Bound States Due to a Pair of Interacting Magnetic Impurities in Metals. II

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The bound states of conduction electrons due to a pair of magnetic impurities which interact with each other by an exchange interaction are investigated by the Yosida theory. Calculations of the previous work by the present authors are generalized by including the vertex correction. The binding energy is calculated within the most divergent approximation for some limiting cases of the strength of the exchange interaction $W$ between impurities, and its behavior as a function of $W$ is obtained by interpolation. Some unphysical features of the previous results caused by the neglect of the vertex correction are corrected. It is found that the binding energy is essentially given by the Kondo temperature defined as an energy where a perturbational series of the most divergent terms diverges.

§ 1. Introduction

The Kondo effect of an isolated magnetic impurity in metals has been extensively investigated by many authors theoretically as well as experimentally and has been essentially understood. There is also some work concerning the effect of correlation between impurities on the Kondo anomaly. However, its feature still remains unclear, especially from a theoretical point of view.

In a previous paper (which will be referred to as I hereafter), we developed a theory of bound states due to a pair of interacting magnetic impurities, applying the Yosida theory to the problem in the zeroth approximation. Though the result showed a reasonable behavior in some aspects, it also had some unsatisfactory properties. In particular the following points are important.

1) The binding energy of an isolated impurity is given by $De^{-1/|z|\rho}$ with usual notations. Then the binding energy of two impurities will be $2De^{-1/|z|\rho}$ if they are infinitely separated. The result of I gives $2De^{-3/|z|\rho}$ in this limit, i.e., the exponent is incorrect.

2) When two impurities couple strongly with each other by an antiferromagnetic exchange interaction $W$, they form a singlet state and behave as a nonmagnetic impurity. Therefore the bound state should disappear in this limit. The result of I gives a bound state with the binding energy $D\exp\{-\alpha/J^2\rho^4\log(D/W)}), \alpha$ being a constant of the order unity.

3) When the exchange interaction between impurities vanishes, a perturbational calculation gives the Kondo temperature as $De^{-3/|z|\rho}$ independently of the distance between impurities. Therefore it is expected in this case that the binding
energy also reduces to $2D e^{-1/|D|}$. The result of I shows it depends on the distance even in this case.

As discussed in I, these defects of our calculation in I are due to the approximation we took there, and will be overcome by taking account of higher-order corrections, especially the vertex correction between electrons and impurities. Ishii actually showed that this expectation is correct by calculating the binding energy of a doublet bound state for $W=0$, including the vertex correction. The purpose of this paper is to extend our calculation of the binding energy of singlet bound states due to a pair of magnetic impurities for general $W$ by taking account of the vertex correction, and to show how the result of I discussed above are modified by it. In other words it is to apply the Yosida-Yoshimori theory to the problem in its complete form.

Throughout this paper we restrict ourselves to the approximation where the most divergent terms in each order of perturbation are only taken into account, though, as will be discussed in § 6, it is very desirable to extend the calculation by including next divergent terms. Calculations we give here are rather complicated. The final results, however, are very simple, i.e., we find the binding energy is equal to the Kondo temperature determined by perturbational calculations.

In § 2 we give the Yoshimori equation in a general form where the two-particle vertex correction is taken into account. The two-particle irreducible vertex is calculated in § 3 by using the Abrikosov theory. In § 4 an explicit form of the Yoshimori equation is given and solved for some special cases. It is solved in § 5 in more general cases by introducing some approximations. In § 6 we give a summary of the results and discussion. In the Appendix we give the detail of calculations necessary for the calculation in § 5.

§ 2. Vertex correction

As in I, we consider a system of conduction electrons and two magnetic impurities with spin 1/2 interacting with each other via an antiferromagnetic $s$-$d$ exchange interaction. We take account of a direct exchange interaction between two impurities instead of calculating the normal part of energy (or the self-energy correction of spin propagators). The Hamiltonian is given by

$$H = \sum_{k \alpha} \epsilon_k c_{k\alpha}^\dagger c_{k\alpha} - \frac{J}{2N} \sum_{k \alpha} \sum_{k' \alpha'} \langle c_{k-k'} S + i s_{k-k'} d \rangle \cdot \sigma_{\alpha \alpha'} c_{k\alpha}^\dagger c_{k'\alpha'} - WS_1 \cdot S_2, \quad (2.1)$$

where

$$S = S_1 + S_2, \quad d = S_1 - S_2, \quad (2.2)$$

$$c_k = \cos(k \cdot R/2), \quad s_k = \sin(k \cdot R/2), \quad (2.3)$$

*) We will call this type of approximation the MD (most divergent) approximation hereafter.
and \( S_1 \) and \( S_2 \) are spin operators of two impurities locating at \( \pm \mathbf{R}/2 \), respectively. Notations are the same as in I.

The wave function of the singlet ground state is written as

\[
\Psi = \Psi_0 + \Psi'.
\]  

(2.4)

Here \( \Psi_0 \) takes the same form as the wave function in the zeroth approximation given in I:

\[
\Psi_0 = \sum_{kk'} \left( \Gamma_{kk'}^{(0)} (c^c_{k1} c^c_{k2} \beta_1 \beta_2 + c^c_{k2} c^c_{k1} \alpha_1 \alpha_2) 
+ (\Gamma_{kk'}^{(0)} - \Gamma_{k'k}^{(0)}) (c^c_{k1} c^c_{k2} \alpha_1 \beta_2 + c^c_{k2} c^c_{k1} \beta_1 \alpha_2) \right) \Phi_0,
\]  

(2.5)

where \( \Phi_0 \) is the wave function of the Fermi vacuum, and \( \alpha_i \) and \( \beta_i (i = 1, 2) \) are wave functions of the impurity spins with \( S_i = \pm 1/2 \), respectively. The coefficients \( \Gamma^{(0)} \) and \( \Gamma^{(0)} \) satisfy symmetry relations

\[
\Gamma_{kk'}^{(0)} = -\Gamma_{k'k}^{(0)}, \quad \Gamma_{kk'}^{(0)} = \Gamma_{k'k}^{(0)}.
\]  

(2.6)

\( \Psi' \) is the amplitude containing electron-hole pairs.

We have to derive the equations for \( \Gamma^{(0)} \) and \( \Gamma^{(0)} \) including the effect of \( \Psi' \).

In Nakajima formalism,\(^10\) it means that we take account of the vertex correction as well as the self-energy correction of spin propagators. Among them, an important part of the self-energy correction has already been included in the starting Hamiltonian as a direct exchange interaction. The remaining part of the self-energy correction only gives a constant energy shift, which we are not interested in. Therefore we have only to consider the vertex correction.

In the present case, we generally need three-particle vertices where two electrons interact with the impurity spins (or a quasi-fermion in Abrikosov's sense).*\(^1\) A simple example of them is shown in Fig. 1(a), where full and dotted lines represent electron and spin propagators, respectively. We can however neglect such diagrams, since they do not contribute to the most divergent term.\(^6\)

Therefore diagrams which have to be taken into account are those where one

\[ \text{Fig. 1. Examples of the three-particle vertices of third order, among which (b) does not contribute to the most divergent term and (a) does not.} \]

\footnote{\( * \) In the case of one-impurity, Abrikosov\(^6\) introduced quasi-fermions associated with each of \((2S+1)\) degenerate spin states of the impurity. In the present case, we introduce them for each of one singlet and three triplet states of the impurity-spin pair. The difference between them is the energy splitting of the spin states due to the exchange interaction \( W \) in the latter case. Thus the spin propagators denoted by dotted lines in Fig. 1 are given by \((\omega - W + i\delta)^{-1} \), \( W \) being given by Eq. (2.11).}
electron interacts with the impurity spins and the other electron passes away (Fig. 1(b)).

We denote the irreducible two-particle vertex correction where an electron interact with the impurity spins by $A^{(2)}_{k\delta, \kappa'\alpha'\gamma'}(\omega, \omega - \omega_1; \omega_2, \omega - \omega_2)$, where the definition of suffices and arguments are given in Fig. 2. Here $\beta$ denotes spin states of the impurities, i.e., three triplet states (denoted by $t$) and a singlet state (denoted by $s$). The spin dependence of the vertex correction is given by

$$
A^{(2)}_{k\delta, \kappa'\alpha'\gamma'} = A^{(2)}_{k\delta, \kappa'\alpha'\gamma'}(\beta, \gamma') = A^{(2)}_{k\delta, \kappa'\alpha'\gamma'}(\sigma \cdot S)_{\alpha, \alpha'},
$$

$$
A^{(2)}_{k\delta, \kappa'\alpha'\gamma'} = A^{(2)}_{k\delta, \kappa'\alpha'\gamma'}(\sigma \cdot d)_{\alpha, \alpha'},
$$

$$
A^{(2)}_{k\delta, \kappa'\alpha'\gamma'} = A^{(2)}_{k\delta, \kappa'\alpha'\gamma'}(\sigma \cdot d)_{\alpha, \alpha'}.
$$

We are interested in singlet spin states of two electrons and two impurity spins. There are two independent singlet states; one is formed by a triplet of impurity spins and a triplet of electrons and denoted by $|t\rangle$, and the other is formed by a singlet of impurity spins and a singlet of electrons and denoted by $|s\rangle$. Then the nonvanishing matrix elements of spin operators in Eq. (2.7) in this $2 \times 2$ subspace are given by

$$
\langle t|\sigma \cdot S|t\rangle = -2,
$$

$$
\langle s|\sigma \cdot d|t\rangle = \langle t|\sigma \cdot d|s\rangle = -\sqrt{3}.
$$

Noting that the $\Gamma^{(2)}$ coefficients $\Gamma^{(2)}$ and $\sqrt{3} \Gamma^{(2)}$ correspond to these spin states $|t\rangle$ and $|s\rangle$, respectively, and using above relations, we find the equations for $\Gamma^{(2)}$ and $\Gamma^{(2)}$ as

$$
(\epsilon_k + \epsilon_{k'} + W_t - E)\Gamma_{kk'}^{(2)}
$$

$$
+ \frac{J}{N} \sum_{k'} \left\{ c_{k-k'} \Gamma_{kk'}^{(2)} + c_{k'-k} \Gamma_{kk'}^{(2)} \right\}
$$

$$
+ \frac{iJ}{2N} \sum_{k'} \left\{ s_{k-k'} \Gamma_{kk'}^{(2)} + s_{k'-k} \Gamma_{kk'}^{(2)} \right\}
$$

$$
+ \sum_{k'} \left\{ A_{kk'}^{(2)}(\epsilon_k, E - \epsilon_k - \epsilon_{k'}; \epsilon_{k'}, E - \epsilon_{k'} - \epsilon_k) \Gamma_{kk'}^{(2)}
$$

$$
+ A_{kk'}^{(2)}(\epsilon_{k'}, E - \epsilon_k - \epsilon_{k'}; \epsilon_k, E - \epsilon_k - \epsilon_{k'}) \Gamma_{kk'}^{(2)} \right\}
$$

$$
+ A_{kk'}^{(2)}(\epsilon_k, E - \epsilon_k - \epsilon_{k'}; \epsilon_{k'}, E - \epsilon_{k'} - \epsilon_k) \Gamma_{kk'}^{(2)}
$$

$$
+ A_{kk'}^{(2)}(\epsilon_{k'}, E - \epsilon_k - \epsilon_{k'}; \epsilon_k, E - \epsilon_k - \epsilon_{k'}) \Gamma_{kk'}^{(2)} \right\}
$$

Fig. 2. The two-particle irreducible vertex.
\[-\sum k' \{ A_{k'k'}^{(0)}(\varepsilon_{k'}, E - \varepsilon_{k'} - \varepsilon_{k'}'; \varepsilon_{k'}, E - \varepsilon_{k'} - \varepsilon_{k'}) \Gamma_{k'k'}^{0}(k') \}
\left\{ A_{k'k'}^{(0)}(\varepsilon_{k'}, E - \varepsilon_{k'} - \varepsilon_{k'}'; \varepsilon_{k'}, E - \varepsilon_{k'} - \varepsilon_{k'}) \Gamma_{k'k'}^{0}(k') \right\} = 0 ,
\]

\((2\cdot9)\)

\(\varepsilon_k + \varepsilon_k' + W - E \}) \Gamma_{k'k'}^{0}(k') \}
\]

\((2\cdot10)\)

where summations over \(k'\) are restricted to the region above the Fermi energy, and

\[ W_1 = -\frac{W}{4} , \quad W_2 = \frac{3}{4} W , \]

\[(2\cdot11)\]

\[ A_{k'k'}^{(0)} = A_{k'k'}^{(0)} - 2 A_{k'k'}^{(1)} . \]

\[(2\cdot12)\]

If we neglect terms with \(A\) in Eqs. (2\cdot9) and (2\cdot10), they reduce to Eq. (2\cdot4) of \(I\).

\[\text{§ 3. Calculation of irreducible vertex}\]

In this section we consider the scattering of an electron by the impurity spins and calculate the vertex function \(L_{a\beta, a'\beta'}(\omega_1, \omega_2; \omega_2, \omega_1)\) by summing up all parquet diagrams. The definition of suffices and arguments of \(L\) are the same as shown in Fig. 2 for \(A^{(0)}\). In general the vertex function depends on three independent frequency variables \(\omega_1\) and \(\omega_2\). In the MD approximation, however, it suffices to consider a function of one variable defined by

\[ L_{a\beta, a'\beta'}(\omega) = L_{a\beta, a'\beta'}(\omega - W_1, W_1; \omega - W_2, W_2) \]

\[(3\cdot1)\]

Following Abrikosov, we put

\[ L_{a\beta, a'\beta'}(\omega) = -\frac{J}{2N} (c_{k-k'}\sigma \cdot S + i\delta_{k-k'}\sigma \cdot A)_{a\beta, a'\beta'} \]

\[ + A_{a\beta, a'\beta'}^{(0)}(\omega) + A_{a\beta, a'\beta'}^{(0)}(\omega) . \]

\[(3\cdot2)\]

Here the first term is the bare vertex given in Eq. (2\cdot1), while \(A^{(0)}(A^{(0)})\) is the contribution from diagrams which cannot be divided into two separate pieces by cutting antiparallel (parallel) electron and quasifermion lines. They are expressed as

\[ A_{a\beta, a'\beta'}^{(0)}(\omega) = \sum_{k' \alpha' \beta'} \frac{\theta(\varepsilon_{k'})}{\omega - \varepsilon_{k'} - W_\beta'} L_{a\beta, a'\beta'}(\omega - \varepsilon_{k'}) L_{k'\alpha' \beta', a'\beta'}(\omega - \varepsilon_{k'}) , \]
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\[ A_{k\alpha\delta, k'\alpha'\delta'}^{(2)}(\omega) = \sum_{k, k', \alpha, \beta, \delta} \frac{\theta(-\epsilon_{k\alpha})}{-\epsilon_{k\alpha} - W_{\beta} - W_{\delta} + W_{\delta'}} L_{k\alpha\delta, k'\alpha'\delta'}(\omega - \epsilon_{k\alpha} + W_{\beta} - W_{\delta}) \times L_{k\alpha\delta, k'\alpha'\delta'}(\omega - \epsilon_{k\alpha} + W_{\beta} - W_{\delta}), \]  
\((3.3)\)

where

\[ \theta(\epsilon) = \begin{cases} 1 & \text{for } \epsilon > 0, \\ 0 & \text{for } \epsilon < 0. \end{cases} \]

Similarly to Eq. (2.7), we can generally put the spin dependence of the vertex function as

\[ L_{k\alpha\delta, k'\alpha'\delta'}(\omega) = L_{k\alpha\delta, k'\alpha'\delta'}^{(\alpha\beta)}(\omega) \delta_{\alpha\alpha'}; \]

\[ L_{k\alpha\delta, k'\alpha'\delta'}(\omega) = L_{k\alpha\delta, k'\alpha'\delta'}^{(\alpha\beta)}(\omega) \delta_{\alpha\alpha'} + L_{k\alpha\delta, k'\alpha'\delta'}^{(\alpha\beta)}(\omega) \left( \sigma \cdot S \right)_{\alpha\alpha'}; \]  
\((3.4)\)

Then after some manipulation we find

\[ L_{k\alpha\delta, k'\alpha'\delta'}^{(\alpha\beta)}(\omega) = 0, \quad L_{k\alpha\delta, k'\alpha'\delta'}^{(\alpha\beta)}(\omega) = 0 \]  
\((3.5)\)

in the MD approximation. Further we put the wave vector dependence of \( L_{k\alpha\beta}(\omega) \) as

\[ L_{k\alpha\beta}^{(\alpha\beta)}(\omega) = c_k c_k \varphi_1(\omega) + s_k s_k \varphi_2(\omega), \]

\[ L_{k\alpha\beta}^{(\alpha\beta)}(\omega) = -L_{k\alpha\beta}^{(\alpha\beta)}(\omega) = i[s_k c_k \varphi_3(\omega) - c_k s_k \varphi_4(\omega)]. \]  
\((3.6)\)

Substituting Eqs. (3.4) to (3.6) into Eqs. (3.2) and (3.3), we obtain equations for \( \varphi_1(\omega) \) as

\[ \varphi_1(\omega) = -\frac{J}{2N} + \rho \alpha_e \int_{-x}^{x} \frac{dx}{x + W_i} \varphi_1(x) + \rho \alpha_s \int_{-x}^{x} \frac{dx}{x - W_i} \varphi_1(x) \]

\[ + \rho \alpha_e \int_{-x}^{x} \frac{dx}{x + W_i} \varphi_2(x) + \rho \alpha_s \int_{-x}^{x} \frac{dx}{x - W_i} \varphi_2(x), \]

\[ \varphi_3(\omega) = -\frac{J}{2N} + 2\rho \alpha_e \int_{-x}^{x} \frac{dx}{x + W_i} \varphi_3(x) + 2\rho \alpha_s \int_{-x}^{x} \frac{dx}{x - W_i} \varphi_3(x) \]  
\((3.7)\)

Equations for \( \varphi_2(\omega) \) and \( \varphi_4(\omega) \) are obtained from Eq. (3.7) by the replacement \( \varphi_1 \leftrightarrow \varphi_2, \varphi_3 \leftrightarrow \varphi_4 \) and \( \alpha_e \leftrightarrow \alpha_s \). Here \( \rho \) denotes the density of states of conduction electrons on the Fermi surface, and \( D \) the band width. \( \alpha_e \) and \( \alpha_s \) are defined by

\[ \alpha_e = \langle c_k \rangle = \frac{1}{2} \left( 1 + \frac{\sin k_F R}{k_F R} \right), \]

\[ \alpha_s = \langle s_k \rangle = \frac{1}{2} \left( 1 - \frac{\sin k_F R}{k_F R} \right), \]  
\((3.8)\)
where $\langle \cdots \rangle$ denotes the average over the direction of $\mathbf{k}$. Though $\alpha_\epsilon$ and $\alpha_\iota$ depend on the magnitude of $\mathbf{k}$, we have approximated them by their value at $k = k_F$ (Fermi wave number).

In solving Eq. (3.7), there appear terms such as $\log \frac{|(\omega + W)/(\omega - W)|}{|\omega|}$. Though they are divergent at $\omega = \pm W$, we neglect them assuming $|\omega| \ll |W|$ or $|\omega| \gg |W|$. After some manipulation we find the solution of Eq. (3.7) as

$$
\varphi_1(\omega) = \varphi_3(\omega) = -\frac{J}{2N} \left[ 1 + \gamma_\epsilon \log \frac{D}{|\omega + W_i|} + \gamma_\iota \log \frac{D}{|\omega + W_i|} \right]^{-1},
$$

$$
\varphi_2(\omega) = \varphi_4(\omega) = -\frac{J}{2N} \left[ 1 + \gamma_\iota \log \frac{D}{|\omega + W_i|} + \gamma_\epsilon \log \frac{D}{|\omega + W_i|} \right]^{-1},
$$

where

$$
\gamma_\iota = \gamma_\iota \epsilon, \quad \gamma_\epsilon = \gamma_\iota \epsilon, \quad \gamma = J \rho.
$$

Equations (3.9) agree with our previous result obtained by the direct perturbational calculation.\(^4\)

In order to get the Yoshimori equation, we need the irreducible vertex $A^{(3)}$. Using above solutions, we obtain

$$
A^{(3)}_{\mathbf{k}k'}(\omega_1, \omega - \omega_1; \omega_2, \omega - \omega_2) = 3\rho \int_{x_1 + x_2 = 0}^{x} dx \frac{1}{x + W_1} \{ \alpha_s \phi_3(\phi_3(x) + \alpha_s \phi_3(\phi_3(x)) \}
$$

$$
= 3J \frac{\alpha_s \phi_3(\phi_3(\phi_3(x) + \alpha_s \phi_3(\phi_3(x)))}{4N} (\alpha_s \phi_3(\phi_3(\phi_3(x) + \alpha_s \phi_3(\phi_3(x)))I(\omega_1 + \omega_2 + \omega + W_i),
$$

$$
A^{(3)}_{kk'}(\omega_1, \omega - \omega_1; \omega_2, \omega - \omega_2) = -\rho \int_{x_1 + x_2 = 0}^{x} dx \frac{1}{x + W_1} \{ \alpha_s \phi_3(\phi_3(x) + \alpha_s \phi_3(\phi_3(x)) \}
$$

$$
= -J \frac{\alpha_s \phi_3(\phi_3(\phi_3(x) + \alpha_s \phi_3(\phi_3(x)))}{4N} (\alpha_s \phi_3(\phi_3(\phi_3(x) + \alpha_s \phi_3(\phi_3(x)))I(\omega_1 + \omega_2 + \omega + W_i),
$$

$$
A^{(3)}_{kk'}(\omega_1, \omega - \omega_1; \omega_2, \omega - \omega_2) = -A^{(3)}(\omega_2, \omega - \omega_2; \omega_1, \omega - \omega_1)
$$

$$
= -2i\rho \int_{x_1 + x_2 = 0}^{x} dx \frac{1}{x + W_1} \{ \alpha_s \phi_3(\phi_3(x) - \alpha_s \phi_3(\phi_3(x)) \}
$$

$$
= iJ \frac{\alpha_s \phi_3(\phi_3(\phi_3(x) - \alpha_s \phi_3(\phi_3(x)))}{2N} (\alpha_s \phi_3(\phi_3(\phi_3(x) - \alpha_s \phi_3(\phi_3(x)))I(\omega_1 + \omega_2 + \omega + W_i),
$$

where

$$
I(\omega) = \frac{\gamma \log(D/|\omega|)}{1 + \gamma \log(D/|\omega|)}.
$$
§ 4. The Yoshimori equation and its solution for special cases

Substitution of Eq. (3·11) in Eqs. (2·9) and (2·10) gives the Yoshimori equation for $G^{(v)}$ and $y^{(v)}$. We introduce the functions $\phi_i(\epsilon_k, \epsilon_k')$ and $\psi_i(\epsilon_k, \epsilon_k')$ defined by

$$\langle s_{kk'} \Gamma^{(v)}_{kk'} \rangle = \frac{\phi_1(\epsilon_k, \epsilon_k')}{\epsilon_k + \epsilon_k' + W_z - E},$$

$$\langle c_{kk'} \Gamma^{(v)}_{kk'} \rangle = \frac{\phi_2(\epsilon_k, \epsilon_k')}{\epsilon_k + \epsilon_k' + W_z - E},$$

$$\langle s_{kk'} \gamma^{(v)}_{kk'} \rangle = \frac{i \phi_1(\epsilon_k, \epsilon_k')}{\epsilon_k + \epsilon_k' + W_z - E},$$

$$\langle c_{kk'} \gamma^{(v)}_{kk'} \rangle = \frac{i \phi_2(\epsilon_k, \epsilon_k')}{\epsilon_k + \epsilon_k' + W_z - E}.$$

(4·1)

Then equations for them are obtained as

$$\phi_1(\epsilon, \epsilon') + \frac{1}{2} \gamma \int_0^\infty d\epsilon'' \left\{ \frac{\alpha \phi_1(\epsilon, \epsilon'')}{\epsilon + \epsilon'' + W_z - E} + \frac{\alpha \phi_2(\epsilon, \epsilon')}{\epsilon'' + \epsilon' + W_z - E} \right\}$$

$$+ \frac{1}{2} \gamma \int_0^\infty d\epsilon'' \left\{ \frac{\alpha \phi_1(\epsilon, \epsilon'')}{\epsilon + \epsilon'' + W_z - E} + \frac{\alpha \phi_2(\epsilon, \epsilon')}{\epsilon'' + \epsilon' + W_z - E} \right\}$$

$$- \frac{1}{4} \gamma \alpha \psi_1(\epsilon, \epsilon) I(\epsilon + \epsilon' + \epsilon'' + W_z - E) \left\{ \frac{\phi_1(\epsilon, \epsilon'')}{\epsilon + \epsilon'' + W_z - E} + \frac{\phi_2(\epsilon, \epsilon')}{\epsilon'' + \epsilon' + W_z - E} \right\} = 0,$$

(4·2)

$$\phi_1(\epsilon, \epsilon') + \frac{3}{2} \gamma \alpha \int_0^\infty d\epsilon'' \left\{ \frac{\phi_1(\epsilon, \epsilon'')}{\epsilon + \epsilon'' + W_z - E} + \frac{\phi_2(\epsilon, \epsilon')}{\epsilon'' + \epsilon' + W_z - E} \right\}$$

$$- \frac{3}{2} \gamma \alpha \int_0^\infty d\epsilon'' I(\epsilon + \epsilon' + \epsilon'' + W_z - E) \left\{ \frac{\phi_1(\epsilon, \epsilon'')}{\epsilon + \epsilon'' + W_z - E} + \frac{\phi_2(\epsilon, \epsilon')}{\epsilon'' + \epsilon' + W_z - E} \right\}$$

$$+ \frac{3}{2} \gamma \alpha \int_0^\infty d\epsilon'' I(\epsilon + \epsilon' + \epsilon'' + W_z - E) \left\{ \frac{\phi_1(\epsilon, \epsilon'')}{\epsilon + \epsilon'' + W_z - E} + \frac{\phi_2(\epsilon, \epsilon')}{\epsilon'' + \epsilon' + W_z - E} \right\} = 0.$$  

(4·3)

Two other equations are obtained from Eqs. (4·2) and (4·3) by replacing the suffixes 1 and 2 of $\phi$ and $\psi$ and the suffixes $c$ and $s$ of $\alpha$ with each other simultaneously. In the following we shall explicitly give equations for $\phi_1$ and $\psi_1$ only. Equations for $\phi_2$ and $\psi_2$ will be obtained from them in the same way. From Eq. (2·6) we see $\phi_1(\epsilon, \epsilon')$ and $\psi_1(\epsilon, \epsilon')$ satisfy symmetry relations

$$\phi_1(\epsilon, \epsilon') = \phi_1(\epsilon', \epsilon), \quad \psi_1(\epsilon, \epsilon') = \psi_1(\epsilon', \epsilon), \quad \phi_1(\epsilon, \epsilon') = \phi_1(\epsilon', \epsilon).$$  

(4·4)
The equations can easily be solved for some special cases: 1) $W > 0$, $W \to \infty$; 2) $W < 0$, $|W| \to \infty$; 3) $\alpha_e = 1$, $\alpha_s = 0$; 4) $W = 0$, $\alpha_e = \alpha_s = 1/2$. Among them, Cases 1) ~ 3) are trivial, since in these cases the vertex correction disappears and the equations reduce to those in the zeroth approximation. The ground-state energy for these cases is given in I as

1) $E = -\frac{1}{4} W - D e^{i\pi \alpha_e} - D e^{i\pi \alpha_s}$,

2) $E = \frac{1}{4} W$,

3) $E = \begin{cases} -\frac{1}{4} W - D e^{i\pi} & \text{for } W > -D e^{i\pi}, \\ \frac{1}{4} W & \text{for } W < -D e^{i\pi}. \end{cases}$

In Case 4) four equations for $\phi_1$, $\phi_2$, $\psi_1$ and $\psi_2$ can be reduced to one equation for $\phi(\epsilon', \epsilon')$ defined by

$$\phi(\epsilon, \epsilon') = [\phi_1(\epsilon, \epsilon') + \phi_2(\epsilon, \epsilon')] + \frac{1}{d} [\psi_1(\epsilon, \epsilon') + \psi_2(\epsilon, \epsilon')].$$

(4.5)

The equation for $\phi$ is obtained as

$$\phi(\epsilon, \epsilon') + \frac{3}{4} \int_0^\rho d\epsilon'' \left\{ \frac{\phi(\epsilon, \epsilon'')}{\epsilon + \epsilon'' - E} + \frac{\phi(\epsilon'', \epsilon')}{\epsilon'' + \epsilon' - E} \right\}$$

$$- \frac{3}{16} \int_0^\rho d\epsilon'' I(\epsilon + \epsilon' + \epsilon'' - E) \left\{ \frac{\phi(\epsilon, \epsilon'')}{\epsilon + \epsilon'' - E} + \frac{\phi(\epsilon'', \epsilon')}{\epsilon'' + \epsilon' - E} \right\} = 0. \quad (4.6)$$

Equation (4.6) is of the same form as derived by Okada and Yosida\textsuperscript{11} for the case of a magnetic impurity with many $d$ electrons. According to Okada-Yosida, the solution of Eq. (4.6) is given by

$$\phi(\epsilon, \epsilon') = A(\epsilon + \epsilon') \left\{ \frac{A(\epsilon)}{\epsilon - E/2} + \frac{A(\epsilon')}{\epsilon' - E/2} \right\},$$

(4.7)

where

$$A(\epsilon) = \left( 1 + \gamma \log \frac{D}{|\epsilon - E/2|} \right)^{-1/4},$$

$$E = -2D e^{i\pi \gamma}. \quad (4.8)$$

The ground state energy for this case obtained in I is $-2De^{i\pi \gamma}$. Here the exponent is modified to the correct one as expected.

§ 5. Solution for general cases

In order to solve the equations for more general cases, we have to introduce further approximations which are allowed within logarithmic accuracy. The method is essentially the same as taken in I, though the procedure becomes more complicated because $\phi_1$ and $\psi_1$ are functions of two variables in the present case.

Now we divide the region of variables into three:
Region I. \( \epsilon, \epsilon' < F \),
Region II. \( \epsilon < F < \epsilon' \) or \( \epsilon' < F < \epsilon \),
Region III. \( F < \epsilon, \epsilon' \),

where
\[
F = |W| - \Delta E, \tag{5.1}
\]
and \( \Delta E \) is the binding energy defined by
\[
E = W + \Delta E \quad \text{for} \quad W > 0,
\]
\[
E = W + \Delta E \quad \text{for} \quad W < 0. \tag{5.2}
\]
The functions \( \psi \) and \( \phi \) defined in each region are denoted by \( \psi^{(i)}, \phi^{(i)} \) and so on. The procedure we take is to derive the equation for \( \phi^{(i)} \) and \( \psi^{(i)} \) by eliminating Region II and III. In doing so, we take the approximation that terms of the order \( r, \log D \) and \( r \log D \) times \( \phi^{(i)} \) or \( \psi^{(i)} \) are retained and terms smaller than them by a factor \( r^n (n \geq 1) \) are neglected.

Within the logarithmic accuracy, we have only to consider three limiting cases: 1) \( W > 0, D \gg W \gg |\Delta E| \); 2) \( W < 0, D \gg |W| \gg |\Delta E| \); 3) \( |W| \ll |\Delta E| \). The case \( |W| \sim D \) is essentially the same as Cases 1) and 2) of § 4. The case \( |W| \sim |\Delta E| \) cannot be discussed from the above equations, since terms of the type \( \log |(W + \omega)/(W - \omega)| \) which we have neglected may play a role in this region. We can, however, find the qualitative behavior of the solution in the whole region of \( W \) by interpolating the solutions for these limiting cases.

1) \( W > 0, D \gg W \gg |\Delta E| \)

In deriving the equation for \( \phi^{(i)}(\epsilon, \epsilon') \) from Eq. (4.2), we rewrite each integral as a sum of two parts in such a way as
\[
\int_0^\rho \! \! d\epsilon'' = \int_0^\rho \! \! d\epsilon'' + \int_0^\rho \! \! d\epsilon''.
\]
In the integrands there appear energy sums of various types such as \( \epsilon + \epsilon'' - \Delta E \) or \( \epsilon + \epsilon'' + F \). Within the logarithmic accuracy we have only to retain the largest one among the energy terms, neglecting other smaller ones. For instance, an integral on the second line of Eq. (4.2) is approximated for \( \epsilon < F \) as
\[
\int_0^\rho \! \! d\epsilon'' \frac{\phi^{(i)}(\epsilon, \epsilon'')}{\epsilon + \epsilon'' + F} = \int_0^\rho \! \! d\epsilon'' \frac{\phi^{(i)}(\epsilon, \epsilon'')}{\epsilon + \epsilon'' + F} + \int_0^\rho \! \! d\epsilon'' \frac{\psi^{(i)}(\epsilon, \epsilon'')}{\epsilon + \epsilon'' + F}
\approx \frac{1}{F} \int_0^\rho \! \! d\epsilon'' \frac{\phi^{(i)}(\epsilon, \epsilon'')}{\epsilon''} + \int_0^\rho \! \! d\epsilon'' \frac{\psi^{(i)}(\epsilon, \epsilon'')}{\epsilon''}. \tag{5.3}
\]
In the integrand of the first term the largest term among \( \epsilon, \epsilon'' \) and \( F \) is \( F \), while in the integrand of the second term it is \( \epsilon'' \). Thus we get the second expression. Further we neglect the first term, for its contribution to the equation
for $\phi_{1}^{(I)}$ is of the order $\gamma \phi_{1}^{(I)}$.

In this way we finally obtain the approximate equation for $\phi_{1}^{(I)}$ as

$$\phi_{1}^{(I)}(\epsilon, \epsilon') + \gamma \int_{0}^{F} d\epsilon'' \left\{ \alpha_{s} \left[ 1 - \frac{1}{4} \alpha_{s} I(F) \right] \frac{\phi_{1}^{(I)}(\epsilon, \epsilon'')}{\epsilon + \epsilon'' - \Delta E} + \alpha_{s} \left[ 1 - \frac{1}{4} \alpha_{s} I(F) \right] \frac{\phi_{1}^{(I)}(\epsilon'', \epsilon')}{\epsilon'' + \epsilon' - \Delta E} \right\}$$

$$+ \frac{\gamma}{\epsilon'} \int_{F}^{\infty} d\epsilon'' \left\{ \alpha_{s} \left[ \phi_{1}^{(I)}(\epsilon, \epsilon'') + \frac{1}{2} \phi_{2}^{(I)}(\epsilon, \epsilon'') \right] \right\}$$

$$+ \frac{1}{2} \phi_{1}^{(I)}(\epsilon'', \epsilon') + \phi_{2}^{(I)}(\epsilon'', \epsilon') \right\} = 0. \quad (5.4)$$

The function $\phi_{1}^{(I)}$ couples with functions in Region II.

Similarly we can derive the equations for $\phi_{1}^{(II)}$ and $\phi_{1}^{(III)}$. If $\epsilon < F < \epsilon'$, integrals on the first line of Eq. (4.3) become

$$\int_{0}^{\epsilon} d\epsilon'' \phi_{1}^{(I)}(\epsilon, \epsilon'') = \int_{0}^{\epsilon} d\epsilon'' \phi_{1}^{(I)}(\epsilon, \epsilon'') + \int_{F}^{\epsilon} d\epsilon'' \phi_{1}^{(I)}(\epsilon, \epsilon''), \quad (5.5)$$

$$\int_{0}^{\epsilon} d\epsilon'' \frac{\phi_{1}^{(II)}(\epsilon'', \epsilon')}{\epsilon'' + \epsilon' - \Delta E} \sim \frac{1}{\epsilon'} \int_{0}^{\epsilon} d\epsilon'' \phi_{1}^{(I)}(\epsilon'', \epsilon') + \int_{F}^{\epsilon} d\epsilon'' \phi_{1}^{(I)}(\epsilon'', \epsilon'). \quad (5.6)$$

If we solve the equations iteratively, we find contributions of two terms of Eq. (5.6) to be of the order

$$\gamma \int_{F}^{\epsilon} d\epsilon' \int_{0}^{\epsilon} d\epsilon'' \phi_{1}^{(I)}(\epsilon'', \epsilon') \sim \gamma^{2} \phi_{1}^{(I)}$$

$$\gamma \int_{F}^{\epsilon} d\epsilon' \int_{0}^{\epsilon} d\epsilon'' \frac{\phi_{1}^{(II)}(\epsilon'', \epsilon')}{\epsilon'' + \epsilon' - \Delta E} \sim \gamma^{2} \log \frac{D}{F} \phi_{1}^{(I)} \quad (5.7)$$

respectively, which can be neglected. In this estimation we took $\phi_{1}^{(I)} \sim \phi_{1}^{(II}) \sim \phi_{1}^{(III)}$ since the energy dependence of $\phi_{1}$ is logarithmic and very weak compared with other factors. Finally we obtain

$$\phi_{1}^{(I)}(\epsilon, \epsilon') + \gamma \alpha_{s} \int_{F}^{\epsilon} d\epsilon'' \frac{\phi_{1}^{(I)}(\epsilon, \epsilon'')}{\epsilon'' + \epsilon' - \Delta E}$$

$$- \frac{1}{2} \gamma \alpha_{s} \alpha_{s} \int_{F}^{\epsilon} d\epsilon'' I(\epsilon'') \left[ \frac{1}{2} \phi_{2}^{(I)}(\epsilon', \epsilon'') + \phi_{1}^{(I)}(\epsilon', \epsilon'') \right]$$

$$= - \alpha_{s} \left[ 1 - \frac{1}{4} \alpha_{s} I(\epsilon') \right] \Phi_{1}(\epsilon) - \frac{1}{2} \alpha_{s} \left[ 1 - \alpha_{s} I(\epsilon') \right] \Psi_{1}(\epsilon), \quad (5.8)$$

where we put
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\[ \Phi_1(\epsilon) = \gamma \int_{E'}^{\epsilon} \frac{\phi_1^{(b)}(\epsilon, \epsilon')}{\epsilon + \epsilon' + W_1 - E} d\epsilon', \quad (5.9) \]

\[ \Psi_1(\epsilon) = \gamma \int_{E'}^{\epsilon} \frac{\psi_1^{(b)}(\epsilon, \epsilon')}{\epsilon + \epsilon' + W_1 - E} d\epsilon'. \]

Though \( \Psi_1(\epsilon) \) can be neglected compared with \( \Phi_1(\epsilon) \) in the present case, we have kept it for later convenience.

The equation for \( \phi_1^{(a)}(\epsilon) \) can be obtained in a similar way. We get for \( \epsilon < F < \epsilon' \)

\[ \phi_1^{(a)}(\epsilon, \epsilon') + \frac{3}{2} \gamma \alpha_s \int_{F}^{\epsilon} \frac{d\epsilon''}{\epsilon''} \phi_1^{(b)}(\epsilon, \epsilon'') 
- \frac{3}{2} \gamma \alpha_s \int_{F}^{\epsilon} \frac{d\epsilon''}{\epsilon''} I(\epsilon' + \epsilon'') \left\{ \alpha_e \phi_1^{(a)}(\epsilon, \epsilon'') - \frac{1}{2} \alpha_e \phi_1^{(b)}(\epsilon, \epsilon'') \right\} 
= -\frac{3}{2} \gamma \alpha_s (1 - \alpha_s I(\epsilon')) \Phi_1(\epsilon) - \frac{3}{4} \alpha_e \alpha_s I(\epsilon') \Psi_1(\epsilon). \quad (5.10) \]

Comparing these equations, we can easily see

\[ \phi_1^{(a)}(\epsilon, \epsilon') - [\phi_1^{(b)}(\epsilon, F) + \phi_1^{(b)}(F, \epsilon')] = 0. \quad (5.11) \]

Thus, we have to solve Eqs. (5.11), (5.8) and (5.10), putting \( \Psi_1 = 0 \).

2) \( W < 0, D \gg |W| \gg |\Delta E| \)

In this case we need the equation for \( \phi_1^{(a)} \). The procedure of getting it is quite similar to the above calculation. We obtain

\[ \phi_1^{(a)}(\epsilon, \epsilon') + \frac{3}{4} \gamma \alpha_s \alpha_s I(F) \int_{F}^{\epsilon} d\epsilon'' \left\{ \frac{\phi_1^{(b)}(\epsilon, \epsilon'')}{\epsilon + \epsilon'' - \Delta E} + \frac{\psi_1^{(b)}(\epsilon'', \epsilon')}{\epsilon'' + \epsilon' - \Delta E} \right\} 
+ \frac{3}{2} \gamma \alpha_s \int_{F}^{\epsilon} \frac{d\epsilon''}{\epsilon''} \left\{ \phi_1^{(b)}(\epsilon, \epsilon'') + \phi_2^{(b)}(\epsilon'', \epsilon') \right\} 
- \frac{3}{2} \gamma \alpha_s \int_{F}^{\epsilon} \frac{d\epsilon''}{\epsilon''} I(\epsilon'') \left\{ \alpha_e \phi_1^{(a)}(\epsilon, \epsilon'') - \frac{1}{2} \alpha_e \phi_1^{(b)}(\epsilon, \epsilon'') \right\} 
+ \alpha_e \phi_2^{(b)}(\epsilon'', \epsilon') - \frac{1}{2} \alpha_e \psi_1^{(b)}(\epsilon'', \epsilon') \right\} = 0. \quad (5.12) \]

Equations for Region II are exactly the same as before (i.e., Eqs. (5.8) and (5.10)) except that \( \Phi_1 \) can be neglected compared with \( \Psi_1 \) in this case. Similarly to Eq. (5.11), we find

\[ \phi_1^{(a)}(\epsilon, \epsilon') - [\phi_1^{(b)}(\epsilon, F) + \phi_1^{(b)}(F, \epsilon')] = 0. \quad (5.13) \]

3) \( |W| \ll |\Delta E| \)

In this case we neglect \( W \) compared with \( E \). Equations for \( \phi_1^{(a)} \) and \( \psi_1^{(a)} \)
are obtained in the same way as before. We finally find Eqs. (5.11), (5.13), (5.8) and (5.10) hold again if we put \( W_s = W_t = 0 \) and \( F = |E| \). In this case \( \phi \) and \( \psi \) are of the same order, and equations for \( \phi^{(i)} \) and \( \psi^{(i)} \) are coupled with each other and should be solved simultaneously.

There is no essential difficulty to solve the equations in the region II, though calculations are somewhat lengthy. Therefore, we shall give here only the results necessary for determining the ground-state energy and show the detail of the calculation in the Appendix. We obtain

\[
\begin{align*}
\phi^{(ii)}_1 (\epsilon, F) + \phi^{(ii)}_1 (F, \epsilon') &= -\frac{1}{1 + \gamma \log D/F} \left\{ \alpha_c \left[ \phi_1 (\epsilon) + \frac{1}{2} \psi_1 (\epsilon) \right] + \alpha_s \left[ \phi_1 (\epsilon') + \frac{1}{2} \psi_1 (\epsilon') \right] \right\}, \\
\phi^{(ii)}_1 (\epsilon, F) + \phi^{(ii)}_1 (F, \epsilon') &= -\frac{3 \alpha_s}{2} \frac{1}{1 + \gamma \log D/F} \left[ \phi_1 (\epsilon) + \phi_1 (\epsilon') \right].
\end{align*}
\]

Using Eqs. (5.11), (5.13), (5.14) and (5.15), we can easily determine the ground-state energy. We shall discuss three cases separately.

1) \( W > 0, \ D > W \gg |\Delta E| \)

Substituting Eq. (5.14) into Eq. (5.11) and putting \( \psi_i = 0 \), we obtain

\[
\phi^{(i)}_1 (\epsilon, \epsilon') + \gamma \int_0^F \frac{\phi^{(i)}_1 (\epsilon, \epsilon'')}{\epsilon + \epsilon'' - \Delta E} d\epsilon'' + \gamma \int_0^F \frac{\phi^{(i)}_1 (\epsilon'', \epsilon')}{\epsilon'' + \epsilon' - \Delta E} d\epsilon'' = 0,
\]

where

\[
\gamma_\epsilon = \frac{\frac{\gamma \alpha_c}{1 + \gamma \log D/F}}{1 + \gamma \log D/F}, \quad \gamma_s = \frac{\frac{\gamma \alpha_s}{1 + \gamma \log D/F}}{1 + \gamma \log D/F}.
\]

The equation is of the same form as obtained in I by the zeroth approximation except that the coupling constant is replaced by an effective one. As shown in I, its solution is easily found to be

\[
\phi^{(i)}_1 (\epsilon, \epsilon') = \frac{A}{\epsilon - E_1} + \frac{A}{\epsilon' - E_2},
\]

\[
E_1 = -F \exp \left( \frac{1}{\gamma_s} \right), \quad E_2 = -F \exp \left( \frac{1}{\gamma_\epsilon} \right), \quad E = E_1 + E_2.
\]

In the present case we can put \( F = W \). Then Eqs. (5.18) and (5.19) give the solution in an explicit form.

2) \( W < 0, \ D \gg |W| \gg |\Delta E| \)

Using Eqs. (5.13) and (5.15) and putting \( \phi_i = 0 \), we find

\[
\phi^{(ii)}_1 (\epsilon, \epsilon') = 0.
\]
This means that there is no bound-state solution at all in this case. A fictitious bound state obtained in I disappears here.

3) $|W| \ll |AE|$

If we neglect $W$, the equations for $\phi_1^{(I)}$ and $\psi_1^{(I)}$ are given by

$$
\phi_1^{(I)}(\epsilon, \epsilon') + \bar{\gamma}_e \int_{0}^{[E]} \frac{d \epsilon''}{\epsilon'' - E} \left[ \phi_1^{(I)}(\epsilon, \epsilon'') + \frac{1}{2} \psi_1^{(I)}(\epsilon, \epsilon'') \right] + \bar{\gamma}_s \int_{0}^{[E]} \frac{d \epsilon''}{\epsilon'' + \epsilon' - E} \left[ \phi_1^{(I)}(\epsilon'', \epsilon') + \frac{1}{2} \psi_1^{(I)}(\epsilon'', \epsilon') \right] = 0 ,
$$

$$
\psi_1^{(I)}(\epsilon, \epsilon') + \frac{3}{2} \bar{\gamma}_s \int_{0}^{[E]} \frac{d \epsilon''}{\epsilon'' - E} \phi_1^{(I)}(\epsilon, \epsilon'') + \frac{3}{2} \bar{\gamma}_s \int_{0}^{[E]} \frac{d \epsilon''}{\epsilon'' + \epsilon' - E} \phi_1^{(I)}(\epsilon'', \epsilon')
$$

$$
= 0 ,
$$

(5.21)

(5.22)

where

$$
\bar{\gamma}_e = \frac{\gamma \alpha_e}{1 + \gamma \log D/|E|} , \quad \bar{\gamma}_s = \frac{\gamma \alpha_s}{1 + \gamma \log D/|E|} .
$$

They are solved by putting

$$
\phi_1^{(I)}(\epsilon, \epsilon') = \frac{A}{\epsilon - E_1} + \frac{A}{\epsilon' - E_2} ,
$$

$$
\phi_1^{(I)}(\epsilon, \epsilon') = \frac{B}{\epsilon - E_1} + \frac{B}{\epsilon' - E_1} ,
$$

$$
\psi_1^{(I)}(\epsilon, \epsilon') = \frac{B}{\epsilon - E_2} + \frac{B}{\epsilon' - E_2} ,
$$

(5.23)

(5.24)

Substitution of Eqs. (5.23) and (5.24) into Eqs. (5.21) and (5.22) gives

$$
(1 + g) A + \frac{1}{2} g B = 0 ,
$$

$$
B + \frac{1}{2} g A = 0 ,
$$

(5.25)

where

$$
g = \bar{\gamma}_e \int_{0}^{[E]} \frac{d \epsilon}{\epsilon - E_2} = \bar{\gamma}_s \int_{0}^{[E]} \frac{d \epsilon}{\epsilon - E_1} .
$$

(5.26)

From Eq. (5.25) $g$ is determined by

$$
1 + g - \frac{4}{3} g^2 = 0 ,
$$

i.e.,

$$
g = 2 \text{ or } -\frac{1}{3} .
$$

(5.27)
Among them \( g = -3/2 \) should be chosen. Substituting this value of \( g \) into Eqs. (5.26) and (5.24), we finally obtain

\[
\exp\left(\frac{3}{2g}\right) + \exp\left(-\frac{3}{2g}\right) = 1. \tag{5.28}
\]

This relation can be satisfied only when

\[
1 + \gamma \log \frac{D}{|E|} = O(\gamma).
\]

Thus we obtain the ground-state energy as

\[
E \simeq -De^{1/r} \tag{5.29}
\]

independently of \( \alpha_e \) and \( \alpha_s \). The result agrees with that obtained by Ishii\(^9\) for a doublet bound state.

§ 6. Summary and discussion

The results obtained in this paper are summarized as follows: The ground-state energy \( E \) of the system is given by

1) for \( W > 0 \) and \( W \sim D \),

\[
E = -\frac{1}{4} W - D e^{1/r_{\alpha_e}} - D e^{1/r_{\alpha_s}};
\]

2) \( W > 0 \) and \( T_{K0} \ll W \ll D \),

\[
E = -\frac{1}{4} W - D \left( \frac{D}{W} \right)^{1/\alpha_e - 1} - D \left( \frac{D}{W} \right)^{1/\alpha_s - 1} e^{1/r_{\alpha_e}};
\]

3) for \( |W| \ll T_{K0} \),

\[
E = -2De^{1/r};
\]

4) for \( W < 0 \) and \( |W| \gg T_{K0} \),

\[
E = \frac{3}{4} W.
\]

In Case 4) there is no bound state. Here \( T_{K0} = De^{1/r} \) is the Kondo temperature of an isolated impurity, \( \gamma = J_0 \) and \( \alpha_e \) and \( \alpha_s \) are given by Eq. (3.8). When the distance between impurities \( R \) vanishes or \( \alpha_e = 1 \) and \( \alpha_s = 0 \), in particular, the ground-state energy reduces to

5) for \( W > -T_{K0} \) and \( R = 0 \),

\[
E = -\frac{1}{4} W - D e^{1/r};
\]

6) for \( W < -T_{K0} \) and \( R = 0 \),
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\[ E = \frac{3}{4} W. \]

We see the defects of the result of I discussed in § 1 have been completely removed as expected, i.e., Case 4) of the above resolves the problem 2) of § 1, while Case 3) is the answer to 1) and 3) of § 1.

In the low-energy region (i.e., lower than \( |W| + |\Delta E| \), \( \Delta E \) being the binding energy), wave functions are essentially of the same form as those in the zeroth approximation. In the high-energy region, they are obtained from Eqs. (A·2), (A·7), (A·16), (A·17) and (A·18) and have a more complicated form.

In order to see the behavior of the ground-state energy as a function of \( W \), we have to interpolate the above results for various limiting cases. To do so, we have to know how correction arises from small but finite \( W \) in Case 3). Unfortunately, however, our calculation cannot give any answer to this question, since we performed calculations within logarithmic accuracy. For instance, the term \( \log(A+B) \) was approximated by \( \log A \) if \( A>B \), since the correction gives only lower divergent contributions. Therefore, as far as we restrict ourselves to the MD approximation, we cannot discuss these corrections.

In this connection, we have to mention to the work by Klein and Tsay,\(^7\) and by Matho and Béal-Monod.\(^9\) Applying the Green's function method to the problem of an impurity-pair and to that of many impurities, Klein and Tsay found the effective Kondo temperature of an impurity under the influence of the interaction with other impurities as

\[ T_K = T_{K0} \{1 - (W'/T_{K0})^6\}^{1/8}, \quad (6·1) \]

where \( W' \) is an effective impurity-impurity interaction potential and is approximately proportional to \( W \). From this expression of the Kondo temperature they concluded that the Kondo effect is completely suppressed by the impurity-impurity interaction if \( |W'|>T_{K0} \) irrespectively of the sign of \( W \). This conclusion was criticized by Matho and Béal-Monod. The situation is essentially different between the cases \( W>0 \) and \( W<0 \). If \( W>0 \), the triplet state of impurity spins is lower than the singlet, and the impurity pair reduces to a magnetic impurity with \( S=1 \) for sufficiently large \( W \). On the other hand, if \( W<0 \), the singlet is lower and the impurity pair behaves as a nonmagnetic impurity for sufficiently large \( |W| \). The Kondo effect disappears in the latter case, while it does not in the former. The expression of the Kondo temperature obtained by Matho and Béal-Monod by the third-order perturbation is essentially different from Eq. (6·1) and asymmetric for the cases \( W>0 \) and \( W<0 \).

Here we are interested in whether there is a term linear to \( W \) in the expression of the binding energy when \( |W| \ll T_{K0} \). If the binding energy is identified with the Kondo temperature, Eq. (6·1) does not give such a linear term. However, as pointed out by Matho and Béal-Monod and discussed above,
Eq. (6-1) seems essentially wrong on this point. The expression obtained by Matho and Béal-Monod contains a linear term for general $R$. It disappears only when $\alpha_a = \alpha_c = 1/2$. It is quite plausible that a linear term vanishes when $R = \infty$, since in this case two impurities form singlet bound states at each site and behave as two nonmagnetic impurities.

In our calculation we could determine the ground-state energy in the whole region of $W$ without any interpolation for a special case where $R = 0$ (Cases 5) and 6) above). Thus we know the behavior of the ground-state energy as a function of $W$ for two limiting cases $R = 0$ and $R = \infty$ (or $\alpha_a = 0$ and $\alpha_c = 1/2$). We may reasonably expect that the energy is a smooth function of $R$ or $\alpha_a$. Thus we expect for $|W| \ll T_K$

$$E = -D e^{\gamma'} - \frac{1}{2} p(\alpha_a) W,$$  

(6-2)

where $p(\alpha_a)$ is a smooth function of $\alpha_a$ and $p(0) = 1$ and $p(1/2) = 0$. The behavior of the ground-state energy as a function of $W$ is illustrated qualitatively in Fig. 3. This is exactly the same as expected in I.

In cases where the concentration of magnetic impurities is not so high, weakly coupled pairs of impurities may play important roles. To treat a weakly coupled pair, we have to verify the expression (6-2) derived by physical considerations and to determine the function $p(\alpha_a)$ explicitly. In addition, it should be noticed that even when $W = 0$, some effects of the impurity correlation may occur.

If $R$ is finite, there is nonvanishing overlapping between the bound state wavefunctions. By analogy with the usual one-particle problem, it is natural to expect such overlapping splits the bound state. We found, however, no such effect in our results obtained by the MD approximation. The reason why we did not seems to be as follows. The energy splitting caused by the overlapping will be at most of the same order as the binding energy of a single impurity $T_K$. Thus the overlapping modifies the binding energy by a factor of the order unity. On the other hand, in the MD approximation we can only determine the exponent of the binding energy, and to determine the factor of the order unity is beyond the approximation. Thus to discuss the behavior of a weakly coupled pair, we have to extend the calculation by including the lower divergent contributions.

**Appendix**

We solve a set of simultaneous equations (5-8) and (5-10) for $\phi_1^{(2)}$ and $\phi_1^{(3)}$, $\Phi_1$ and $T_1$ being given. In order to solve them, we approximate the
the integrals on the second line of Eqs. (5.8) and (5.10) in such a way as

\[
\int_{\epsilon}^{\epsilon''} \frac{d\epsilon''}{\epsilon''} I(\epsilon'' + \epsilon') \phi^{(\text{II})}_{2}(\epsilon, \epsilon'')
\]

\[
= I(\epsilon') \int_{\epsilon'}^{\epsilon''} \frac{d\epsilon''}{\epsilon''} \phi^{(\text{II})}_{1}(\epsilon, \epsilon'') + \int_{\epsilon'}^{\epsilon''} \int_{\epsilon'}^{\epsilon''} \frac{d\epsilon''}{\epsilon''} I(\epsilon'') \phi^{(\text{II})}_{1}(\epsilon, \epsilon''). \quad (A.1)
\]

This is the same approximation as we took in Eq. (5.5), for instance. Let us put

\[
\phi^{(\text{II})}_{1}(\epsilon, \epsilon') = f(x), \quad (A.2)
\]

\[
\phi^{(\text{II})}_{2}(\epsilon, \epsilon') = g(x), \quad (A.3)
\]

where we have not shown the \( \epsilon \)-dependence of the functions explicitly. Then equations for \( f(x) \) and \( g(x) \) are given by

\[
f(x) - \alpha_{e} \int_{0}^{x} dx' \left[ f(x') + \frac{1}{2} g(x') \right] - \frac{1}{2} \alpha_{e} \alpha_{s} \int_{0}^{x} dx' \frac{x'}{1-x'} \left[ \frac{1}{2} f(x') + g(x') \right] = -\alpha_{e} (1 + \frac{1}{4} \alpha_{s} x \frac{1}{1-x}) \phi_{1} - \frac{1}{2} \alpha_{e} \left( 1 + \alpha_{s} x \frac{1}{1-x} \right) \psi_{1}, \quad (A.4)
\]

\[
g(x) - \frac{3}{2} \alpha_{s} \int_{0}^{x} dx' f(x') - \frac{3}{2} \alpha_{s} \int_{0}^{x} dx' \frac{x'}{1-x'} \left[ \alpha_{s} f(x') - \frac{1}{2} \alpha_{e} g(x') \right] - \frac{3}{2} \alpha_{s} \int_{x}^{1} dx' \left[ \alpha_{s} f(x') - \frac{1}{2} \alpha_{e} g(x') \right] = -\frac{3}{2} \alpha_{s} \left[ 1 + \alpha_{s} x \frac{1}{1-x} \right] \phi_{1} + \frac{3}{4} \alpha_{s} \alpha_{s} x \frac{1}{1-x} \psi_{1}, \quad (A.5)
\]

where

\[
t = -\gamma \log \frac{D}{\epsilon}. \quad (A.6)
\]

We can solve these equations by putting

\[
f(x) = \sum_{i=1}^{4} A_{i} (1-x)^{p_{i}},
\]

\[
g(x) = \sum_{i=1}^{4} B_{i} (1-x)^{q_{i}},
\]
Substitution of Eq. (A.7) into Eqs. (A.4) and (A.5) gives equations determining $A_t, B_t$ and $p_t$, i.e.,

\[
\sum_{t=1}^{4} \frac{(1-t)^{p_t+1}}{p_t+1} A_t = -\Phi_1, \tag{A.10}
\]

\[
\sum_{t=1}^{4} \frac{(1-t)^{p_t+1}}{p_t+1} B_t = -\Psi_1, \tag{A.11}
\]

\[
\sum_{t=1}^{4} \frac{1}{p_t+1} \left\{ \left( 1 + \frac{\alpha_t}{p_t} \right) A_t - \frac{\alpha_t}{2p_t} B_t \right\} = 0, \tag{A.12}
\]

\[
\sum_{t=1}^{4} \frac{1}{p_t+1} \left\{ \left( 1 + \frac{\alpha_t}{4p_t} \right) A_t + \frac{1}{2}\left( 1 + \frac{\alpha_t}{p_t} \right) B_t \right\} = 0. \tag{A.13}
\]

The exponents $p_t$ are determined by putting $\det=0$ from Eqs. (A.8) and (A.9), i.e.,

\[
p(p+1) + (p+1)\alpha_t - \frac{3}{4} \alpha_t \alpha_t = 0 \tag{A.14}
\]

or

\[
p(p+1) - p\alpha_t - \frac{3}{4} \alpha_t \alpha_t = 0. \tag{A.15}
\]

We denote the solutions of Eq. (A.14) by $p_1$ and $p_2$, and those of Eq. (A.15) by $p_3$ and $p_4$. Then we find

\[
A_2 = A_4 = B_2 = B_4 = 0 \tag{A.16}
\]

and

\[
A_1 = -\frac{1}{(1-t)^{p_1+1}} \frac{p_1+1}{p_1-p_2} \left\{ (\alpha_t - (p_2+1)\Phi_1 + \frac{1}{2} \alpha_t \Psi_1 \right\}, \tag{A.17}
\]

\[
B_1 = -\frac{1}{(1-t)^{p_1+1}} \frac{p_1+1}{p_1-p_2} \left\{ \frac{3}{2} \alpha_t \Phi_1 - (p_2+1)\Psi_1 \right\}, \tag{A.17}
\]

where

\[
p_{1,2} = \frac{1}{2} \left[ -(1+\alpha_t) \pm \sqrt{\alpha_t^2 + 3\alpha_t \alpha_t} \right]. \tag{A.18}
\]

Expressions for $A_2$ and $B_2$ are obtained from Eq. (A.17) by replacing $p_1$ and $p_2$ with each other.
Thus the solution in Region II has been determined as a function of $\Phi_1$ and $\mathcal{V}_1$. In order to get the equation for $\phi_1^{(1)}$ and $\phi_1^{(2)}$, we have only to know $\phi_1^{(1)}(\epsilon, F)$, $\phi_1^{(2)}(\epsilon, F)$ and so on which appear in Eqs. (5·11) and (5·13). They are obtained as

$$
\phi_1^{(1)}(\epsilon, F) = \sum_{i=1}^{N} A_i (1-t)^{p_i} = -\frac{\alpha_1}{1-t} \left( \Phi_1 + \frac{1}{2} \mathcal{V}_1 \right),
$$
(A·19)

$$
\phi_1^{(2)}(\epsilon, F) = \sum_{i=1}^{N} B_i (1-t)^{p_i} = -\frac{3}{2} \frac{\alpha_2}{1-t} \Phi_1.
$$
(A·20)

By the use of symmetry relations, other functions such as $\phi_1^{(1)}(F, \epsilon)$, $\phi_1^{(2)}(F, \epsilon)$ are also obtained. Combining these results, we finally obtain Eqs. (5·14) and (5·15).

References

1) As a review of the Kondo effect, see, e.g.,
5) K. Sato and Y. Nagaoka, Prog. Theor. Phys. 50 (1973), 37, referred to as I.
9) A. A. Abrikosov, Physics 2 (1965), 5.