho/N, \quad (3.5)$$

$\rho$  denoting the density of states of conduction electrons of pure metal near the Fermi surface.

Let us examine the self-energy part in Eq. (3.3). We put

$$G^0(\omega) = K(\omega) - iL(\omega), \quad (3.6)$$

where  $K(\omega)$  and  $L(\omega)$  are real functions of  $\omega$  defined by

$$K(\omega) = \frac{1}{N} \sum_{\mathbf{k}} P \frac{f_{\mathbf{k}} - \frac{1}{2}}{\omega - \xi_{\mathbf{k}}}, \quad (3.7)$$

$$L(\omega) = \pi\rho [f(\omega) - \frac{1}{2}]. \quad (3.8)$$

In calculating  $K(\omega)$ , we replace the summation over  $\mathbf{k}$  by the integration over  $\xi_{\mathbf{k}}$ . Then, if we assume the density of states to be independent of  $\omega$ , the integral diverges. Therefore we should cut off the integration at

some energy. We calculate  $K(\omega)$  as follows:

$$\begin{aligned} K(\omega) &= \frac{1}{N} \int_{-\infty}^{\infty} P \frac{f(\xi) - \frac{1}{2}}{\omega - \xi} \rho(\xi) d\xi \\ &\cong \frac{\rho}{N} \int_{-D}^D P \frac{f(\xi) - \frac{1}{2}}{\omega - \xi} d\xi \\ &= -\frac{\rho}{2N} \int_{-D}^D P \frac{1}{\omega - \xi} \tanh\left(\frac{\xi}{2T}\right) d\xi, \quad (3.9) \end{aligned}$$

where the cutoff energy should be of the order of band width. In particular at  $T=0$  we have

$$K(\omega) = -(\rho/N) \ln|\omega/D|. \quad (3.10)$$

Although the approximation taken above is rather crude, it does not seem that inclusion of actual band structures and  $k, k'$  dependence of  $J$  affects, at least qualitatively, the behavior of  $K(\omega)$  near  $\omega=0$ , which is our main interest. At finite temperatures  $K(\omega)$  has a sharp maximum at  $\omega=0$ .

By the use of Eqs. (3.5) and (3.6), Eq. (3.3) becomes

$$\begin{aligned} \frac{1}{2\pi} G_{kk}(\omega)^{-1} &= \omega - \xi_k - \frac{3\pi J^2 \rho}{16N^2} \frac{JL(\omega)}{[1+JK(\omega)]^2 + [JL(\omega)]^2} \\ &+ i \frac{3\pi J^2 \rho}{16N^2} \frac{1+JK(\omega)}{[1+JK(\omega)]^2 + [JL(\omega)]^2}. \quad (3.11) \end{aligned}$$

It should be noticed here that, if  $J < 0$  and the temperature is low enough, the imaginary part of the above expression, which is equal to the inverse of the lifetime of conduction electrons, becomes negative near  $\omega=0$ . This means that the conduction-electron states become unstable near the Fermi surface. The *critical* temperature  $T_c$  below which this instability arises is determined by

$$1 = \frac{|J|\rho}{N} \int_0^D \frac{1}{\xi} \tanh\left(\frac{\xi}{2T_c}\right) d\xi, \quad (3.12)$$

or

$$T_c = 1.14\Delta_0 \quad (3.13)$$

with

$$\Delta_0 = D \exp(-N/|J|\rho). \quad (3.14)$$

It should be noticed that the expression for  $T_c$  is quite similar to that for the transition temperature of superconductors. If  $D \sim 5$  eV and  $|J|\rho/N \sim 10^{-1}$ , we have  $\Delta_0 \sim 2.5 \times 10^{-4}$  eV and  $T_c \sim 3^\circ\text{K}$ .

When  $J < 0$  and  $T < T_c$ , we have to solve the equations more carefully. In this case  $m_k$  is expected not to be small, but to have a quite large value near the Fermi surface.

#### 4. SELF-CONSISTENT TREATMENT: SOLUTION AT LOW TEMPERATURES

Now we shall consider the case  $J < 0$  and  $T < T_c$ , and solve Eqs. (2.24)–(2.27) in a self-consistent way. As was

discussed in the last section,  $m_k$  is expected to be quite large near  $\xi_k=0$ . In fact it will be shown later that  $m_k$  has a logarithmic singularity at  $\xi_k=0$  at  $T=0$ . Because of this singularity of  $m_k$ ,  $\Gamma(\omega)$  is also expected to be anomalous as a function of  $\omega$  near  $\omega=0$ . By the use of these properties of  $m_k$  and  $\Gamma(\omega)$ , we can find an approximate solution of Eqs. (2.24)–(2.27) which is valid near the Fermi surface.

Let us assume the relation<sup>7</sup>

$$m_k - \frac{3}{4} = \alpha(n_k - \frac{1}{2})/\xi_k, \quad (\alpha > 0), \quad (4.1)$$

where  $\alpha$  is a parameter to be determined in a self-consistent way. Then  $G(\omega)$  becomes

$$G(\omega) = -\Gamma(\omega) - \frac{1}{N} \sum_{\mathbf{k}} \frac{n_k - \frac{1}{2}}{\xi_k}.$$

Assuming

$$1 + \frac{|J|}{N} \sum_{\mathbf{k}} \frac{n_k - \frac{1}{2}}{\xi_k} = 0, \quad (4.2)$$

we have a simple expression for  $G_k$ :

$$G_k(\omega) = \frac{1}{2\pi} \frac{\omega}{(\omega - \xi_k)(\omega + i\Delta)}, \quad (4.3)$$

where

$$\Delta = (\pi/4N) |J| \rho \alpha > 0 \quad (4.4)$$

and we have made use of Eq. (3.5). Similarly Eq. (2.25) becomes

$$\Gamma_k(\omega) = i \frac{|J|\rho m_k - \frac{3}{4}}{4N \omega + i\Delta}. \quad (4.5)$$

From Eqs. (2.26) and (4.3), we obtain

$$\begin{aligned} n_k - \frac{1}{2} &= \frac{\xi_k^2}{\xi_k^2 + \Delta^2} (f_k - \frac{1}{2}) + \frac{1}{\pi} \frac{\Delta \xi_k}{\xi_k^2 + \Delta^2} \\ &\times \int_{-D}^D \left( P \frac{1}{\omega - \xi_k} - \frac{\omega}{\omega^2 + \Delta^2} \right) \frac{1}{e^{\omega/T} + 1} d\omega, \quad (4.6) \end{aligned}$$

which reduces to

$$\begin{aligned} n_k - \frac{1}{2} &= \frac{\xi_k^2}{\xi_k^2 + \Delta^2} (f_k^0 - \frac{1}{2}) + \frac{1}{\pi} \frac{\Delta \xi_k}{\xi_k^2 + \Delta^2} \ln \left| \frac{\xi_k}{\Delta} \right|, \\ &\text{at } T=0, \quad (4.7) \end{aligned}$$

where we have taken the same approximation as we did in calculating Eq. (3.9).

<sup>7</sup> The parameter  $\alpha$  has been taken to be positive; for, if otherwise,  $G_k(\omega)$  has a pole in the upper half-plane of complex  $\omega$ , which contradicts the required analytic property of  $G_k(\omega)$ . However, negative  $\alpha$  can also satisfy the self-consistent condition, because Eq. (4.8) determines only the magnitude of  $\alpha$  and not its sign. It is not so clear what this unstable solution means physically.

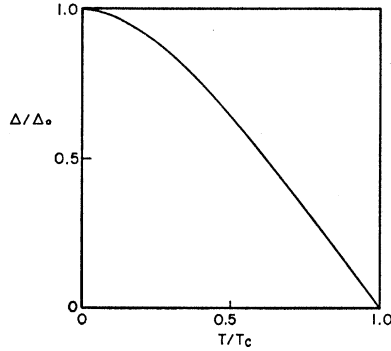


FIG. 1. Temperature dependence of  $\Delta$ .  $\Delta$  is normalized by its value at  $T=0$ .

Substitution of Eq. (4.6) in Eq. (4.2) gives

$$1 = \frac{|J|\rho}{N} \int_0^D \frac{\xi}{\xi^2 + \Delta^2} \tanh\left(\frac{\xi}{2T}\right) d\xi - \frac{|J|\rho}{\pi N} \int_{-D}^D \frac{\Delta}{\xi^2 + \Delta^2} \left( P \frac{1}{\omega - \xi} - \frac{\omega}{\omega^2 + \Delta^2} \right) \frac{1}{e^{\omega/T} + 1} d\omega d\xi.$$

The integral of the last term is shown to be of the order of  $(\Delta/D) \ln(\Delta/D)$ . It will be shown later that  $\Delta/D \ll 1$ , so we can neglect the second term of the above expression. Thus we have a relation

$$1 = \frac{|J|\rho}{N} \int_0^D \frac{\xi}{\xi^2 + \Delta^2} \tanh\left(\frac{\xi}{2T}\right) d\xi, \quad (4.8)$$

which determines  $\Delta$  as a function of  $T$ .

$m_{\mathbf{k}}$  is calculated by Eqs. (4.1) and (4.6). We have

$$m_{\mathbf{k}} - \frac{3}{4} = \frac{4\Delta}{\pi |J|\rho/N} \left\{ \frac{\xi_{\mathbf{k}}}{\xi_{\mathbf{k}}^2 + \Delta^2} \left( f_{\mathbf{k}} - \frac{1}{2} \right) + \frac{1}{\pi} \frac{\Delta}{\xi_{\mathbf{k}}^2 + \Delta^2} \times \int_{-D}^D \left( P \frac{1}{\omega - \xi_{\mathbf{k}}} - \frac{\omega}{\omega^2 + \Delta^2} \right) \frac{1}{e^{\omega/T} + 1} d\omega \right\} \quad (4.9)$$

and, in particular,

$$m_{\mathbf{k}} - \frac{3}{4} = -\frac{4}{\pi^2 |J|\rho/N} \ln\left(\frac{T_c}{T}\right), \quad \text{at } \xi_{\mathbf{k}} = 0, \quad (4.10)$$

where  $T_c$  is given by Eq. (3.13). [The calculation of Eq. (4.10) will be given in the Appendix.] From Eq. (4.10) it can be seen that  $|(m_{\mathbf{k}})_{\xi_{\mathbf{k}}=0}| \gg \frac{3}{4}$  except in the region  $|T_c - T| \leq T_c(J\rho/N)$ .

Next we consider Eqs. (2.27) and (4.5). Inserting Eq. (4.5) in Eq. (2.27), we have

$$m_{\mathbf{k}} = \left[ \frac{|J|\rho}{N} \int_0^D \frac{\xi}{\xi^2 + \Delta^2} \tanh\left(\frac{\xi}{2T}\right) d\xi \right] (m_{\mathbf{k}} - \frac{3}{4}). \quad (4.11)$$

At first glance, Eq. (4.11) is inconsistent with Eq. (4.9). However, it can be seen from Eq. (4.9) that  $|m_{\mathbf{k}}| \gg 1$

at  $-\Delta \leq \xi_{\mathbf{k}} \leq \Delta$ . If we confine our calculation to this region, we can neglect  $\frac{3}{4}$  in Eq. (4.11) compared with  $m_{\mathbf{k}}$ . Then Eq. (4.11) reduces to Eq. (4.8) which was already obtained. This means that Eqs. (4.6) and (4.9) together with Eq. (4.8) are the self-consistent solution of our problem which is valid near  $\xi_{\mathbf{k}} = 0$ .

It should be said, however, that there remains some ambiguity. In the above discussion we used the relation (4.1) in the whole range of  $\mathbf{k}$  in calculating  $G(\omega)$  and  $\Gamma(\omega)$ , while Eq. (4.1) has been proved to be valid only in the region near the Fermi surface. However, it can be seen from Eqs. (4.6) and (4.9) that, as  $|\xi_{\mathbf{k}}|$  increases,  $n_{\mathbf{k}}$  and  $m_{\mathbf{k}}$  tend to their zeroth-order values (3.1) rapidly. It seems that a deviation of  $n_{\mathbf{k}}$  and  $m_{\mathbf{k}}$  from Eqs. (4.6) and (4.9) in the region  $|\xi_{\mathbf{k}}| > \Delta$  does not affect  $G(\omega)$  and  $\Gamma(\omega)$ , in particular their behavior near  $\omega = 0$ , seriously.

Equation (4.8) has a solution when  $T < T_c$ . In particular we have

$$\Delta \cong \Delta_0 \left[ 1 - \frac{1}{6} \pi^2 (T/\Delta_0)^2 \right] \quad \text{at } T \sim 0, \quad (4.12)$$

$$\Delta \cong (4/\pi)(T_c - T) \quad \text{at } T \lesssim T_c, \quad (4.13)$$

where  $\Delta_0$  and  $T_c$  are given by Eqs. (3.14) and (3.13), respectively. [Calculation of Eqs. (4.12) and (4.13) will be given in the Appendix.]  $T$  dependence of  $\Delta$  is shown in Fig. 1. Although Eq. (4.8) has a solution as long as  $T < T_c$ , we must notice that the inequality  $|m_{\mathbf{k}}| \gg \frac{3}{4}$  does not hold when  $|T - T_c| \sim T_c(|J|\rho/N)$ . Therefore the solution obtained above is meaningful in the region

$$|T - T_c| \gg T_c(|J|\rho/N). \quad (4.14)$$

By the use of the above results Eqs. (2.17) and (2.18) are reduced to

$$G_{\mathbf{k}\mathbf{k}'}(\omega) = \frac{1}{2\pi} \left\{ \frac{\delta_{\mathbf{k}\mathbf{k}'}}{\omega - \xi_{\mathbf{k}}} + \frac{1}{\pi\rho} \frac{1}{(\omega - \xi_{\mathbf{k}})(\omega - \xi_{\mathbf{k}'})} \frac{\Delta}{\omega + i\Delta} \right\}, \quad (4.15)$$

$$\Gamma_{\mathbf{k}\mathbf{k}'}(\omega) = \frac{1}{2\pi} \frac{J}{2N} \frac{m_{\mathbf{k}'} - \frac{3}{4}}{(\omega - \xi_{\mathbf{k}})(\omega + i\Delta)}; \quad (4.16)$$

in particular, we have

$$\frac{1}{2\pi} G_{\mathbf{k}\mathbf{k}}(\omega)^{-1} = \omega - \xi_{\mathbf{k}} - \frac{1}{\pi\rho} \frac{\Delta}{\omega + i\Delta}. \quad (4.17)$$

From Eq. (4.17) it can be seen that the lifetime of conduction electrons is positive in the whole region of energy.

The physical meaning of the additional pole  $\omega = -i\Delta$  becomes clear if we examine how conduction-electron spins are polarized around the impurity. The behavior of the conduction-electron spin polarization is seen by calculating the quantity

$$\begin{aligned} \rho(\mathbf{R}) &= \sum_{\mathbf{k}\mathbf{k}'} \langle C_{\mathbf{k}\uparrow}^\dagger C_{\mathbf{k}'\downarrow} S_- \rangle e^{i(\mathbf{k}-\mathbf{k}')\cdot\mathbf{R}} \\ &= \frac{2}{3} \sum_{\mathbf{k}\mathbf{k}'} \int d\omega f(\omega) \{-2 \text{Im}\Gamma_{\mathbf{k}\mathbf{k}'}(\omega)\} e^{i(\mathbf{k}-\mathbf{k}')\cdot\mathbf{R}}. \end{aligned} \quad (4.18)$$

For simplicity we consider the case  $T=0$ . Then after some calculations we get

$$p(\mathbf{R}) = -(4\Delta N^2/3\pi\rho)[a(R)]^2$$

$$a(\mathbf{R}) = \frac{1}{N} \sum_{\mathbf{k}} \left\{ \frac{\xi_{\mathbf{k}}}{\xi_{\mathbf{k}}^2 + \Delta^2} (f_{\mathbf{k}}^0 - \frac{1}{2}) + \frac{1}{\pi} \frac{\Delta}{\xi_{\mathbf{k}}^2 + \Delta^2} \ln \left| \frac{\xi_{\mathbf{k}}}{\Delta} \right| \right\} e^{i\mathbf{k}\cdot\mathbf{R}}. \quad (4.19)$$

If  $R \ll v_F/\Delta$ ,  $v_F$  being the Fermi velocity,  $\mathbf{k}$  dependence of the exponential factor in Eq. (4.19) is slower than that of the factor in the wavy brackets, and hence, the former can be replaced by its average over the Fermi surface. Then we obtain

$$p(R) \cong -(\Delta N^2/3\pi J^2 \rho) (\sin k_F R / k_F R)^2 \quad \text{for } R \ll v_F/\Delta. \quad (4.20)$$

For  $R \geq v_F/\Delta$ ,  $p(R)$  will vanish more rapidly. Equation (4.20) is compared with the usual Ruderman-Kittel-Yosida type polarization,<sup>1</sup> which is proportional to  $\sin(k_F R)/(k_F R)^3$  when  $k_F R \gg 1$ . First of all we see that the polarization has a much longer range in this case, and that it is negative, or antiparallel to the localized spin, in the whole region of space rather than oscillating. If  $\Delta \sim 5 \times 10^{-4}$  eV,  $\epsilon_F \sim 5$  eV, and  $k_F \sim 10^8$  cm<sup>-1</sup>, we have  $v_F/\Delta \cong (\epsilon_F/\Delta) k_F^{-1} \sim 10^{-4}$  cm.

Thus it is concluded that, when the temperature becomes lower than  $T_c$ , there appears a quasibound state around the localized spin, whose range is of the order  $v_F/\Delta$ . However, it should also be remarked that  $T_c$  is not a transition temperature in an ordinary sense, because, if  $T_c - T \leq T_c (|J|\rho/N)$ , the quasibound state obtained here is no longer stable. Although we could not get the solution in this transitional region of temperature, it seems that the quasibound state appears gradually rather than suddenly at  $T = T_c$ .

## 5. RESISTIVITY AND SPECIFIC HEAT

So far we have considered the case of one impurity. It is not difficult, however, to extend the result to the case of many impurities, if their concentration  $c$  is small enough and the interaction between them can be neglected. In this case we have only to multiply by  $cN$  those terms which come from the interaction with the impurity. Thus we have from Eqs. (3.11) and (4.15)

$$\frac{1}{2\pi} G_{\mathbf{k}\mathbf{k}}(\omega)^{-1} = \omega - \xi_{\mathbf{k}} + i \frac{3\pi J^2 \rho c}{16N} \frac{1}{1 + JK(\omega)}, \quad \text{for } T > T_c, \quad (5.1)$$

$$\frac{1}{2\pi} G_{\mathbf{k}\mathbf{k}}(\omega)^{-1} = \omega - \xi_{\mathbf{k}} - \frac{cN}{\pi\rho} \frac{\Delta}{\omega + i\Delta}, \quad \text{for } T < T_c. \quad (5.2)$$

In Eq. (5.1) we have neglected higher order terms of  $J$ . By the use of Eqs. (5.1) and (5.2) we shall calculate the resistivity and the specific heat of the system.

## A. Resistivity

The static conductivity  $\sigma$  is calculated by the formula

$$\sigma = -\frac{2e^2}{3} \int \tau_{\mathbf{k}} v_{\mathbf{k}}^2 \frac{\partial f}{\partial \xi_{\mathbf{k}}} \rho d\xi_{\mathbf{k}}, \quad (5.3)$$

where  $v_{\mathbf{k}}$  is the velocity of the conduction electron with wave vector  $\mathbf{k}$  and  $\tau_{\mathbf{k}}$  is its mean free time. If we use Eq. (5.1) for the Green's function,  $\tau_{\mathbf{k}}$  is given by

$$\frac{1}{\tau_{\mathbf{k}}} = \frac{3\pi J^2 \rho c}{16N} \frac{1}{1 - |J|K(\xi_{\mathbf{k}})}. \quad (5.4)$$

Then  $\sigma$  is calculated as

$$\sigma = \frac{2e^2 \rho v_F^2}{3} \frac{16N}{3\pi J^2 \rho c} \int (1 - |J|K(\xi)) \left( -\frac{\partial f}{\partial \xi} \right) d\xi$$

$$= \frac{ne^2}{m^*} \frac{16}{3\pi |J|c} \ln \left| \frac{T}{0.68T_c} \right|, \quad (5.5)$$

where  $n$  is the total number of conduction electrons and we put  $\rho = 3n/2m^*v_F^2$ ,  $m^*$  denoting the effective mass of conduction electrons. Thus we get the resistivity  $\rho_{\text{res}} = 1/\sigma$  as

$$\rho_{\text{res}} = \frac{m^*}{ne^2} \frac{3\pi |J|c}{16} \left( \ln \left| \frac{T}{0.68T_c} \right| \right)^{-1}. \quad (5.6)$$

If the temperature is high enough above  $T_c$ , Eq. (5.6) reduces to

$$\rho_{\text{res}} = \frac{m^*}{ne^2} \frac{3\pi J^2 \rho c}{16N} \left[ 1 + \frac{|J|\rho}{N} \ln \left| \frac{0.77D}{T} \right| \right], \quad (5.7)$$

which is essentially the same as the result obtained by Kondo.<sup>2</sup> It should be noticed, however, that Eq. (5.7) is correct only at high temperatures. Equation (5.6) itself diverges at  $T = 0.68T_c$  and becomes negative for  $T < 0.68T_c$ , which corresponds to the instability mentioned before.

For  $T < T_c$ , we should use Eq. (5.2). Then we have

$$\frac{1}{\tau_{\mathbf{k}}} = \frac{cN}{\pi\rho} \frac{\Delta^2}{\xi_{\mathbf{k}}^2 + \Delta^2}, \quad (5.8)$$

$$\sigma = \frac{ne^2}{m^*} \frac{\pi\rho}{cN} \left[ 1 + \frac{\pi^2}{3} \left( \frac{T}{\Delta} \right)^2 \right], \quad (5.9)$$

$$\rho_{\text{res}} = \frac{m^*}{ne^2} \frac{cN}{\pi\rho} \left[ 1 + \frac{\pi^2}{3} \left( \frac{T}{\Delta} \right)^2 \right]^{-1}. \quad (5.10)$$

It should be noticed here that  $\rho_{\text{res}}$  tends to a finite value, which is independent of the magnitude of  $J$ , as the temperature decreases, and that there is no term proportional to  $\ln T$  at low temperatures. The  $T$  dependence

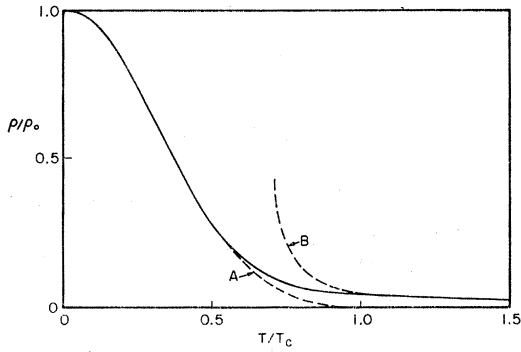


FIG. 2. Temperature dependence of resistivity.  $\rho_{\text{res}}$  is normalized by its value at  $T=0$ . Curve *A* is calculated by Eq. (5.10) and curve *B* by Eq. (5.7) ( $|J|\rho/N=0.01$ ). For  $T\sim T_c$ , we interpolate these two curves.

of Eqs. (5.10) and (5.6) is shown in Fig. 2. For  $T\sim T_c$ , we interpolate the two expressions, because both of them are incorrect there. If we add the contribution from the electron-phonon interaction to the above result for the resistivity, it is clear that there appears a resistance minimum near  $T=T_c$ .

### B. Specific Heat

The appearance of quasibound states changes the density of states of conduction electrons, which is given by

$$\bar{\rho}(\omega) = \sum_{\mathbf{k}} \{-2 \text{Im}G_{\mathbf{k}\mathbf{k}}(\omega)\}. \quad (5.11)$$

Inserting Eq. (5.2) in Eq. (5.11), we get the change in density of states as

$$\delta\rho(\omega) = -\frac{cN^2}{\pi^2\rho} \left\{ I' \frac{\Delta^2}{\omega^2 + \Delta^2} + \frac{\pi\rho'}{N} \frac{\Delta\omega}{\omega^2 + \Delta^2} \right\}, \quad (5.12)$$

where the derivatives of  $I(\omega) = \text{Re}F(\omega)$  and  $\rho(\omega) = -(N/\pi) \text{Im}F(\omega)$  with respect to  $\omega$  have been replaced by their values at the Fermi surface,  $I'$  and  $\rho'$ .

The change in the total energy of the system is calculated as

$$\begin{aligned} \delta E &= \int \omega \delta\rho(\omega) f(\omega) d\omega \\ &= -\frac{cN^2}{\pi^2\rho} \left\{ \Delta^2 I' \int \frac{\omega}{\omega^2 + \Delta^2} f(\omega) d\omega \right. \\ &\quad \left. + \frac{\pi\Delta\rho'}{N} \int \frac{\omega^2}{\omega^2 + \Delta^2} f(\omega) d\omega \right\}. \quad (5.13) \end{aligned}$$

By the use of Eq. (4.8) the first term in the brackets reduces to  $I'\Delta^2/J(\rho/N)$ . In the calculation of the second term there remains some ambiguity. In the above we used Eq. (5.11), which is valid only in the neighborhood

of the Fermi surface, as if it were correct over the whole region of  $\omega$ . Such extrapolation is allowed only when the integral to be calculated converges rapidly. In the second integral contributions come from the whole region of  $\omega$  to the same order. Therefore, to calculate it precisely, we have to know  $G_{\mathbf{k}\mathbf{k}}(\omega)$  in the whole region of  $\omega$ . Instead of doing so, we estimate it by cutting off the integration at  $\omega \sim \pm\Delta$ . The second term then gives a contribution of the order  $\rho'\Delta^2/N$ , which is at most of the same order of the first term. Thus we have

$$\delta E = \frac{cNI'}{\pi^2|J|(\rho/N)^2} \Delta^2, \quad (5.14)$$

where  $I'$  should be considered as a parameter of the order  $\epsilon_F^{-2}$ .

The contribution to the specific heat is given by  $\delta C = \partial(\delta E)/\partial T$ . To calculate the derivative of  $\Delta$  with  $T$ , we differentiate both sides of Eq. (4.8) with  $T$  and obtain

$$\frac{d\Delta^2}{dT} = -\frac{2\Delta^2}{T} \left\{ \frac{1}{A(\Delta/T)} - 1 \right\} \quad (5.15)$$

$$A(\delta) = 2\delta^2 \int_0^\infty \frac{\chi}{(\chi^2 + \delta^2)^2} \tanh \frac{\chi}{2} d\chi. \quad (5.16)$$

For the cases  $\delta \gg 1$  and  $\delta \ll 1$ ,  $A(\delta)$  becomes

$$\begin{aligned} A(\delta) &= 1 - (\pi^2/3)(1/\delta^2), \quad \text{for } \delta \gg 1, \\ &= (\pi/4)\delta, \quad \text{for } \delta \ll 1. \end{aligned} \quad (5.17)$$

Thus we obtain the anomalous part of the specific heat, which is due to the appearance of quasibound states, as

$$\delta C = -\frac{cNI'}{\pi^2|J|(\rho/N)^2} \frac{2\Delta^2}{T} \left\{ \frac{1}{A(\Delta/T)} - 1 \right\}, \quad (5.18)$$

particular,

$$\delta C = -\frac{2cNI'}{3|J|(\rho/N)^2} T, \quad \text{for } T \sim 0 \quad (5.19)$$

$$\delta C = -\frac{32cNI'}{\pi^4|J|(\rho/N)^2} (T_c - T), \quad \text{for } T \sim T_c. \quad (5.20)$$

The  $T$  dependence of  $\delta C$  is shown in Fig. 3, where  $I'$  is assumed to be negative.

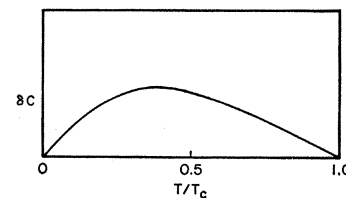


FIG. 3. Temperature dependence of the anomalous part of the specific heat in an arbitrary scale.

The order of magnitude of  $\delta C$  is  $(cN/|J|)T$ , for  $I' \sim \epsilon_F^{-2}$  and  $\rho \sim N\epsilon_F^{-1}$ , while the specific heat of pure metals is of the order  $(N/\epsilon_F)T$ . Therefore the relative magnitude of  $\delta C$  is of the order  $(c\epsilon_F/|J|) \approx 10^{-1}$  if we take  $c = 10^{-2}$  and  $|J|/\epsilon_F = 10^{-1}$ . The contribution to the specific heat seems to be rather small.

## 6. DISCUSSION

As was suggested in Sec. 1, our problem has been solved by a method similar to the theory of superconductivity. The results, however, have some differences from the case of superconductivity. In the energy spectrum of conduction electrons appeared an anomaly near the Fermi surface, corresponding to the quasibound state, rather than an energy gap. Further, the appearance of the quasibound state seems to take place gradually in a transitional region of temperature, although we could not determine the behavior of the system in the transition.

Our model treated in this paper looks oversimplified compared with the actual case of dilute alloys. First of all we neglected Coulomb interaction between the conduction electrons. To see the effect of Coulomb interaction, we calculate the charge density of electrons associated with the quasibound state. It is calculated from Eq. (4.15) in a way similar to the calculation of Eq. (4.18), and is found to be smaller than the spin polarization density by a factor  $(J/\epsilon_F)^2 \ll 1$ . This means that the bound state is essentially a bound state of electron-spin density, and not that of electron-charge density. Therefore it cannot be destroyed by Coulomb interaction as long as Coulomb interaction is taken into account in Hartree approximation. Our theory is not applicable to the case where the exchange interaction between the conduction electrons plays an important role.

If we do not neglect  $\text{Re}F(\omega)$  [i.e., if we do not assume Eq. (3.5)],  $\Delta$  becomes complex and the energy of the quasibound state shifts upwards or downwards from the Fermi surface according to the sign of  $\text{Re}F(\omega)$ . Some of the expressions will be a little more complicated, but the main results are not modified, at least qualitatively. In addition, it can be seen that, if this is the case, there appears some space charge around the localized spin. It is, therefore, expected that  $\Delta$  effectively becomes real if the Coulomb interaction is taken into account.

There is no essential difficulty in generalizing the treatment to the case  $S > \frac{1}{2}$ , although it might be much more complicated. It is quite reasonable to believe that the main result obtained here, i.e., the appearance of the quasibound state at low temperatures, is not modified even in the case  $S > \frac{1}{2}$ .

The main defect of our theory seems to be that the equations are solved only in the neighborhood of the Fermi surface and the solution is extrapolated to the whole region of energy when we calculate some integrals.

Because of this approximation we could not see how the quasibound state appears in the transitional region of temperature. It is very desirable to refine the treatment of this point.

The same problem of Kondo's effect has also been treated by Suhl<sup>8</sup> by the method of Chew and Low in scattering theory. Though his result seems to have some similarity to ours, it is not so easy to see the relation between these two treatments.

There also remains an interesting problem of the magnetic susceptibility at low temperatures. The polarization of conduction-electron spins associated with the quasibound state is expected to behave as a part of localized spin, and hence, the effective magnitude of localized spin will be reduced at low temperatures. However, the calculation of the magnetic susceptibility is beyond the scope of this paper, because it requires calculation of the two-particle Green's functions. In addition the interaction between localized spins, which we have neglected throughout this paper, will play an important role there. This problem will be left for future investigations.

*Note added in proof.* It should be said that the calculation in Sec. 3 for the case of high temperatures has only a qualitative meaning. The lifetime of conduction electrons obtained in (3.11) differs from that of the perturbational calculation<sup>2</sup> in the third order of  $J$ , when the former is expanded in powers of  $J$ . This is because we put  $m_k = 0$  in (3.1), which is correct only to the zeroth order. From Eq. (2.18) we get to the lowest order of  $J$

$$\Gamma_{kk'}(\omega) = -(3J/16\pi N) \cdot [(\omega - \xi_k)(\omega - \xi_{k'})]^{-1}.$$

It is then easy to see that  $m_k$  is proportional to  $J \log |\xi_k|$  in this order (for  $T=0$ ). From this term there arises another contribution to the lifetime which is proportional to  $J^3 \log |\omega|$  (for  $T=0$ ), and the final result is, as it should be, the same as Kondo's.

A different expression for the lifetime of conduction electrons has been obtained by Suhl<sup>8</sup> by a dispersion theoretical method. His expression gives no negative lifetime even near the Fermi surface. However, as pointed out by Suhl himself, it has a pole in the upper-half plane of complex frequency at low temperatures. The existence of such a pole usually means that the unperturbed Fermi surface has some instability. In this case it is expected that the Fermi surface is unstable locally, in the vicinity of the paramagnetic impurity. If this is the case, the self-consistent treatment in Sec. 4 has an essential importance in the present problem.

## ACKNOWLEDGMENTS

The author would like to express his sincere thanks to Professor H. Suhl and Dr. K. Sawada for suggesting the problem and for many enlightening discussions.

<sup>8</sup> H. Suhl, Phys. Rev. **138**, A515 (1965).



## APPENDIX

(1) *Proof of Eq. (4.10)*: Putting  $\xi_{\mathbf{k}}=0$  in Eq. (4.9), we have

$$\begin{aligned} (m_{\mathbf{k}} - \frac{3}{4})_{\xi_{\mathbf{k}}=0} &= \frac{4}{\pi^2 (J\rho/N)^2} \left\{ 1 + \frac{|J|\rho}{N} \int_{-D}^D \frac{1}{\omega} \frac{1}{e^{\omega/T} + 1} d\omega \right\} \\ &= \frac{4}{\pi^2 (J\rho/N)^2} \left\{ 1 - \frac{|J|\rho}{N} \int_0^{D/T} \frac{1}{\chi} \frac{\chi}{2} \tanh^{-1} d\chi \right\}. \quad (\text{A1}) \end{aligned}$$

The integral is divided into two parts as

$$\int_0^{D/T} = \int_0^{D/T_c} \frac{1}{\chi} \frac{\chi}{2} \tanh^{-1} d\chi + \int_{D/T_c}^{D/T} \frac{1}{\chi} \frac{\chi}{2} \tanh^{-1} d\chi,$$

where  $T_c$  is given by Eq. (3.13). By the use of Eq. (3.12) the first integral becomes  $N/|J|\rho$ , while in the second integral  $\tanh(\frac{1}{2}\chi)$  can be approximated by unity because  $D/T_c \gg 1$ . Thus we have

$$\frac{|J|\rho}{N} \int_0^{D/T} \frac{1}{\chi} \frac{\chi}{2} \tanh^{-1} d\chi = 1 + \frac{|J|\rho}{N} \ln\left(\frac{T_c}{T}\right). \quad (\text{A2})$$

Substitution of Eq. (A2) in Eq. (A1) gives Eq. (4.10).

(2) *Proof of Eqs. (4.12) and (4.13)*: Equation (4.8) is rewritten as

$$1 = \frac{|J|\rho}{N} \int_0^{D/T} \frac{\chi}{\chi^2 + \delta^2} \tanh\left(\frac{\chi}{2}\right) d\chi, \quad (\text{A3})$$

with

$$\delta = \Delta/T. \quad (\text{A4})$$

When  $T \ll T_c$ , we have  $\delta \gg 1$ , for  $\Delta$  tends to a finite value for  $T \rightarrow 0$ . In this case the integral in Eq. (A3) is divided into two parts as

$$\begin{aligned} \int_0^{D/T} &= \int_0^A \frac{\chi}{\chi^2 + \delta^2} \tanh^{-1} d\chi \\ &\quad + \int_A^{D/T} \frac{\chi}{\chi^2 + \delta^2} \tanh^{-1} d\chi, \quad (\text{A5}) \end{aligned}$$

where  $A$  is a constant such as  $1 \ll A \ll \delta$ . In the first integral  $\chi^2$  can be neglected compared with  $\delta^2$ , and it becomes

$$\begin{aligned} \int_0^A &\cong \frac{1}{\delta^2} \int_0^A \chi \tanh^{-1} d\chi \\ &= \frac{1}{\delta^2} \int_0^A \chi \left( \tanh^{-1} - 1 \right) d\chi + \frac{A^2}{2\delta^2}. \end{aligned}$$

In calculating the integral in the last expression, we can replace the region of integration by  $(0, \infty)$ , for the integrand vanishes rapidly for  $\chi \gg 1$ . Thus we have

$$\int_0^A = -\frac{\pi^2}{6} \frac{1}{\delta^2} + \frac{A^2}{2\delta^2}. \quad (\text{A6})$$

In the second integral of Eq. (A5),  $\tanh(\frac{1}{2}\chi)$  is approximated by unity, and we have

$$\int_A^{D/T} = \int_A^{D/T} \frac{\chi}{\chi^2 + \delta^2} d\chi \cong \ln\left(\frac{D}{\Delta}\right) - \frac{A^2}{2\delta^2}. \quad (\text{A7})$$

By the use of Eqs. (A6), (A7), and (A5), Eq. (A3) becomes

$$1 = \frac{|J|\rho}{N} \left\{ \ln\left(\frac{D}{\Delta}\right) - \frac{\pi^2}{6} \left(\frac{T}{\Delta}\right)^2 \right\}. \quad (\text{A8})$$

Solving Eq. (A8) for  $\Delta$ , we finally obtain Eq. (4.12).

When  $T \sim T_c$ , we have  $\delta \ll 1$ . We divide the integral as Eq. (A5), but in this case  $A$  is chosen as  $\delta \ll A \ll 1$ . In the first integral  $\tanh(\frac{1}{2}\chi)$  is expanded with  $\chi$ , and it becomes

$$\int_0^A \cong \frac{1}{2} \int_0^A \frac{\chi^2}{\chi^2 + \delta^2} d\chi \cong \frac{A}{2} - \frac{\pi}{4} \delta. \quad (\text{A9})$$

In the second integral  $\delta^2$  is neglected compared with  $\chi^2$  and it is calculated as follows:

$$\begin{aligned} \int_A^{D/T} &\cong \int_A^{D/T} \frac{1}{\chi} \frac{\chi}{2} \tanh^{-1} d\chi \\ &= \int_0^{D/T_c} \frac{1}{\chi} \frac{\chi}{2} \tanh^{-1} d\chi + \int_{D/T_c}^{D/T} \frac{1}{\chi} \frac{\chi}{2} \tanh^{-1} d\chi \\ &\quad - \int_0^A \frac{1}{\chi} \frac{\chi}{2} \tanh^{-1} d\chi. \end{aligned}$$

The first term becomes  $N/|J|\rho$  by the use of Eq. (4.8). In the second term  $\tanh(\frac{1}{2}\chi)$  is approximated by 1, and in the third by  $\frac{1}{2}\chi$ . Then

$$\int_A^{D/T} \cong \frac{N}{|J|\rho} + \ln\left(\frac{T_c}{T}\right) - \frac{A}{2}. \quad (\text{A10})$$

Inserting Eqs. (A9), (A10), and (A5) in Eq. (A3), we have

$$\Delta = (4/\pi)T \ln(T_c/T), \quad (\text{A11})$$

which becomes Eq. (4.13) for  $|T - T_c| \ll T_c$ .