

Magnetic-Field Dependence of the Local Electronic Structure in the Ground State of the s - d Exchange System and Magnetoresistance at 0°K

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(Received September 24, 1969)

Recent two publications by Yosida and Yoshimori have clarified the detailed electronic structure of the singlet collective bound state developed so far by them and by Okiji. In this paper, by means of their method, the magnetic-field dependence of the local electronic structure of the ground state is investigated. In particular, it is shown that the z -component of the spin correlation which sticks around the impurity remains unchanged even in the limit of increasing field. From this calculation, an expression for the magnetoresistance is inferred with the aid of the Friedel sum rule:

$$R(\mathcal{A}) = R_0 \cos^2 \frac{\pi}{2} \frac{\mathcal{A}}{(\tilde{E}_0^2 + \mathcal{A}^2)^{1/2}},$$

where \tilde{E}_0 denotes the binding energy of the singlet state and \mathcal{A} the Zeeman energy of the free spin. It is to be noticed that this has no logarithmic field dependence. It is further shown that the relation $\langle \sigma \rangle = (\rho J / 2N) \langle S_z \rangle$ holds generally between the spin polarization of the conduction electrons and the induced localized spin.

§ 1. Introduction

Since Yosida¹⁾ has shown by the generalized perturbation method that the singlet collective bound state is realized as the ground state of the system consisting of conduction electrons and a localized spin which are coupled with an antiferromagnetic s - d exchange interaction, theories^{2)~9)} have been developed on the basis of this work and many properties of this singlet bound state have been clarified.

Among these, Yoshimori and Yosida⁷⁾ (hereafter referred to as I) revealed partially the local electronic structure of the singlet bound state by calculating the charge density and the spin correlation density at the impurity site. According to this, the charge density at the impurity site which is finite at the starting approximation of the generalized perturbation theory completely vanishes in the final stage. This fact indicates that the bound state is not of the charge density but of the spin correlation density. Moreover, the recent work of Yosida and Yoshimori⁹⁾ (hereafter referred to as II) has completely proved the physical picture of the singlet bound state as has been drawn in I by calculating the total charge and the total spin correlation accumulated around the localized spin.

That is, one of the two components of the singlet bound state is composed by the up-spin state of the localized spin and down-spin cloud made of half an electron with down-spin and half a hole with up-spin which are both trapped around the impurity, and the other component is the one obtained from the former by the reverse of all spin directions. The anomalous binding energy \tilde{E} is understood as a consequence of the formation of such a bound state. From the consideration of the phase shift for the conduction electrons, they have also proved the unitarity limit value for the electrical resistivity.

In previous papers,^{4),8)} as part of a series of work, we have partially made the extension of this theory to the case in which the magnetic field is applied. Magnetic field tends to fix the spin direction so as to gain the Zeeman energy and it has an effect of preventing the spin flip process due to the exchange interaction which is essential to the anomalous binding energy. By these two factors the ground state is determined. The obtained energy is expressed as a function of the applied field and from it an induced magnetization and a finite susceptibility are obtained at 0°K. It is further concluded within a weak coupling limit that the bound state does not vanish at a finite value of magnetic field, but approaches the normal state asymptotically at high field. Though calculations have been done for the magnetic field acting on only the localized spin, it has been shown⁴⁾ that there arises no change in the local character of the results for the case where the applied field also interacts with the conduction electrons.

It is the purpose of the present paper to investigate the magnetic field-dependence of the results obtained in I and II according to the method developed in them, namely the local distributions of the charge and the spin polarization in each of the two components ψ_α and ψ_β by calculating their densities at the impurity site and the total localized amounts of them, where ψ_α and ψ_β are two components of the ground state wave function associated with up- and down-spin states of the localized spin, respectively. As combinations of these quantities, the spin correlation, the spin polarization and the charge localized around the impurity are obtained. Further, the interpretation of these in terms of the phase shift makes it possible to derive the magnetoresistance at 0°K. All calculations in later sections will be made in the case where the applied field interacts only with the localized spin. Section 2 is devoted to a brief summary of the results obtained previously^{4),8)} which are necessary for later sections. In § 3, densities of the charge, of the spin polarization and of the z -component of the spin correlation at the impurity site are calculated, and by the use of these and also of the Feynman relation the spin correlation density at the impurity site, the kinetic energy and the exchange energy of the system are obtained. In § 4, the total localized charge and the spin polarization are calculated separately for ψ_α and ψ_β components. With this result, we make a consideration for the magnetoresistance in § 5. In § 6, by the use of the general method valid for a nondegenerate state it is shown that the relation between the total localized spin polari-

zation of the conduction electrons and the magnitude of the localized spin induced in the ground state is a general one common to that obtained in the second order perturbation theory or RKY theory¹⁰⁾ and that in the usual perturbation theory up to an infinite order.¹¹⁾ Conclusion and discussion are given in the last section.

§ 2. Results obtained in previous papers

In this section we summarize the main results obtained in the previous two papers which treated the effect of a magnetic field on the singlet ground state.

We consider the system consisting of a localized spin and conduction electrons which are coupled with an antiferromagnetic s - d exchange interaction. For the purpose of investigating the effect of the magnetic field on the local property of this system, it is sufficient to consider the field applied only to the localized spin, as mentioned in § 1. The Hamiltonian is written as

$$H = \sum_{k\sigma} \epsilon_k a_{k\sigma}^* a_{k\sigma} + 2\Delta S_z - \frac{J}{2N} \sum_{kk'} [(a_{k'\uparrow}^* a_{k\uparrow} - a_{k'\downarrow}^* a_{k\downarrow}) S_z + a_{k'\uparrow}^* a_{k\downarrow} S_- + a_{k'\downarrow}^* a_{k\uparrow} S_+], \quad (1)$$

where

$$\Delta = \frac{1}{2} g \mu_B H_z, \quad (2)$$

and the notations are the same as those given in the previous papers.^{4), 8)} In Yosida's theory, the ground state wave function is constructed as follows:

$$\begin{aligned} \psi = & [\sum_1 (\Gamma_1^\alpha a_{1\uparrow}^* \alpha + \Gamma_1^\beta a_{1\uparrow}^* \beta) \\ & + \sum_{123} (\Gamma_{12,3}^{\alpha\downarrow} a_{1\downarrow}^* a_{2\downarrow}^* a_{3\downarrow} \alpha + \Gamma_{12,3}^{\beta\uparrow} a_{1\uparrow}^* a_{2\uparrow}^* a_{3\uparrow} \beta + \Gamma_{12,3}^{\alpha\uparrow} a_{1\downarrow}^* a_{2\uparrow}^* a_{3\uparrow} \alpha + \Gamma_{12,3}^{\beta\downarrow} a_{1\uparrow}^* a_{2\downarrow}^* a_{3\downarrow} \beta) \\ & + \sum_{12345} (\Gamma_{123,45}^{\alpha\downarrow\downarrow} a_{1\downarrow}^* a_{2\downarrow}^* a_{3\downarrow}^* a_{4\downarrow} a_{5\downarrow} \alpha + \Gamma_{123,45}^{\beta\uparrow\uparrow} a_{1\uparrow}^* a_{2\uparrow}^* a_{3\uparrow}^* a_{4\uparrow} a_{5\uparrow} \beta \\ & + \Gamma_{123,45}^{\alpha\uparrow\downarrow} a_{1\downarrow}^* a_{2\downarrow}^* a_{3\uparrow}^* a_{4\downarrow} a_{5\uparrow} \alpha + \Gamma_{123,45}^{\beta\downarrow\uparrow} a_{1\uparrow}^* a_{2\uparrow}^* a_{3\downarrow}^* a_{4\uparrow} a_{5\downarrow} \beta \\ & + \Gamma_{123,45}^{\alpha\uparrow\uparrow} a_{1\downarrow}^* a_{2\uparrow}^* a_{3\uparrow}^* a_{4\uparrow} a_{5\uparrow} \alpha + \Gamma_{123,45}^{\beta\downarrow\downarrow} a_{1\uparrow}^* a_{2\downarrow}^* a_{3\downarrow}^* a_{4\downarrow} a_{5\downarrow} \beta) \\ & + \dots] \psi_0, \end{aligned} \quad (3)$$

where α and β respectively denote the spin-up and spin-down states of the localized spin of which magnitude is assumed to be one half, ψ_0 the state of the unpolarized Fermi sea, and the coefficients $\Gamma_{12,3}^{\alpha\uparrow}$ and $\Gamma_{12,3}^{\beta\downarrow}$ are defined in the same way as in references 1), 4) and 8), so that $\Gamma_{12,3}^{\alpha\uparrow}$ defined in references 2) and 9) is given by $-\Gamma_{21,3}^{\alpha\uparrow}$ in the present definition. In later calculations, we will often consider the components of the wave function separated as

$$\psi = \psi_\alpha + \psi_\beta, \quad (4)$$

where

$$\psi_\alpha = |\alpha\rangle \langle \alpha | \psi \rangle \quad \text{and} \quad \psi_\beta = |\beta\rangle \langle \beta | \psi \rangle.$$

Inserting Eqs. (1) and (3) into the Schrödinger equation,

$$(H - E)\psi = 0, \quad (5)$$

we set up an infinite set of the simultaneous equations for the coefficients Γ . The first parts of these are as follows:

$$\Gamma_1^\alpha (\varepsilon_1 - E + \Delta) + \frac{J}{4N} \sum_1 \Gamma_1^\alpha - \frac{J}{2N} \sum_1 \Gamma_1^\beta - \frac{J}{4N} \sum_{23} (\Gamma_{[21],3}^{\alpha\downarrow} + \Gamma_{12,3}^{\alpha\uparrow} - 2\Gamma_{21,3}^{\beta\downarrow}) = 0, \quad (6)$$

$$\begin{aligned} \Gamma_{[12],3}^{\alpha\downarrow} (\varepsilon_1 + \varepsilon_2 - \varepsilon_3 - E + \Delta) + \frac{J}{4N} (\Gamma_1^\alpha - \Gamma_2^\alpha) + \frac{J}{4N} \sum_4 (\Gamma_{[42],3}^{\alpha\downarrow} + \Gamma_{[14],3}^{\alpha\downarrow} + \Gamma_{[21],4}^{\alpha\downarrow} \\ - 2\Gamma_{42,3}^{\beta\downarrow} + 2\Gamma_{41,3}^{\beta\downarrow}) + \frac{J}{4N} \sum_{45} (\Gamma_{[412],53}^{\alpha\downarrow\downarrow} + \Gamma_{[12]4,35}^{\alpha\downarrow\uparrow} + 2\Gamma_{4[12],35}^{\beta\downarrow\downarrow}) = 0, \end{aligned} \quad (7)$$

$$\begin{aligned} \Gamma_{12,3}^{\alpha\uparrow} (\varepsilon_1 + \varepsilon_2 - \varepsilon_3 - E + \Delta) - \frac{J}{4N} (\Gamma_1^\alpha - 2\Gamma_2^\beta) + \frac{J}{4N} \sum_4 (\Gamma_{42,3}^{\alpha\uparrow} - \Gamma_{14,3}^{\alpha\uparrow} + \Gamma_{12,4}^{\alpha\uparrow} - 2\Gamma_{[42],3}^{\beta\uparrow} \\ - 2\Gamma_{21,4}^{\beta\downarrow}) - \frac{J}{4N} \sum_{45} (\Gamma_{[14]2,53}^{\alpha\downarrow\uparrow} + \Gamma_{1[24],53}^{\alpha\uparrow\uparrow} + 2\Gamma_{[42]1,35}^{\beta\uparrow\downarrow}) = 0, \end{aligned} \quad (8)$$

$$\begin{aligned} \Gamma_{[123],45}^{\alpha\downarrow\downarrow} (\varepsilon_1 + \varepsilon_2 + \varepsilon_3 - \varepsilon_4 - \varepsilon_5 - E + \Delta) + \frac{J}{4N} (-\Gamma_{[12],4}^{\alpha\downarrow} + \Gamma_{[12],5}^{\alpha\downarrow} + \Gamma_{[13],4}^{\alpha\downarrow} \\ - \Gamma_{[13],5}^{\alpha\downarrow} - \Gamma_{[23],4}^{\alpha\downarrow} + \Gamma_{[23],5}^{\alpha\downarrow}) + \frac{J}{4N} \sum_6 (\Gamma_{[623],45}^{\alpha\downarrow\downarrow} + \Gamma_{[163],45}^{\alpha\downarrow\downarrow} + \Gamma_{[126],45}^{\alpha\downarrow\downarrow} \\ - \Gamma_{[123],65}^{\alpha\downarrow\downarrow} - \Gamma_{[123],46}^{\alpha\downarrow\downarrow} - 2\Gamma_{6[23],45}^{\beta\downarrow\downarrow} - 2\Gamma_{6[31],45}^{\beta\downarrow\downarrow} - 2\Gamma_{6[12],45}^{\beta\downarrow\downarrow}) + \dots = 0, \end{aligned} \quad (9)$$

$$\begin{aligned} \Gamma_{[12]3,45}^{\alpha\downarrow\uparrow} (\varepsilon_1 + \varepsilon_2 + \varepsilon_3 - \varepsilon_4 - \varepsilon_5 - E + \Delta) + \frac{J}{4N} (\Gamma_{[12],4}^{\alpha\downarrow} + \Gamma_{23,5}^{\alpha\uparrow} - \Gamma_{13,5}^{\alpha\uparrow} + 2\Gamma_{31,4}^{\beta\downarrow} \\ - 2\Gamma_{32,4}^{\beta\downarrow}) + \frac{J}{4N} \sum_6 (\Gamma_{[62]3,45}^{\alpha\downarrow\uparrow} + \Gamma_{[16]3,45}^{\alpha\downarrow\uparrow} - \Gamma_{[12]6,45}^{\alpha\downarrow\uparrow} - \Gamma_{[12]3,65}^{\alpha\downarrow\uparrow} + \Gamma_{[12]3,46}^{\alpha\downarrow\uparrow} \\ + 2\Gamma_{[63]1,54}^{\beta\downarrow\downarrow} - 2\Gamma_{[63]2,54}^{\beta\downarrow\downarrow} + 2\Gamma_{3[12],46}^{\beta\downarrow\downarrow}) + \dots = 0, \end{aligned} \quad (10)$$

$$\begin{aligned} \Gamma_{1[23],45}^{\alpha\uparrow\uparrow} (\varepsilon_1 + \varepsilon_2 + \varepsilon_3 - \varepsilon_4 - \varepsilon_5 - E + \Delta) + \frac{J}{4N} (\Gamma_{12,4}^{\alpha\uparrow} - \Gamma_{12,5}^{\alpha\uparrow} - \Gamma_{13,4}^{\alpha\uparrow} + \Gamma_{13,5}^{\alpha\uparrow} \\ + 2\Gamma_{[23],4}^{\beta\uparrow} - 2\Gamma_{[23],5}^{\beta\uparrow}) + \frac{J}{4N} \sum_6 (\Gamma_{6[23],45}^{\alpha\uparrow\uparrow} - \Gamma_{1[63],45}^{\alpha\uparrow\uparrow} - \Gamma_{1[26],45}^{\alpha\uparrow\uparrow} \\ + \Gamma_{1[23],65}^{\alpha\uparrow\uparrow} + \Gamma_{1[23],46}^{\alpha\uparrow\uparrow} - 2\Gamma_{[623],45}^{\beta\uparrow\uparrow} + 2\Gamma_{[23]1,46}^{\beta\uparrow\downarrow} - 2\Gamma_{[23]1,56}^{\beta\uparrow\downarrow}) + \dots = 0, \end{aligned} \quad (11)$$

where $[12]$, etc., attached to the coefficients denote the antisymmetrized sum. Equations corresponding to Γ^β , $\Gamma^{\beta\uparrow}$, ... are obtained from Eqs. (6)~(11) by replacing Δ with $-\Delta$ and reversing all spin suffixes. Eliminating $\Gamma_{12,3}$ and also higher order terms from these equations, we can obtain simultaneous integral equations for Γ_1^α and Γ_1^β . By the method of collecting all the most divergent

terms in the integration kernel⁶⁾ and by the assumption of a constant density of states ρ for $|\varepsilon| < D$ (D is the half of the band width), these equations are solved⁸⁾ in a closed form for a magnetic field such as

$$\log \left(1 + \frac{A}{\tilde{E}} \right) / \log \frac{-\tilde{E}}{D} \ll 1, \quad (12)$$

where \tilde{E} is an anomalous part of the energy given below.

The obtained results which are correct with respect to the most divergent terms are as follows. The ground state energy consists of two parts,

$$E = \Delta E + (\tilde{E} + A), \quad (13)$$

where ΔE is the energy shift of the normal part,³⁾

$$\Delta E = -A - \frac{3}{4} \left(\frac{\rho J}{N} \right)^2 D \log 2 + \dots, \quad (14)$$

and \tilde{E} is the anomalous part,

$$\tilde{E} = -(\tilde{E}_0^2 + A^2)^{1/2} \quad (15)$$

with \tilde{E}_0 , the binding energy in the absence of the field,^{6),7)}

$$\tilde{E}_0 = -D e^{N/\rho J}. \quad (16)$$

Though the energy shift obtained by the usual perturbation theory has also a field dependence, it is smaller than A and \tilde{E} by the factor of $\rho J/N$, and therefore it should be neglected in the present approximation. The wave functions $I^\alpha(\varepsilon)$ and $I^\beta(\varepsilon)$ associated with the energy, Eq. (13), are expressed as

$$I^\alpha(\varepsilon) = \frac{-1}{\varepsilon - \tilde{E} + A} \left[\left(1 - \frac{\rho J}{N} \log \frac{\varepsilon - \tilde{E}_0}{D} \right)^{-1/4} - \frac{1}{3} \left(1 - \frac{\rho J}{N} \log \frac{-\tilde{E}_0}{D} \right)^{1/2} \left(1 - \frac{\rho J}{N} \log \frac{\varepsilon - \tilde{E}_0}{D} \right)^{-3/4} \right], \quad (17a)$$

$$I^\beta(\varepsilon) = \frac{1}{\varepsilon - \tilde{E} - A} \left[\left(1 - \frac{\rho J}{N} \log \frac{\varepsilon - \tilde{E}_0}{D} \right)^{-1/4} - \frac{1}{3} \left(1 - \frac{\rho J}{N} \log \frac{-\tilde{E}_0}{D} \right)^{1/2} \left(1 - \frac{\rho J}{N} \log \frac{\varepsilon - \tilde{E}_0}{D} \right)^{-3/4} \right]. \quad (17b)$$

As stated in II, the second term in the parentheses of Eqs. (17a, b) cannot be omitted for later calculations in spite of the factor of $[1 - (\rho J/N) \log(-\tilde{E}_0/D)]^{1/2}$, because the first term becomes of the same order as the second at $\varepsilon = 0$. In deriving the simultaneous equations for $I^\alpha(\varepsilon)$ and $I^\beta(\varepsilon)$ of which solution is given above and for later calculations, we use the following expansion forms for the coefficients $\Gamma_{[12],3}^{\alpha\downarrow}$, $\Gamma_{12,3}^{\alpha\uparrow}$, $\Gamma_{[123],[45]}^{\alpha\downarrow\downarrow}$, $\Gamma_{[12],3,45}^{\alpha\downarrow\uparrow}$ and $\Gamma_{1[23],[45]}^{\alpha\uparrow\uparrow}$:

$$\Gamma_{[12],3}^{\alpha\downarrow} D_{123} = -\frac{J}{4N} (\Gamma_1^\alpha - \Gamma_2^\alpha) + \left(\frac{J}{4N} \right)^2 \sum_4 \left[\frac{-5\Gamma_2^\alpha + \Gamma_4^\alpha + \Gamma_4^\beta}{D_{423}} + \frac{5\Gamma_1^\alpha - \Gamma_4^\alpha - 2\Gamma_4^\beta}{D_{143}} \right]$$

$$\begin{aligned}
& -\frac{\Gamma_1^\alpha - \Gamma_2^\alpha}{D_{124}} \Big] - \left(\frac{J}{4N}\right)^3 \sum_{45} \Big[\frac{1}{D_{143}} \left(\frac{13\Gamma_1^\alpha - 5\Gamma_5^\alpha - 4\Gamma_5^\beta}{D_{153}} \right. \\
& + \frac{-5\Gamma_4^\alpha - 3\Gamma_5^\alpha + 2\Gamma_4^\beta + 2\Gamma_5^\beta}{D_{453}} + \frac{7\Gamma_1^\alpha + \Gamma_4^\alpha - 10\Gamma_4^\beta}{D_{145}} \Big) \\
& - \frac{1}{D_{243}} \left(\frac{13\Gamma_2^\alpha - 5\Gamma_5^\alpha - 4\Gamma_5^\beta}{D_{253}} + \frac{-5\Gamma_4^\alpha - 3\Gamma_5^\alpha + 2\Gamma_4^\beta + 2\Gamma_5^\beta}{D_{453}} \right. \\
& + \frac{7\Gamma_2^\alpha + \Gamma_4^\alpha - 10\Gamma_4^\beta}{D_{245}} \Big) + \frac{1}{D_{124}} \left(\frac{-5\Gamma_1^\alpha + \Gamma_5^\alpha + 2\Gamma_5^\beta}{D_{154}} + \frac{5\Gamma_2^\alpha - \Gamma_5^\alpha - 2\Gamma_5^\beta}{D_{254}} \right. \\
& + \frac{\Gamma_1^\alpha - \Gamma_2^\alpha}{D_{125}} \Big) + \frac{1}{D_{12345}} \left(\frac{2\Gamma_2^\alpha + \Gamma_4^\alpha}{D_{245}} - \frac{2\Gamma_1^\alpha + \Gamma_4^\alpha}{D_{145}} + \frac{7\Gamma_1^\alpha + \Gamma_4^\alpha - 4\Gamma_4^\beta}{D_{143}} \right. \\
& \left. \left. - \frac{7\Gamma_2^\alpha + \Gamma_4^\alpha - 4\Gamma_4^\beta}{D_{243}} + \frac{-5\Gamma_1^\alpha + 5\Gamma_2^\alpha}{D_{125}} \right) \right] + \dots, \quad (18)
\end{aligned}$$

$$\begin{aligned}
\Gamma_{12,3}^{\alpha\uparrow} D_{123} &= \left(\frac{J}{4N}\right) (\Gamma_1^\alpha - 2\Gamma_2^\beta) + \left(\frac{J}{4N}\right)^2 \sum_4 \Big[\frac{-\Gamma_4^\alpha + 4\Gamma_2^\beta - 2\Gamma_4^\beta}{D_{423}} + \frac{\Gamma_1^\alpha - 2\Gamma_4^\beta}{D_{143}} \\
& + \frac{-5\Gamma_1^\alpha + 4\Gamma_2^\beta}{D_{124}} \Big] + \left(\frac{J}{4N}\right)^3 \sum_{45} \Big[\frac{1}{D_{143}} \left(\frac{\Gamma_1^\alpha - 2\Gamma_5^\beta}{D_{153}} + \frac{-\Gamma_5^\alpha + 4\Gamma_4^\beta - 2\Gamma_5^\beta}{D_{453}} \right. \\
& + \frac{-5\Gamma_1^\alpha + 4\Gamma_4^\beta}{D_{145}} \Big) - \frac{1}{D_{243}} \left(\frac{5\Gamma_5^\alpha - 14\Gamma_2^\beta + 4\Gamma_5^\beta}{D_{253}} + \frac{-\Gamma_4^\alpha - 4\Gamma_5^\alpha + 10\Gamma_4^\beta}{D_{453}} \right. \\
& + \frac{5\Gamma_4^\alpha - 2\Gamma_2^\beta - 2\Gamma_4^\beta}{D_{245}} \Big) + \frac{1}{D_{124}} \left(\frac{7\Gamma_1^\alpha - 4\Gamma_5^\alpha}{D_{154}} + \frac{-3\Gamma_5^\alpha - 2\Gamma_2^\beta + 2\Gamma_5^\beta}{D_{254}} \right. \\
& + \frac{13\Gamma_1^\alpha - 14\Gamma_2^\beta}{D_{125}} \Big) + \frac{1}{D_{12345}} \left(\frac{-4\Gamma_4^\alpha + 4\Gamma_2^\beta - 2\Gamma_4^\beta}{D_{245}} + \frac{-2\Gamma_1^\alpha - \Gamma_4^\alpha}{D_{145}} \right. \\
& \left. + \frac{-5\Gamma_1^\alpha + 10\Gamma_4^\beta}{D_{143}} + \frac{-\Gamma_4^\alpha - 2\Gamma_2^\beta + 4\Gamma_4^\beta}{D_{243}} + \frac{7\Gamma_1^\alpha - 2\Gamma_2^\beta}{D_{125}} \right) \Big] + \dots, \quad (19)
\end{aligned}$$

$$\begin{aligned}
\Gamma_{[123],[45]}^{\alpha\downarrow\downarrow} D_{12345} &= \left(\frac{J}{4N}\right)^2 \Big[\frac{-\Gamma_1^\alpha + \Gamma_2^\alpha}{D_{124}} + \frac{\Gamma_1^\alpha - \Gamma_2^\alpha}{D_{125}} + \frac{\Gamma_1^\alpha - \Gamma_3^\alpha}{D_{134}} - \frac{\Gamma_1^\alpha - \Gamma_3^\alpha}{D_{135}} \\
& - \frac{\Gamma_2^\alpha - \Gamma_3^\alpha}{D_{234}} + \frac{\Gamma_2^\alpha - \Gamma_3^\alpha}{D_{235}} \Big] + \dots, \quad (20)
\end{aligned}$$

$$\begin{aligned}
\Gamma_{[12]3,[45]}^{\alpha\downarrow\uparrow} D_{12345} &= \left(\frac{J}{4N}\right)^2 \Big[\frac{\Gamma_1^\alpha - \Gamma_2^\alpha}{D_{124}} + \frac{\Gamma_1^\alpha - 2\Gamma_3^\beta}{D_{135}} - \frac{\Gamma_2^\alpha - 2\Gamma_3^\beta}{D_{235}} - \frac{2\Gamma_3^\beta - 4\Gamma_1^\alpha}{D_{134}} \\
& + \frac{2\Gamma_3^\beta - 4\Gamma_2^\alpha}{D_{234}} \Big] + \dots, \quad (21)
\end{aligned}$$

$$\begin{aligned}
\Gamma_{[123],[45]}^{\alpha\uparrow\uparrow} D_{12345} &= \left(\frac{J}{4N}\right)^2 \Big[-\frac{\Gamma_1^\alpha - 2\Gamma_2^\beta}{D_{124}} + \frac{\Gamma_1^\alpha - 2\Gamma_2^\beta}{D_{125}} + \frac{\Gamma_1^\alpha - 2\Gamma_3^\beta}{D_{134}} \\
& - \frac{\Gamma_1^\alpha - 2\Gamma_3^\beta}{D_{135}} + \frac{2\Gamma_2^\beta - 2\Gamma_3^\beta}{D_{234}} - \frac{2\Gamma_2^\beta - 2\Gamma_3^\beta}{D_{235}} \Big] + \dots, \quad (22)
\end{aligned}$$

where

$$D_{123} = \varepsilon_1 + \varepsilon_2 - \varepsilon_3 - \tilde{E}_0,$$

$$D_{12345} = \varepsilon_1 + \varepsilon_2 + \varepsilon_3 - \varepsilon_4 - \varepsilon_5 - \tilde{E}_0.$$

Coefficients with the index β corresponding to Eqs. (18)~(22) are obtained from them by reversing all spin directions.

We should add a remark on these expressions. When these are derived first from Eqs. (6)~(11) by the iteration method, $(\varepsilon_1 + \varepsilon_2 - \varepsilon_3 - \tilde{E} \pm \Delta)$ and $(\varepsilon_1 + \varepsilon_2 + \varepsilon_3 - \varepsilon_4 - \varepsilon_5 - \tilde{E} \pm \Delta)$ occur in place of D_{123} and D_{12345} , respectively. However, in calculations so far and later $\Gamma_{12,3}$, $\Gamma_{123,45}$ are used only in the integrated form and at that time $1/(\varepsilon_1 + \varepsilon_2 - \varepsilon_3 - \tilde{E} \pm \Delta)$ comes in a form such as $\log(\varepsilon_1 + \varepsilon_2 - \varepsilon_3 - \tilde{E} \pm \Delta)/D$, which is rewritten as

$$\log \frac{\varepsilon_1 + \varepsilon_2 - \varepsilon_3 - \tilde{E} \pm \Delta}{D} = \log \frac{\varepsilon_1 + \varepsilon_2 - \varepsilon_3 - \tilde{E}_0}{D} + \log \frac{\varepsilon_1 + \varepsilon_2 - \varepsilon_3 - \tilde{E} \pm \Delta}{\varepsilon_1 + \varepsilon_2 - \varepsilon_3 - \tilde{E}_0},$$

the second term of this expression is very small compared with the first by the condition of (12). On the other hand, $1/(-\tilde{E} \pm \Delta)$ comes directly from the normalization integral (23a, b) given below and also from $\Gamma^\alpha(0)$ and $\Gamma^\beta(0)$ which appear in the calculation of § 4. Field dependence in the argument of logarithm is thus very small compared with that of $1/(-\tilde{E} \pm \Delta)$ and can be neglected. Therefore the field dependence of Eqs. (18)~(22) appears only through that of $\Gamma^\alpha(\varepsilon)$ and $\Gamma^\beta(\varepsilon)$ and such an approximation is sufficient for the calculations of the following sections. Similar circumstances have been seen in Eqs. (17a, b) where the effect of the magnetic field appears only in the first factor. This fact makes calculations remarkably easy.

In order to calculate physical quantities, the normalization integral of the wave function ψ is obtained in the same manner as I,

$$\langle \psi | \psi \rangle = \langle \psi_\alpha | \psi_\alpha \rangle + \langle \psi_\beta | \psi_\beta \rangle, \quad (23)$$

$$\langle \psi_\alpha | \psi_\alpha \rangle = \sum_1 (\Gamma_1^\alpha)^2 + \frac{1}{2} \sum_{123} (\Gamma_{[12],3}^{\alpha\uparrow})^2 + \sum_{123} (\Gamma_{12,3}^{\alpha\uparrow})^2 + \dots$$

Contributions from Γ_{123} and other higher order terms to $\langle \psi_\alpha | \psi_\alpha \rangle$ can be neglected in comparison with the first term, and the first term is calculated by the use of Eq. (17a) as

$$\langle \psi_\alpha | \psi_\alpha \rangle = \sum_1 (\Gamma_1^\alpha)^2 = \frac{4}{9} \rho \frac{1}{-\tilde{E} + \Delta} \left(1 - \frac{\rho J}{N} \log \frac{-\tilde{E}_0}{D} \right)^{-1/2}. \quad (23a)$$

In the same way we obtain

$$\langle \psi_\beta | \psi_\beta \rangle = \sum_1 (\Gamma_1^\beta)^2 = \frac{4}{9} \rho \frac{1}{-\tilde{E} - \Delta} \left(1 - \frac{\rho J}{N} \log \frac{-\tilde{E}_0}{D} \right)^{-1/2}. \quad (23b)$$

Induced localized spin is calculated by the use of these equations:

$$\langle S_z \rangle = \frac{\langle \psi | S_z | \psi \rangle}{\langle \psi | \psi \rangle} = \frac{1}{2} \frac{\langle \psi_\alpha | \psi_\alpha \rangle - \langle \psi_\beta | \psi_\beta \rangle}{\langle \psi | \psi \rangle} = -\frac{1}{2} \frac{\Delta}{(\tilde{E}_0^2 + \Delta^2)^{1/2}}, \quad (24)$$

and from this a finite susceptibility can be obtained. This field-dependence of the magnetization is particularly significant in the sense that it does not include any logarithmic function of field. These results are completely incompatible with those obtained by the Suhl-Nagaoka theories.¹²⁾

As mentioned before, all these results have been derived under the condition of (12), which can be rewritten with the use of Eq. (15) as $\Delta \ll -\tilde{E}_0 \times \exp(-N/3\rho J)$. Another condition which is omitted in references 4) and 8) is caused by the following consideration. Equation (15) indicates that $\tilde{E} + \Delta$ is always negative and this means that the bound state is more stable than that obtained by the usual perturbation theory including the magnetic field. However, for increasing field, $\tilde{E} + \Delta$ decreases gradually and if it becomes the order of $\Delta\rho J/N$, any decisive conclusion cannot be drawn down, because at that field $\tilde{E} + \Delta$ is comparable with terms neglected in the calculations. This leads to another condition about the applied field:

$$\frac{\rho J}{N} \frac{\Delta}{\tilde{E} + \Delta} \ll 1, \quad (25)$$

which is rewritten as $\Delta \ll -\tilde{E}_0/\sqrt{\rho|J|/N}$ by the use of Eq. (15), and it is a more severe condition than (12). Anyway for a magnetic field such as

$$\Delta = c|\tilde{E}_0|, \quad c: \text{any finite value independent of } \rho J/N, \quad (26)$$

namely for much larger field than $|\tilde{E}_0|$, inequalities (12) and (25) are both satisfied thoroughly in the weak coupling limit. Therefore, a significant result is that the anomalous binding energy decreases but never vanishes by an external field.

§ 3. Spin polarization density and spin correlation density at the impurity site

In this section and the next one, local electron distributions with up- and down-spins are investigated separately in each of two components ψ_α and ψ_β by the use of the results described in the previous section, in parallel with II. In order to calculate these quantities, we calculate summations of $\langle \psi_\alpha | a_{k'\uparrow}^* a_{k\uparrow} | \psi_\alpha \rangle$ and $\langle \psi_\alpha | a_{k'\downarrow}^* a_{k\downarrow} | \psi_\alpha \rangle$, of which expressions have different forms according as k or k' is an electron state or a hole state, as given in Eqs. (18)~(23) of II in slightly different notations. For simplicity we omit the contribution from the Fermi sphere, and only deviations from it are given.

We calculate first the charge density at the impurity site in the component ψ_α :

$$\begin{aligned} n_{\alpha\uparrow}(0) + n_{\alpha\downarrow}(0) &= \frac{1}{V} \frac{1}{\langle \psi | \psi \rangle} \sum_{kk'} \langle \psi_\alpha | a_{k'\uparrow}^* a_{k\uparrow} + a_{k'\downarrow}^* a_{k\downarrow} | \psi_\alpha \rangle \\ &= \frac{1}{V} \frac{1}{\langle \psi | \psi \rangle} \left\{ (\sum_1 \Gamma_1^\alpha)^2 + 2 \sum_{123} \Gamma_1^\alpha (\Gamma_{12,3}^{\alpha\uparrow} + \Gamma_{[12],3}^{\alpha\downarrow}) \right\} \end{aligned}$$

$$\begin{aligned}
& + \sum_{1234} \left[\Gamma_{12,3}^{\alpha\uparrow} (\Gamma_{14,3}^{\alpha\uparrow} - \Gamma_{12,4}^{\alpha\uparrow} + \Gamma_{42,3}^{\alpha\uparrow}) + \Gamma_{[12],3}^{\alpha\downarrow} \left(\Gamma_{[14],3}^{\alpha\downarrow} - \frac{1}{2} \Gamma_{[12],4}^{\alpha\downarrow} \right) \right] \\
& - \sum_{12345} \left[\Gamma_{[12],3}^{\alpha\downarrow} (\Gamma_{[12],4,35}^{\alpha\downarrow\uparrow} - \Gamma_{[124],[35]}^{\alpha\downarrow\uparrow}) - 2\Gamma_{12,3}^{\alpha\uparrow} (\Gamma_{1[24],[35]}^{\alpha\uparrow\uparrow} + \Gamma_{[14]2,53}^{\alpha\uparrow\uparrow}) \right] + \dots \Big\}, \quad (27)
\end{aligned}$$

where V denotes the total volume of the crystal. By the use of Eqs. (18) ~ (22), this is expressed with Γ_1^α and Γ_1^β alone. After calculating integrals to be correct for the most divergent contributions, we obtain up to third order in J

$$\begin{aligned}
n_{\alpha\uparrow}(0) + n_{\alpha\downarrow}(0) = \frac{1}{V} \frac{1}{\langle\psi|\psi\rangle} & \left[(\sum_1 \Gamma_1^\alpha)^2 \right. \\
& \left. - \sum_{12} \Gamma_1^\alpha \left(\frac{1}{2} \Gamma_2^\alpha - \Gamma_2^\beta \right) \left(X_{12} + \frac{1}{2} X_{12}^2 + \frac{1}{3} X_{12}^3 + \dots \right) \right], \quad (28)
\end{aligned}$$

where

$$X_{12} = \frac{\rho J}{N} \log \frac{\varepsilon_1 + \varepsilon_2 - \tilde{E}_0}{D},$$

and by assuming that the n -th term in the parentheses is $(1/n) X_{12}^n$, this can be written as

$$n_{\alpha\uparrow}(0) + n_{\alpha\downarrow}(0) = \frac{1}{V} \frac{1}{\langle\psi|\psi\rangle} \left[(\sum_1 \Gamma_1^\alpha)^2 + \sum_{12} \Gamma_1^\alpha \left(\frac{1}{2} \Gamma_2^\alpha - \Gamma_2^\beta \right) \log(1 - X_{12}) \right]. \quad (29)$$

With the use of Eq. (17a), each term in the parentheses is integrated in the weak coupling limit as

$$\begin{aligned}
(\sum_1 \Gamma_1^\alpha)^2 &= \rho^2 \frac{16}{9} \left(\frac{N}{\rho J} \right)^2 \left[1 + \frac{\rho J}{N} \log \frac{-\tilde{E} + D}{-\tilde{E}_0} \left(1 - \frac{\rho J}{N} \log \frac{-\tilde{E}_0}{D} \right)^{-1/4} \right], \\
\sum_{12} \Gamma_1^\alpha \Gamma_2^\alpha \log(1 - X_{12}) &= -\rho^2 \frac{32}{27} \left(\frac{N}{\rho J} \right)^2 \\
&\quad \times \left[1 + 2 \frac{\rho J}{N} \log \frac{-\tilde{E} + D}{-\tilde{E}_0} \left(1 - \frac{\rho J}{N} \log \frac{-\tilde{E}_0}{D} \right)^{-1/4} \right], \\
\sum_{12} \Gamma_1^\alpha \Gamma_2^\beta \log(1 - X_{12}) &= \rho^2 \frac{32}{27} \left(\frac{N}{\rho J} \right)^2. \quad (30)
\end{aligned}$$

In these expressions, field dependence is only in the form of $\log[(-\tilde{E} + D)/-\tilde{E}_0]$ and this part is of the next divergent order for the magnetic field of Eq. (26) compared with the field-independent terms as remarked in the previous section. On the other hand, the normalization integral $\langle\psi|\psi\rangle$ which is given in Eq. (23) has a stronger field dependence of the form of $1/(-\tilde{E} \pm D)$ and other weak field-dependent terms are neglected in the normalization integral as next divergent terms. Therefore for the calculation of Eq. (29), only the most divergent (field independent) terms in Eq. (30) are significant. Thus we obtain

$$n_{\alpha\uparrow}(0) + n_{\alpha\downarrow}(0) = 0, \quad (31)$$

and by the symmetry relation,

$$n_{\beta\uparrow}(0) + n_{\beta\downarrow}(0) = 0. \quad (32)$$

That is, there appears no charge density at the impurity site.

Next we calculate the spin polarization density at the impurity site by the same step of calculations. Its component for ϕ_α is expressed as

$$\begin{aligned} & \frac{1}{2} [n_{\alpha\uparrow}(0) - n_{\alpha\downarrow}(0)] \\ &= \frac{1}{2V} \frac{1}{\langle \phi | \phi \rangle} \sum_{kk'} \langle \phi_\alpha | a_{k'\uparrow}^* a_{k\uparrow} - a_{k'\downarrow}^* a_{k\downarrow} | \phi_\alpha \rangle \\ &= \frac{1}{2V} \frac{1}{\langle \phi | \phi \rangle} \left\{ -(\sum_1 \Gamma_1^\alpha)^2 + 2 \sum_{123} \Gamma_1^\alpha (\Gamma_{12,3}^{\alpha\uparrow} - \Gamma_{[12],3}^{\alpha\downarrow}) \right. \\ & \quad + \sum_{1234} \left[\Gamma_{12,3}^{\alpha\uparrow} (\Gamma_{14,3}^{\alpha\uparrow} - \Gamma_{12,4}^{\alpha\uparrow} - \Gamma_{42,3}^{\alpha\uparrow}) - \Gamma_{[12],3}^{\alpha\downarrow} \left(\Gamma_{[14],3}^{\alpha\downarrow} - \frac{1}{2} \Gamma_{[12],3}^{\alpha\downarrow} \right) \right] \\ & \quad \left. - \sum_{12345} [\Gamma_{[12],3}^{\alpha\downarrow} (\Gamma_{[12]4,35}^{\alpha\uparrow} - \Gamma_{[124],53}^{\alpha\downarrow}) - 2\Gamma_{12,3}^{\alpha\uparrow} (\Gamma_{1[24],35}^{\alpha\uparrow} - \Gamma_{[14]2,53}^{\alpha\downarrow})] + \dots \right\}. \end{aligned} \quad (33)$$

Combining this with $n_{\beta\uparrow}(0) - n_{\beta\downarrow}(0)$ which is obtained from Eq. (33) by the symmetry relation and by the same procedure from Eq. (27) to Eq. (28), we obtain the expression for the spin polarization density at the impurity site as

$$\begin{aligned} & \frac{1}{2} [n_{\alpha\uparrow}(0) - n_{\alpha\downarrow}(0) + n_{\beta\uparrow}(0) - n_{\beta\downarrow}(0)] \\ &= \frac{1}{2V} \frac{1}{\langle \phi | \phi \rangle} \left\{ (\sum_1 \Gamma_1^\beta)^2 - (\sum_1 \Gamma_1^\alpha)^2 \right. \\ & \quad + \frac{1}{2} \sum_{12} (\Gamma_1^\alpha \Gamma_2^\alpha - \Gamma_1^\beta \Gamma_2^\beta) \left[X_{12} + \frac{1}{2} X_{12}^2 + \frac{1}{3} X_{12}^3 + \dots \right] \\ & \quad \left. + \frac{J}{N} \sum_{123} \left[(\Gamma_1^\alpha)^2 \frac{1}{\varepsilon_1 + \varepsilon_2 - \varepsilon_3 - \tilde{E} + D} - (\Gamma_1^\beta)^2 \frac{1}{\varepsilon_1 + \varepsilon_2 - \varepsilon_3 - \tilde{E} - D} \right] \right\}, \end{aligned} \quad (34)$$

where the last term is calculated in logarithmic accuracy as

$$\begin{aligned} \sum_{123} (\Gamma_1^\alpha)^2 \frac{1}{\varepsilon_1 + \varepsilon_2 - \varepsilon_3 - \tilde{E} + D} &= \rho^2 \sum_1 (\Gamma_1^\alpha)^2 \left[2D \log 2 + (\varepsilon_1 - \tilde{E} + D) \log \frac{\varepsilon_1 - \tilde{E} + D}{D} \right] \\ &\simeq 2D\rho^2 \log 2 \sum_1 (\Gamma_1^\alpha)^2 = \sum_1 (\Gamma_1^\alpha)^2 \sum_{23} \frac{1}{\varepsilon_2 - \varepsilon_3}. \end{aligned} \quad (35)$$

Equation (35) is of higher order in J than $(\sum_1 \Gamma_1^\alpha)^2$, etc. in Eq. (34) as is easily shown from Eqs. (23a, b) and (30), so that only the part proportional to D is

retained. The remaining most divergent terms in Eq. (34) cancel with each other in the same way as the charge density does. As a result, the spin polarization density at the impurity site is obtained as

$$\begin{aligned}
 \frac{1}{V} \langle s_z(0) \rangle &= \frac{1}{2} [n_{\alpha\uparrow}(0) - n_{\alpha\downarrow}(0) + n_{\beta\uparrow}(0) - n_{\beta\downarrow}(0)] \\
 &= \frac{J}{2VN} \frac{1}{\langle \phi | \phi \rangle} \sum_1 [(\Gamma_1^\alpha)^2 - (\Gamma_1^\beta)^2] \sum_{kk'} \frac{1}{\epsilon_k - \epsilon_{k'}} \\
 &= \frac{J}{2VN} \frac{1}{\langle \phi | \phi \rangle} [\langle \phi_\alpha | \phi_\alpha \rangle - \langle \phi_\beta | \phi_\beta \rangle] \sum_{kk'} \frac{1}{\epsilon_k - \epsilon_{k'}} \\
 &= \langle S_z \rangle \left(\frac{J}{VN} \right) \sum_{kk'} \frac{1}{\epsilon_k - \epsilon_{k'}}, \tag{36}
 \end{aligned}$$

where use has been made of Eqs. (23a, b) and (24). Equation (36) is just the same expression as obtained in the RKY theory,¹⁰⁾ and the effect of the bound state is included only in the expression of $\langle S_z \rangle$.

Similarly the z -component of the spin correlation density at the impurity is calculated as

$$\begin{aligned}
 &\frac{1}{2V} \frac{1}{\langle \phi | \phi \rangle} \sum_{kk'} \langle \phi | (a_{k'\uparrow}^* a_{k\uparrow} - a_{k'\downarrow}^* a_{k\downarrow}) S_z | \phi \rangle \\
 &= \frac{1}{4} [n_{\alpha\uparrow}(0) - n_{\alpha\downarrow}(0) - n_{\beta\uparrow}(0) + n_{\beta\downarrow}(0)] \\
 &= \frac{1}{4V} \frac{1}{\langle \phi | \phi \rangle} \left\{ -(\sum_1 \Gamma_1^\alpha)^2 - (\sum_1 \Gamma_1^\beta)^2 \right. \\
 &\quad + \sum_{12} (\Gamma_1^\alpha \Gamma_2^\alpha + \Gamma_1^\beta \Gamma_2^\beta) \left[\frac{1}{2} X_{12} + \frac{1}{4} X_{12}^2 + \frac{1}{3} X_{12}^3 + \dots \right] \\
 &\quad + \sum_{12} \Gamma_1^\alpha \Gamma_2^\beta \left[2X_{12} + 2X_{12}^2 + \frac{8}{3} X_{12}^3 + \dots \right] \\
 &\quad \left. + \frac{J}{N} \sum_{kk'} \frac{1}{\epsilon_k - \epsilon_{k'}} \sum_1 [(\Gamma_1^\alpha)^2 + (\Gamma_1^\beta)^2] \right\} \\
 &= \frac{1}{4V} \frac{1}{\langle \phi | \phi \rangle} \left\{ -\frac{3}{4} [(\sum_1 \Gamma_1^\alpha)^2 + (\sum_1 \Gamma_1^\beta)^2] \right. \\
 &\quad + \frac{1}{3} \sum_{12} (\Gamma_1^\alpha \Gamma_2^\alpha + \Gamma_1^\beta \Gamma_2^\beta) \left[-1 + X_{12} + \frac{1}{4} (1 - X_{12})^{-2} \right] \\
 &\quad \left. + \frac{2}{3} \sum_{12} \Gamma_1^\alpha \Gamma_2^\beta [-1 + X_{12} + (1 - X_{12})^{-2}] \right\} \\
 &\quad + \frac{1}{4V} \frac{J}{N} \sum_{kk'} \frac{1}{\epsilon_k - \epsilon_{k'}}. \tag{37}
 \end{aligned}$$

Integrals in Eq. (37) are calculated in a way similar to Eq. (30),

$$\begin{aligned}\sum_{12} \Gamma_1^\alpha \Gamma_2^\alpha X_{12} &= \sum_{12} \Gamma_1^\beta \Gamma_2^\beta X_{12} = -\sum_{12} \Gamma_1^\alpha \Gamma_2^\beta X_{12} = \rho^2 \frac{32}{45} \left(\frac{N}{\rho J} \right)^2, \\ \sum_{12} \Gamma_1^\alpha \Gamma_2^\alpha (1 - X_{12})^{-2} &= \sum_{12} \Gamma_1^\beta \Gamma_2^\beta (1 - X_{12})^{-2} = -\sum_{12} \Gamma_1^\alpha \Gamma_2^\beta (1 - X_{12})^{-2} \\ &= -\rho^2 \left(\frac{N}{\rho J} \right)^2 \left[\frac{16}{3} - \frac{64}{27} \left(1 - \frac{\rho J}{N} \log \frac{-\tilde{E}_0}{D} \right)^{-1/2} \right],\end{aligned}\quad (38)$$

where field-dependent terms are also of the next divergent terms and are thus neglected for the same reason as before. Inserting Eqs. (30) and (38) into Eq. (37), we finally obtain

$$\begin{aligned}\frac{1}{2V} \frac{1}{\langle \psi | \psi \rangle} \sum_{kk'} \langle \psi | (a_{k'\uparrow}^* a_{k\uparrow} - a_{k'\downarrow}^* a_{k\downarrow}) S_z | \psi \rangle \\ = -\frac{1}{3} \left(\frac{N}{\rho J} \right)^2 \frac{\rho}{V} \frac{\tilde{E}_0^2}{(\tilde{E}_0^2 + D^2)^{1/2}} + \frac{J}{4VN} \sum_{kk'} \frac{1}{\varepsilon_k - \varepsilon_{k'}}.\end{aligned}\quad (39)$$

In Eq. (39), we obtain the z -component of the spin correlation density at the impurity site and from this we can prove that other components of this quantity are also equal to Eq. (39) as follows; assuming that all three components are equal to Eq. (39) and by the use of the Feynman relation, we can obtain the correct result Eq. (13) for the total energy. Thus the spin correlation density at the impurity site is obtained in the form

$$\frac{1}{V} \langle \mathbf{s}(0) \cdot \mathbf{S} \rangle = -\left(\frac{N}{\rho J} \right)^2 \frac{\rho}{V} \frac{\tilde{E}_0^2}{(\tilde{E}_0^2 + D^2)^{1/2}} + \frac{3}{4} \frac{J}{VN} \sum_{kk'} \frac{1}{\varepsilon_k - \varepsilon_{k'}}, \quad (40)$$

where the first term expresses the contribution from the formation of the bound state and the second term is that of the normal part. The kinetic energy, the potential energy and the Zeeman energy are obtained separately by the use of Eqs. (13) and (40) as

$$\begin{aligned}E_{\text{zeeman}} &= g\mu_B \langle S_z \rangle H_z = -\frac{D^2}{(\tilde{E}_0^2 + D^2)^{1/2}}, \\ E_{\text{exch}} &= \frac{N}{\rho J} \frac{\tilde{E}_0^2}{(\tilde{E}_0^2 + D^2)^{1/2}} - \frac{3}{4\rho^2} \left(\frac{\rho J}{N} \right)^2 \sum_{kk'} \frac{1}{\varepsilon_k - \varepsilon_{k'}}, \\ E_{\text{kin}} &= E - E_{\text{zeeman}} - E_{\text{exch}} = -\left(1 + \frac{N}{\rho J} \right) \frac{\tilde{E}_0^2}{(\tilde{E}_0^2 + D^2)^{1/2}} + \frac{3}{8\rho^2} \left(\frac{\rho J}{N} \right)^2 \sum_{kk'} \frac{1}{\varepsilon_k - \varepsilon_{k'}}.\end{aligned}\quad (41)$$

The electron densities at the impurity site for the up- and down-spins in ϕ_α and ϕ_β are obtained by combining Eqs. (31), (32), (36) and (39) as

$$n_{\alpha\uparrow}(0) = -n_{\alpha\downarrow}(0) = -\frac{\rho}{3V} \left(\frac{N}{\rho J} \right)^2 \frac{\tilde{E}_0^2}{(\tilde{E}_0^2 + D^2)^{1/2}}$$

$$\begin{aligned}
& + \frac{J}{4VN} \left(1 - \frac{D}{(\tilde{E}_0^2 + D^2)^{1/2}} \right) \sum_{kk'} \frac{1}{\varepsilon_k - \varepsilon_{k'}}, \\
n_{\beta\uparrow}(0) = -n_{\beta\downarrow}(0) = & \frac{\rho}{3V} \left(\frac{N}{\rho J} \right)^2 \frac{\tilde{E}_0^2}{(\tilde{E}_0^2 + D^2)^{1/2}} \\
& - \frac{J}{4VN} \left(1 + \frac{D}{(\tilde{E}_0^2 + D^2)^{1/2}} \right) \sum_{kk'} \frac{1}{\varepsilon_k - \varepsilon_{k'}}. \quad (42)
\end{aligned}$$

Anomalous parts of these are shown in Fig. 1 as the values at the origin. Total amounts of electron and hole trapped around the impurity in ψ_α and ψ_β are investigated in the next section.

§ 4. Total localized electrons with up- and down-spins in each of two components ψ_α and ψ_β

We calculate in this section the total localized electrons with up- and down-spins in each of two components ψ_α and ψ_β . For this purpose we calculate first,

$$n_{\alpha\uparrow} \pm n_{\alpha\downarrow} = \sum_k \lim_{k' \rightarrow k} \langle \psi_\alpha | a_{k'\uparrow}^* a_{k\uparrow} \pm a_{k'\downarrow}^* a_{k\downarrow} | \psi_\alpha \rangle / \langle \psi | \psi \rangle. \quad (43)$$

As mentioned in the previous section, these consist of three parts corresponding to the cases that states k and k' are both electron states, both hole states and one of them is an electron state and the other a hole state. Among them, the electron-electron and hole-hole parts are continuous as k' tends to k and therefore a contribution to Eq. (43) from these parts is equal to the total (not to restrict total local) amount of them in ψ_α . The structure of the wave function, Eq. (3), shows that net one electron with down-spin state is added in ψ_α . From this consideration or by the same calculation as that made in deriving Eqs. (33) and (34) from Eqs. (31) and (32) in II, we obtain

$$(n_{\alpha\uparrow} \pm n_{\alpha\downarrow})_{ee} + (n_{\alpha\uparrow} \pm n_{\alpha\downarrow})_{hh} = \pm \frac{\langle \psi_\alpha | \psi_\alpha \rangle}{\langle \psi | \psi \rangle}. \quad (44)$$

The contribution from electron-hole part distinguishes the total localized quantities from the trivial total quantities, Eq. (44), and makes a crucial effect as described in II. We calculate this part as follows,

$$(n_{\alpha\uparrow} \pm n_{\alpha\downarrow})_{eh} = 2 \sum_k \lim_{\substack{\varepsilon_{k'} \rightarrow 0_+ \\ \varepsilon_k \rightarrow 0_-}} (n_{\alpha\uparrow} \pm n_{\alpha\downarrow})_{eh}^{k'k}, \quad (45)$$

where

$$(n_{\alpha\uparrow} \pm n_{\alpha\downarrow})_{eh}^{k'k} \langle \psi | \psi \rangle = \langle \psi_\alpha | a_{k'\uparrow}^* a_{k\uparrow} \pm a_{k'\downarrow}^* a_{k\downarrow} | \psi_\alpha \rangle_{eh}. \quad (46)$$

The main point of this calculation as remarked in II is that though the contribution to Eq. (45) only comes from the Fermi surface, the integrand $(n_{\alpha\uparrow} \pm n_{\alpha\downarrow})_{eh}^{k'k}$ has a singularity of $(\varepsilon_{k'} - \varepsilon_k)^{-1}$ at that surface, so that a finite value can be obtained. By the use of Eq. (3), Eq. (46) is expressed in the coefficients I as

$$(n_{\alpha\uparrow} \pm n_{\alpha\downarrow})_{eh}^{k'k} \langle \psi | \psi \rangle = \sum_1 \Gamma_1^\alpha (\Gamma_{1k',k}^{\alpha\uparrow} \pm \Gamma_{[1k'],k}^{\alpha\downarrow}) \\ + \sum_{123} [\frac{1}{2} \Gamma_{[12],3}^{\alpha\downarrow} (\pm \Gamma_{[k'12],[k3]}^{\alpha\downarrow} - \Gamma_{[12]k',3k}^{\alpha\uparrow}) + \Gamma_{12,3}^{\alpha\uparrow} (\pm \Gamma_{[k'1]2,k3}^{\alpha\uparrow} - \Gamma_{1[k'2],[k3]}^{\alpha\uparrow})] + \dots \quad (47)$$

The right-hand side of this expression is calculated by the use of the Schrödinger equations (6) ~ (11) in order to draw the factor $(\varepsilon_{k'} - \varepsilon_k)^{-1}$. For example, for $\Gamma_1^\alpha \Gamma_{1k',k}^{\alpha\uparrow}$, we subtract Eq. (6) multiplied by $\Gamma_{1k',k}^{\alpha\uparrow}$ from Eq. (8) multiplied by Γ_1^α and then obtain $\Gamma_1^\alpha \Gamma_{1k',k}^{\alpha\uparrow} (\varepsilon_{k'} - \varepsilon_k)$. In this procedure, A which appears in the left-hand side of Eqs. (6) ~ (11) drops off. For the first term of Eq. (47), we derive

$$(n_{\alpha\uparrow} \pm n_{\alpha\downarrow})_{eh(1-3)}^{k'k} \langle \psi | \psi \rangle (\varepsilon_{k'} - \varepsilon_k) = \sum_1 \Gamma_1^\alpha (\Gamma_{1k',k}^{\alpha\uparrow} \pm \Gamma_{[1k'],k}^{\alpha\downarrow}) (\varepsilon_{k'} - \varepsilon_k) \\ = \frac{J}{4N} (\sum_1 \Gamma_1^\alpha) (\pm \Gamma_{k'}^\alpha - 2\Gamma_{k'}^\beta) \quad (48.1)$$

$$- \frac{J}{4N} \sum_1 (\Gamma_1^\alpha)^2 (\pm 1 - 1) \quad (48.2)$$

$$+ \frac{J}{2N} (\sum_1 \Gamma_1^\alpha) \sum_1 (\pm \Gamma_{1k',k}^{\beta\downarrow} + \Gamma_{[1k'],k}^{\beta\uparrow}) - \frac{J}{2N} (\sum_1 \Gamma_1^\beta) \sum_1 (\Gamma_{1k',k}^{\alpha\uparrow} \pm \Gamma_{[1k'],k}^{\alpha\downarrow}) \quad (48.3)$$

$$- \frac{J}{4N} \sum_{123} (\Gamma_{[21],3}^{\alpha\downarrow} + \Gamma_{12,3}^{\alpha\uparrow} - 2\Gamma_{21,3}^{\beta\downarrow}) (\Gamma_{1k',k}^{\alpha\uparrow} \pm \Gamma_{[1k'],k}^{\alpha\downarrow}) \quad (48.4)$$

$$- \frac{J}{4N} \sum_{12} \Gamma_1^\alpha [-\Gamma_{12,k}^{\alpha\uparrow} + \Gamma_{1k',2}^{\alpha\uparrow} - 2\Gamma_{k'1,2}^{\beta\downarrow} \pm (\Gamma_{[12],k}^{\alpha\downarrow} - \Gamma_{[1k'],2}^{\alpha\downarrow} + 2\Gamma_{21,k}^{\beta\downarrow})] \quad (48.5)$$

$$+ \frac{J}{4N} \sum_1 \Gamma_1^\alpha [\Gamma_{[12]k',3k}^{\alpha\downarrow} + \Gamma_{1[k'2],[3k]}^{\alpha\uparrow} + 2\Gamma_{[2k']1,k3}^{\beta\uparrow} \mp (\Gamma_{[21k'],[3k]}^{\alpha\downarrow} + \Gamma_{[1k']2,k3}^{\alpha\downarrow} + 2\Gamma_{2[k'],[k3]}^{\beta\downarrow})]. \quad (48.6)$$

Equation (48) corresponds to Eqs. (40) and (47) of II, in which the condition for the singlet state makes expressions passably simple.

Next step of calculation is to express the higher order coefficients $\Gamma_{12,3}$, $\Gamma_{123,45}$ in Eq. (48) with Γ_1^α and Γ_1^β by using Eqs. (18) ~ (22) and also corresponding equations with index β , and to calculate them retaining the most divergent contributions. The first term can be calculated as

$$\frac{J}{4N} (\sum_1 \Gamma_1^\alpha) (\pm \Gamma_{k'}^\alpha - 2\Gamma_{k'}^\beta) \\ = \left[\frac{1}{3} + \frac{\rho J}{6N} \left(1 - \frac{\rho J}{N} \log \frac{-\tilde{E}_0}{D} \right)^{-1/4} \log \frac{-\tilde{E} + D}{-\tilde{E}_0} \right] \cdot (\pm \Gamma_{k'}^\alpha - 2\Gamma_{k'}^\beta).$$

In this expression, the second term in the square brackets is a field-dependent one, however, as often mentioned it is very small in comparison with the field dependence of $(\pm \Gamma_{k'}^\alpha - 2\Gamma_{k'}^\beta)$ or of $\langle \psi | \psi \rangle$ in Eq. (48) and hereafter it is to be neglected. Thus we obtain for the first term

$$\frac{J}{4N}(\sum_1 \Gamma_1^\alpha)(\pm \Gamma_{k'}^\alpha - 2\Gamma_{k'}^\beta) = \frac{1}{3}(\pm \Gamma_{k'}^\alpha - 2\Gamma_{k'}^\beta). \quad (49)$$

The second term is the term appearing in the normalization integral Eq. (23) and thus of the next order as compared with Eq. (49). Contributions of other terms of Eq. (48) to the most divergent terms are calculated, in terms of X and X_1 defined by

$$X = \frac{\rho J}{N} \log \frac{-\tilde{E}_0}{D} \quad \text{and} \quad X_1 = \frac{\rho J}{N} \log \frac{\varepsilon_1 - \tilde{E}_0}{D},$$

as follows:

$$\begin{aligned} (48.3) &= \frac{J}{N} [\pm \Gamma_{k'}^\alpha (\sum_1 \Gamma_1^\alpha) - \Gamma_{k'}^\beta (\sum_1 \Gamma_1^\beta)] \left[\frac{1}{4} X + \frac{3}{16} X^2 + \frac{21}{128} X^3 + \dots \right] \\ &\quad + \frac{J}{N} [\pm \Gamma_{k'}^\alpha (\sum_1 \Gamma_1^\beta) - \Gamma_{k'}^\beta (\sum_1 \Gamma_1^\alpha)] \left[\frac{1}{8} X + \frac{9}{64} X^2 + \frac{35}{256} X^3 + \dots \right] \\ &= \frac{J}{4N} [\pm \Gamma_{k'}^\alpha (\sum_1 \Gamma_1^\alpha) - \Gamma_{k'}^\beta (\sum_1 \Gamma_1^\beta)] X (1-X)^{-3/4} \\ &\quad + \frac{J}{2N} [\pm \Gamma_{k'}^\alpha (\sum_1 \Gamma_1^\beta) - \Gamma_{k'}^\beta (\sum_1 \Gamma_1^\alpha)] \left[-1 + (1-X)^{1/4} + \frac{1}{2} X (1-X)^{-3/4} \right]. \end{aligned} \quad (50)$$

$$\begin{aligned} (48.4) &= \pm \frac{J}{4N} \Gamma_{k'}^\alpha \sum_1 (\Gamma_1^\alpha + 4\Gamma_1^\beta) \\ &\quad \times \left(-\frac{1}{32} X_1^2 + \frac{1}{16} X_1 X - \frac{5}{128} X_1^3 + \frac{3}{128} X_1^2 X + \frac{9}{128} X_1 X^2 + \dots \right) \\ &\quad + \frac{J}{4N} \Gamma_{k'}^\beta \sum_1 (\Gamma_1^\alpha + 4\Gamma_1^\beta) \\ &\quad \times \left(-\frac{1}{16} X_1^2 + \frac{1}{8} X_1 X - \frac{3}{32} X_1^3 + \frac{3}{32} X_1^2 X + \frac{3}{32} X_1 X^2 + \dots \right). \end{aligned} \quad (51)$$

$$\begin{aligned} (48.5) &= \mp \frac{J}{4N} \Gamma_{k'}^\alpha \sum_1 \Gamma_1^\alpha \left(\frac{1}{4} X_1 + \frac{3}{32} X_1^2 + \frac{7}{128} X_1^3 + \dots \right) \\ &\quad - \frac{J}{4N} \Gamma_{k'}^\beta \sum_1 \Gamma_1^\alpha \left(X_1 + \frac{15}{16} X_1^2 + \frac{7}{8} X_1^3 + \dots \right). \end{aligned} \quad (52)$$

$$\begin{aligned} (48.6) &= \mp \frac{J}{4N} \Gamma_{k'}^\alpha \sum_1 \Gamma_1^\alpha \left(\frac{3}{8} X_1^2 - \frac{7}{16} X_1 X + \frac{17}{32} X_1^3 - \frac{45}{128} X_1^2 X - \frac{39}{128} X_1 X^2 + \dots \right) \\ &\quad - \frac{J}{4N} \Gamma_{k'}^\beta \sum_1 \Gamma_1^\alpha \left(\frac{1}{8} X_1 X + \frac{1}{16} X_1^3 + \frac{3}{16} X_1 X^2 + \dots \right). \end{aligned} \quad (53)$$

Adding up Eqs. (51), (52) and (53), we obtain

(51) + (52) + (53)

$$\begin{aligned}
&= \pm \frac{J}{4N} \Gamma_{k'}^{\alpha} \sum_1 \Gamma_1^{\alpha} \left[\left(\frac{1}{4} X_1 + \frac{1}{2} X_1^2 + \frac{5}{8} X_1^3 + \dots \right) \right. \\
&\quad \left. - X \left(\frac{1}{2} X_1 + \frac{3}{8} X_1^2 + \dots \right) - X^2 \left(\frac{3}{8} X_1 + \dots \right) \right] \\
&\quad \pm \frac{J}{4N} \Gamma_{k'}^{\alpha} \sum_1 \Gamma_1^{\beta} \left[\left(\frac{1}{8} X_1^2 + \frac{5}{32} X_1^3 + \dots \right) \right. \\
&\quad \left. - X \left(\frac{1}{4} X_1 + \frac{3}{32} X_1^2 + \dots \right) - X^2 \left(\frac{9}{32} X_1 + \dots \right) \right] \\
&\quad + \frac{J}{4N} \Gamma_{k'}^{\beta} \sum_1 \Gamma_1^{\alpha} \left[\left(-X_1 - \frac{7}{8} X_1^2 - \frac{27}{32} X_1^3 + \dots \right) \right. \\
&\quad \left. - X \left(\frac{1}{4} X_1 + \frac{3}{32} X_1^2 + \dots \right) - X^2 \left(\frac{9}{32} X_1 + \dots \right) \right] \\
&\quad + \frac{J}{4N} \Gamma_{k'}^{\beta} \sum_1 \Gamma_1^{\beta} \left[\left(\frac{1}{4} X_1^2 + \frac{3}{8} X_1^3 + \dots \right) \right. \\
&\quad \left. - X \left(\frac{1}{2} X_1 + \frac{3}{8} X_1^2 + \dots \right) - X^2 \left(\frac{3}{8} X_1 + \dots \right) \right]. \quad (54)
\end{aligned}$$

In order to find out functions of X and X_1 whose expansion forms coincide respectively with those in Eq. (54) up to the third order in $\rho J/N$, we can rearrange Eq. (54) as

$$\begin{aligned}
(54) &= \mp \frac{J}{4N} \Gamma_{k'}^{\alpha} \sum_1 \left(\frac{1}{4} \Gamma_1^{\alpha} + \Gamma_1^{\beta} \right) (X_1 + X_1^2 + X_1^3 + \dots) \\
&\quad + \frac{J}{4N} \sum_1 [\pm \Gamma_{k'}^{\alpha} (\Gamma_1^{\beta} - 2\Gamma_1^{\alpha}) - \Gamma_{k'}^{\beta} (\Gamma_1^{\alpha} - 2\Gamma_1^{\beta})] \\
&\quad \times \frac{4}{15} \left[\left(\frac{5}{4} X_1 + \frac{45}{32} X_1^2 + \frac{195}{128} X_1^3 + \dots \right) \right. \\
&\quad \left. - \frac{1}{4} X \left(\frac{5}{4} X_1 + \frac{45}{32} X_1^2 + \dots \right) - \frac{3}{32} X^2 \left(\frac{5}{4} X_1 + \dots \right) + \dots \right] \\
&\quad + \frac{J}{4N} (\pm \Gamma_{k'}^{\alpha} - \Gamma_{k'}^{\beta}) \sum_1 (\Gamma_1^{\alpha} + \Gamma_1^{\beta}) \\
&\quad \times \frac{2}{3} \left[\left(\frac{3}{4} X_1 + \frac{21}{32} X_1^2 + \frac{77}{128} X_1^3 + \dots \right) + \left(\frac{1}{4} X_1 + \frac{3}{32} X_1^2 + \frac{7}{128} X_1^3 + \dots \right) \right. \\
&\quad \left. + \frac{1}{4} X \left(\frac{3}{4} X_1 + \frac{21}{32} X_1^2 + \dots \right) + \frac{5}{4} X \left(\frac{1}{4} X_1 + \frac{3}{32} X_1^2 + \dots \right) \right. \\
&\quad \left. + \frac{5}{32} X^2 \left(\frac{3}{4} X_1 + \dots \right) + \frac{45}{32} X^2 \left(\frac{1}{4} X_1 + \dots \right) \right], \quad (55)
\end{aligned}$$

and it would be allowable to identify (55) with

$$\begin{aligned}
 (54) = & \mp \frac{J}{4N} \Gamma_{k'}^\alpha \sum_1 \left(\frac{1}{4} \Gamma_1^\alpha + \Gamma_1^\beta \right) [(1-X_1)^{-1} - 1] \\
 & + \frac{J}{4N} \sum_1 [\pm \Gamma_{k'}^\alpha (\Gamma_1^\beta - 2\Gamma_1^\alpha) - \Gamma_{k'}^\beta (\Gamma_1^\alpha - 2\Gamma_1^\beta)] \\
 & \times \frac{4}{15} (1-X)^{1/4} [(1-X_1)^{-5/4} - 1] \\
 & + \frac{J}{6N} (\pm \Gamma_{k'}^\alpha - \Gamma_{k'}^\beta) \sum_1 (\Gamma_1^\alpha + \Gamma_1^\beta) \{ (1-X)^{-1/4} [(1-X_1)^{-5/4} - 1] \\
 & - (1-X)^{-5/4} [(1-X_1)^{1/4} - 1] \}. \quad (56)
 \end{aligned}$$

For the second term of Eq. (47), the same procedure of calculations has been taken, where all the most divergent terms cancel with each other. Details are omitted in order to avoid lengthy description. Finally, Eq. (47) consists of Eqs. (49), (50) and (56). Adding up these contributions and performing the summations involved in them in the same way as II, we obtain for the most divergent contributions of Eq. (47)

$$\begin{aligned}
 \lim_{\substack{\varepsilon_{k'} \rightarrow 0_+ \\ \varepsilon_k \rightarrow 0_-}} (n_{\alpha\uparrow} \pm n_{\alpha\downarrow})_{eh}^{k'k} \langle \psi | \psi \rangle (\varepsilon_{k'} - \varepsilon_k) &= \frac{1}{3} (\pm \Gamma_0^\alpha - \Gamma_0^\beta) (1-X)^{-1/4} \\
 &= -\frac{2}{9} \left(\pm \frac{1}{-\tilde{E} + \mathcal{A}} + \frac{1}{-\tilde{E} - \mathcal{A}} \right) (1-X)^{-1/2}, \quad (57)
 \end{aligned}$$

where Γ_0 is defined by $\Gamma_0 = (\Gamma_k)_{\varepsilon_k=0}$. Therefore, using Eqs. (23a, b) for $\langle \psi | \psi \rangle$, we obtain

$$\lim_{\substack{\varepsilon_{k'} \rightarrow 0_+ \\ \varepsilon_k \rightarrow 0_-}} (n_{\alpha\uparrow} \pm n_{\alpha\downarrow})_{eh}^{k'k} (\varepsilon_{k'} - \varepsilon_k) = -\frac{1}{2\rho} \frac{\pm \langle \psi_\alpha | \psi_\alpha \rangle + \langle \psi_\beta | \psi_\beta \rangle}{\langle \psi | \psi \rangle}. \quad (58)$$

Two equations involved in Eq. (58) correspond to Eqs. (46) and (57) of II, respectively. Factor of 1/2 in (58) is attributed to the difference of taking the normalization; for the singlet state it is possible to consider it in one component of the wave function, but it is not the case in the magnetic field. By inserting Eq. (58) into Eq. (45), summation on the Fermi surface can be carried out as is done in Eq. (36) of II and the following results are obtained,

$$(n_{\alpha\uparrow} + n_{\alpha\downarrow})_{eh} = -\frac{1}{2} \quad (59)$$

and

$$(n_{\alpha\uparrow} - n_{\alpha\downarrow})_{eh} = \frac{1}{2} \frac{\langle \psi_\alpha | \psi_\alpha \rangle - \langle \psi_\beta | \psi_\beta \rangle}{\langle \psi | \psi \rangle}. \quad (60)$$

Equation (60) which vanishes completely for $\mathcal{A}=0$ has now a finite value, whereas Eq. (59) does not change. Combining these results with Eq. (44), we obtain,

with the use of Eq. (15),

$$n_{\alpha\uparrow} + n_{\alpha\downarrow} = \frac{\langle\psi_\alpha|\psi_\alpha\rangle - \langle\psi_\beta|\psi_\beta\rangle}{2\langle\psi|\psi\rangle} = \frac{-\Delta}{2(\tilde{E}_0^2 + \Delta^2)^{1/2}} = \langle S_z \rangle \quad (61)$$

and

$$n_{\alpha\uparrow} - n_{\alpha\downarrow} = -\frac{1}{2}, \quad (62)$$

from which, $(n_{\beta\uparrow} \pm n_{\beta\downarrow})$ can be obtained in terms of the symmetry relation, and thus we have the following relations,

$$\begin{aligned} n_{\alpha\uparrow} &= -n_{\beta\uparrow} = \frac{1}{4} \left(-1 - \frac{\Delta}{(\tilde{E}_0^2 + \Delta^2)^{1/2}} \right) = \frac{1}{2} \left(-\frac{1}{2} + \langle S_z \rangle \right), \\ n_{\alpha\downarrow} &= -n_{\beta\downarrow} = \frac{1}{4} \left(1 - \frac{\Delta}{(\tilde{E}_0^2 + \Delta^2)^{1/2}} \right) = \frac{1}{2} \left(\frac{1}{2} + \langle S_z \rangle \right). \end{aligned} \quad (63)$$

For the singlet case ($\Delta=0$), Eq. (63) differs from the corresponding equations (59) and (60) of II by the factor 1/2. This difference is trivial, because here we normalize ψ , whereas in II one component of ψ is normalized. The results of Eq. (63) are shown together with the result (42) schematically in Fig. 1. Here it is to be noted that with increasing field the magnitude of electron- and hole-clouds with up-spin increases, though it becomes thin and tends to twice as large as those for the zero-field case, while clouds for down-spin diminish. The combinations of Eq. (63) give the most divergent contributions for the following physical quantities,

(i) total localized charge

$$n_{\alpha\uparrow} + n_{\alpha\downarrow} + n_{\beta\uparrow} + n_{\beta\downarrow} = 0, \quad (64.1)$$

(ii) total localized spin polarization

$$\frac{1}{2}(n_{\alpha\uparrow} - n_{\alpha\downarrow} + n_{\beta\uparrow} - n_{\beta\downarrow}) = 0, \quad (64.2)$$

(iii) z-component of the total localized spin correlation

$$\frac{1}{4}(n_{\alpha\uparrow} - n_{\alpha\downarrow} - n_{\beta\uparrow} + n_{\beta\downarrow}) = -\frac{1}{4}. \quad (64.3)$$

Since contribution of the RKY term to the spin polarization is of the next order of divergence, it drops in (ii). We will reexamine Eqs. (64.1) and (64.2) rigorously in § 6 without restriction to the most divergent terms,

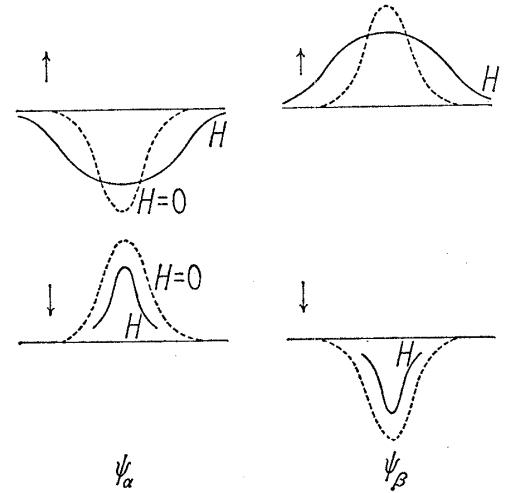


Fig. 1. Local distributions of electrons with up- and down-spins in ψ_α and ψ_β . The solid-line represents those in the presence of the magnetic-field and the dotted-line in the singlet ground state.

For the spin correlation, Eq. (64.3) proves that the z -component does not change and other components are calculated in a same way as is done for the z -component and the result is

$$\begin{aligned} \frac{1}{2} \frac{1}{\langle \phi | \phi \rangle} \sum_k \lim_{k' \rightarrow k} \langle \phi | a_{k'\uparrow}^* a_{k\downarrow} S_- + a_{k'\downarrow}^* a_{k\uparrow} S_+ | \phi \rangle / \langle \phi | \phi \rangle \\ = \sum_k \Gamma_k^\alpha \Gamma_k^\beta = \frac{-\tilde{E}_0^2}{4\Delta(\tilde{E}_0^2 + \Delta^2)^{1/2}} \log \frac{(\tilde{E}_0^2 + \Delta^2)^{1/2} + \Delta}{(\tilde{E}_0^2 + \Delta^2)^{1/2} - \Delta}. \end{aligned} \quad (65)$$

Equation (65) is due to the contributions from electron-electron and hole-hole parts and electron-hole part has no effect on Eq. (65), because a procedure similar to deriving Eq. (48) in which appears a singularity of $(\epsilon_{k'} - \epsilon_k)^{-1}$ now gives rise to the factor of $(\epsilon_{k'} - \epsilon_k \pm 2\Delta)^{-1}$ which is finite when k' tends to k , as is easily seen from the Schrödinger equations for Γ^α 's and Γ^β 's. Equation (65) is a monotonic function and tends to zero for large Δ . Thus the total localized spin correlation behaves Ising-like for large Δ .

§ 5. Magnetoresistance at 0°K

In this section, we give a consideration for the magnetoresistance, using the result of the previous section. The phase shifts for the conduction electrons are related with Eq. (63) by the Friedel sum rule. However, the phase shift obtained in this way is given separately for the components ϕ_α and ϕ_β , and it is the essential point how to relate these with the calculation of the magnetoresistance. We proceed as follows: Since $n_{\alpha\uparrow}$ is normalized in ϕ , the total amounts of up-spin-electron trapped around the impurity in ϕ_α is $n_{\alpha\uparrow} \langle \phi | \phi \rangle / \langle \phi_\alpha | \phi_\alpha \rangle$, which equals $-1/2$ for the singlet state ($\Delta=0$). Thus the phase shift $\eta_{\alpha\uparrow}$ for the up-spin-state amounts to $\pi n_{\alpha\uparrow} \langle \phi | \phi \rangle / \langle \phi_\alpha | \phi_\alpha \rangle$ by the Friedel sum rule, and the other phase shifts $\eta_{\alpha\downarrow}$, $\eta_{\beta\uparrow}$ and $\eta_{\beta\downarrow}$ are considered similarly. When the expression for the magnetoresistance is derived from these phase shifts, we believe by the physical insight that it is relevant to consider the difference of the probabilities for ϕ_α and ϕ_β in weighting them to the phase shifts in themselves, not in weighting them to the components of resistance corresponding to each phase shift. Therefore the magnetoresistance may be written for the present system where only the s -wave scattering is taken into account in the form

$$R(\Delta) = R_0 \sum_{\sigma=\uparrow\downarrow} \frac{1}{4} \left[\sin^2 \left(\eta_{\alpha\sigma} \frac{2\langle \phi_\alpha | \phi_\alpha \rangle}{\langle \phi | \phi \rangle} \right) + \sin^2 \left(\eta_{\beta\sigma} \frac{2\langle \phi_\beta | \phi_\beta \rangle}{\langle \phi | \phi \rangle} \right) \right], \quad (66)$$

where R_0 denotes one s -wave unitarity limit for resistivity. In this expression factor 2 is brought into the arguments of sine in order that Eq. (66) coincides with the correct result of II for the singlet state ($\Delta=0$) where $\pi/2$ or $-\pi/2$ enters the arguments of sine, as discussed below Eq. (63). Inserting Eq. (63) into Eq. (66), we obtain the magnetoresistance in the form

$$R(\Delta) = R_0 \sin^2 \frac{\pi}{2} \left(1 - \frac{\Delta}{(\tilde{E}_0^2 + \Delta^2)^{1/2}} \right) \quad (67)$$

$$\simeq R_0 \left[1 - \frac{\pi}{4} \frac{\Delta^2}{\tilde{E}_0^2} + \dots \right] \quad \text{for } \Delta \sim 0$$

and with the use of Eq. (24) it is written as

$$R(\Delta) = R_0 \cos^2 \pi \langle S_z \rangle. *) \quad (68)$$

Here an important thing is that this expression has no logarithmic field dependence. Equation (67) is shown in Fig. 2(a) in a usual scale and also in Fig. 2(b)

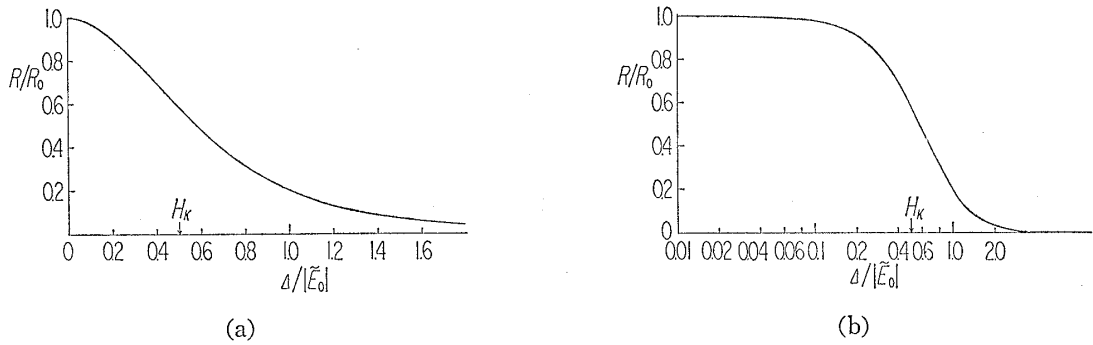


Fig. 2. Magnetoresistance (a) in a usual scale, (b) in a log-scale.

in a log-scale. It is noted in this figure that the log H -like dependence of the magnetoresistance is seen in the neighborhood of H_K , where H_K is defined as $|\tilde{E}_0|/g\mu_B$ at which the usual perturbation calculation diverges.¹⁴⁾

On the other hand, a feature similar to Fig. 2 is seen in the experimental result by Daybell and Steyert¹⁵⁾ who measured the magnetoresistance in a dilute alloy of Cr in Cu down to 40 m°K and up to the magnetic field of several times of T_K . In contrast to the susceptibility, the magnetoresistance becomes flat at low temperatures and it is easy to extrapolate it to the zero-temperature. Moreover, the temperature-dependence of resistivity¹⁶⁾ is also quite similar to Fig. 2a or Fig. 2b, and if we take account of the similarity between temperature and field effects in the present system, the expression similar to Eq. (67) seems to hold plausibly also for temperature-dependence. Magnetoresistance has also been calculated by More and Suhl¹⁷⁾ on the basis of the S -matrix theory, but their result at low temperature shows a complex behaviour and differs completely from ours.

§ 6. General relations

In this section, we show rigorously that the total localized spin polarization is given by $(\rho J/2N) \langle S_z \rangle$ by the method developed in II.

*) The same expression as Eq. (68) can also be derived on the basis of the Takano-Ogawa theory.¹³⁾ However, the expression for $\langle S_z \rangle$ is completely different from ours and it shows a discontinuity in its field derivative at $H=H_K$, while there is no such discontinuity in our case.

Applying the relation $\langle\psi|[H, a_{k'\sigma}^* a_{k\sigma}]_-\psi\rangle=0$ which holds for the eigenstate ψ of the Hamiltonian H to the present system, and assuming that ψ is non-degenerate, we obtain the following expression which corresponds to Eq. (63) of II,

$$\langle\psi|a_{k'\uparrow}^* a_{k\uparrow} - a_{k'\downarrow}^* a_{k\downarrow}|\psi\rangle/\langle\psi|\psi\rangle = -\frac{J}{2N} \frac{L_{k'} - L_k}{\varepsilon_{k'} - \varepsilon_k}, \quad (69)$$

where $L_{k'}$ is defined by

$$L_{k'} = \sum_l \langle\psi|(a_{k'\uparrow}^* a_{l\uparrow} + a_{k'\downarrow}^* a_{l\downarrow}) S_z - a_{k'\downarrow}^* a_{l\uparrow} S_+ + a_{k'\uparrow}^* a_{l\downarrow} S_-|\psi\rangle/\langle\psi|\psi\rangle. \quad (70)$$

Explicit effect of the magnetic field drops out from Eq. (70) because $a_{k'\sigma}^* a_{k\sigma}$ commutes with the Zeeman Hamiltonian. For $\varepsilon_{k'}, \varepsilon_k > 0$ and $\varepsilon_{k'}, \varepsilon_k < 0$, the right-hand side of Eq. (69) tends to $-(J/2N)(dL_k/d\varepsilon_k)$ as k' tends to k , and for $\varepsilon_{k'} > 0, \varepsilon_k < 0$, it is proportional to the discontinuity of L_k at the Fermi surface. Circumstances are the same as those in which Eqs. (65) and (66) are derived from Eq. (64) in II and thus the spin polarization is expressed with L_k as

$$n_{\alpha\uparrow} - n_{\alpha\downarrow} + n_{\beta\uparrow} - n_{\beta\downarrow} = -\frac{\rho J}{2N} [L(D) - L(-D)]. \quad (71)$$

L_k is expressed with coefficients Γ 's from Eq. (70) as

$$\begin{aligned} L_k &= \frac{1}{\langle\psi|\psi\rangle} [(\Gamma_k^\alpha + \Gamma_k^\beta) \sum_l (\Gamma_l^\alpha - \Gamma_l^\beta) + \dots] \quad \text{for } \varepsilon_k > 0, \\ &= \frac{1}{\langle\psi|\psi\rangle} \left[\langle\psi_\alpha|\psi_\alpha\rangle - \langle\psi_\beta|\psi_\beta\rangle + \frac{1}{2} \sum_{12} \Gamma_1^\alpha (\Gamma_{12,k}^{\alpha\uparrow} + \Gamma_{[12],k}^{\alpha\downarrow} + 2\Gamma_{21,k}^{\beta\downarrow}) + \dots \right] \\ &\quad \text{for } \varepsilon_k < 0. \end{aligned} \quad (72)$$

Noticing that $\Gamma_k^\alpha, \Gamma_{12,k}^{\alpha\uparrow}$, etc., are of order $1/D$ at band edge, we obtain

$$L(D) = 0$$

and

$$L(-D) = \frac{\langle\psi_\alpha|\psi_\alpha\rangle - \langle\psi_\beta|\psi_\beta\rangle}{\langle\psi|\psi\rangle} = 2\langle S_z \rangle, \quad (73)$$

where use has been made of Eq. (24). Inserting Eq. (73) into Eq. (71), we finally obtain the total localized spin polarization $\langle\sigma\rangle$,

$$\langle\sigma\rangle = \frac{1}{2} (n_{\alpha\uparrow} - n_{\alpha\downarrow} + n_{\beta\uparrow} - n_{\beta\downarrow}) = \frac{\rho J}{2N} \langle S_z \rangle. \quad (74)$$

Equation (74) corrects the result of the previous section, Eq. (64.2). Equation (74) is the relation first found in the RKY theory¹⁰⁾ and also confirmed by the usual perturbation theory,¹¹⁾ so that this is considered as a general relation holding between the spin polarization and a magnitude of the localized spin. Heeger,

Welsh, Jensen and Gladstone¹⁸⁾ have calculated the magnetic susceptibility for the analysis of their experimental result. Their result shows that $\langle\sigma\rangle$ is equal to $\langle S_z\rangle$ when the g -value of the conduction electron is the same as that of the localized spin. This contradicts the general relation proved above.

If we take another combination of $a_{k'\sigma}^*a_{k\sigma}$ instead of Eq. (69), it can also be shown that the localized charge generally vanishes for the present Hamiltonian as has been proved in II.

§ 7. Conclusion and discussion

We have investigated the magnetic-field dependence of the local electronic structure of the ground state in a weak coupling limit. Here we summarize the results obtained in each section. In the absence of the field, it is the conclusion of II that $\psi_\alpha(\psi_\beta)$ has half of a down-spin-electron (hole) and half of an up-spin-hole (electron) localized around the impurity in total, and in the present case it is shown that with increasing field the magnitude of trapped up-spin-hole (electron) in $\psi_\alpha(\psi_\beta)$ increases and tends to the twice of that in zero-field case and that of down-spin-electron (hole) decreases and tends to zero. Accordingly, it can be said that in the limit of increasing field $\psi_\alpha(\psi_\beta)$ has almost one up-spin-hole (electron) and no down-spin-electron (hole) localized around the impurity. (On the basis of this interpretation, we have derived the magnetoresistance.) On the other hand, densities of these at the impurity site diminish with the field. Accordingly, there remains in $\psi_\alpha(\psi_\beta)$ a cloud of up-spin-hole (electron) clinging to the localized spin even in a high field. This feature is characteristic of the bound state. On the basis of this result, we have obtained a reasonable expression for the magnetoresistance at 0°K, which has no $\log H$ -dependence though it has a part linear in $\log H$ in the vicinity of H_K . Further we have shown the following: The total localized spin correlation varies from $-3/4$ to the limit of $-1/4$ with increasing field. The total spin polarization is related with the induced localized spin as $\langle\sigma\rangle=(\rho J/2N)\langle S_z\rangle$. This has its origin in the RKY spin polarization and is the relation which generally holds between them. Since the spin polarization density at the impurity site also consists of that of the RKY theory, we may expect that all the feature of the spin polarization is given by the RKY theory. The charge does not accumulate in the ground state of the present system. The exchange energy and the kinetic energy are expressed as functions of the field. Finally, guided by the methods of I and II, we have studied all the results obtained in them in the presence of the magnetic field.

Measurements of the magnetic susceptibility¹⁹⁾ have been done mainly in the system such as Cu-Fe, Cu-Mn and Au-V. However, the conclusions drawn from various experimental results do not always agree as to whether the susceptibility tends to the constant value or diverges as $T^{-1/2}$ at $T\rightarrow 0^\circ\text{K}$. Recently Pratt, Schermer and Steyert²⁰⁾ have found the temperature independent susceptibility

in the range $4m^{\circ}\text{K} < T < 10m^{\circ}\text{K}$ by measurements of the anisotropy of γ -ray emission from Mn^{54} doped in Cu which was first done at $10m^{\circ}\text{K}$ and $25m^{\circ}\text{K}$ by Campbell et al.²¹⁾ This suggests the constant susceptibility at 0°K in agreement with our conclusion.

Acknowledgments

The author would like to express his deep thanks to Professor K. Yosida and Professor A. Yoshimori for suggesting the present problem as well as the continual guidance throughout the course of this work. Discussions with Dr. A. Sakurai are also acknowledged. This work has partially been financed by the Sakkokai foundation.

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Note added in proof: By investigating the total localized spin polarization and the spin density at the impurity site, we have concluded that all the feature of the spin polarization is given by the RKY form with $\langle S_z \rangle$ induced by the field. It is possible to prove that this is also true for the spin density at any point \mathbf{r} by examining the expression for $\sigma(\mathbf{r})$ obtained by operating $(1/N)\sum_{\mathbf{k}\mathbf{k}'} \exp[-i(\mathbf{k}'-\mathbf{k})\mathbf{r}]$ to Eq. (69). Details will be published elsewhere.