

## Magnetic-Field Dependence of the Bound State Due to the *s-d* Exchange Interaction

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On the basis of the theory developed by Yosida, Okiji and Yoshimori on the singlet ground state of a system of conduction electrons and a localized spin coupled with an antiferromagnetic exchange interaction, the magnetic-field dependence of the ground state is investigated in logarithmic accuracy by collecting the most divergent terms in the integration kernel. The correctness of a previous result for the susceptibility obtained by an iteration method is confirmed in the weak coupling limit, and it is further concluded that in this limit the bound state does not disappear at a finite value of magnetic field, but approaches the normal state asymptotically at high field.

### § 1. Introduction

It has been shown by Yosida<sup>1)</sup> that the ground state is a singlet collective bound state in a system of conduction electrons and a localized spin coupled with an antiferromagnetic *s-d* exchange interaction. Since then, theories have been developed on the basis of this work.<sup>2)-6)</sup> Among these, Yoshimori<sup>5)</sup> has recently succeeded in deriving a closed form of solution for the singlet bound state by collecting the most divergent terms in the kernel of the secular integral equation. Further, by the use of this method, calculations have been made of such quantities as the normalization integral of the wave function, the kinetic energy and the charge density and more conclusive results of a series of work are derived.<sup>6)</sup>

In a previous paper,<sup>4)</sup> as a part of a series of the work, we have calculated by the iteration method the magnetic susceptibility of the singlet bound state at 0°K and obtained  $\mu_B^2/|\tilde{E}|$  for the susceptibility, where  $\tilde{E}$  denotes its binding energy. It was shown that this result does hold at any stage of approximation. However, as the calculation was restricted in that paper to a weak field, it was impossible to elucidate the behavior of the localized spin in high field. In high field the situation is considered qualitatively as follows. The singlet bound state, which is stable in the absence of the field and at 0°K, will decrease its binding energy as field is increased, because field makes a spin-flip process due to the exchange interaction difficult. In this paper, using the method of collecting the most divergent terms in the integration kernel,<sup>5),6)</sup> we derive an expression for the binding energy as a function of the applied field, which is valid up to a

high field compared with the binding energy in the absence of the field. It is also shown that the expression previously obtained for the susceptibility is correct in the weak coupling limit.

## § 2. Calculation

We consider the system described by the following Hamiltonian:

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

where

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

and the other notations are the usual ones.<sup>4)</sup> Although we consider the Zeeman energy only for the localized spin, the result for the anomalous part of the magnetization does not change for the case in which the conduction electrons also interact with a magnetic field, as discussed in the previous paper.<sup>4)</sup>

The ground state wave function is constructed as follows:<sup>1)</sup>

$$\begin{aligned} \psi = & [\sum_k (\Gamma_k^\alpha a_{k\downarrow}^* \alpha + \Gamma_k^\beta a_{k\uparrow}^* \beta) \\ & + \sum_{k_1 k_2 k_3} (\Gamma_{k_1 k_2 k_3}^{\alpha\downarrow} a_{k_1\downarrow}^* a_{k_2\downarrow}^* a_{k_3\downarrow} \alpha + \Gamma_{k_1 k_2 k_3}^{\beta\uparrow} a_{k_1\uparrow}^* a_{k_2\uparrow}^* a_{k_3\uparrow} \beta \\ & + \Gamma_{k_1 k_2 k_3}^{\alpha\uparrow} a_{k_1\downarrow}^* a_{k_2\uparrow}^* a_{k_3\uparrow} \alpha + \Gamma_{k_1 k_2 k_3}^{\beta\downarrow} a_{k_1\uparrow}^* a_{k_2\downarrow}^* a_{k_3\downarrow} \beta) \\ & + \dots] \psi_v, \quad (3) \end{aligned}$$

where  $\alpha$  and  $\beta$ , respectively, denote the spin-up and spin-down state of the localized spin ( $S = \frac{1}{2}$ ), and  $\psi_v$  denotes the Fermi state. From the Schrödinger equation, we obtain an infinite chain of the simultaneous equations for  $\Gamma_k$ ,  $\Gamma_{k_1 k_2 k_3}$ ,  $\dots$ . Eliminating  $\Gamma_{k_1 k_2 k_3}$  and also higher order terms from these equations, we finally obtain the following integral equation for  $\Gamma_k^\alpha$  and  $\Gamma_k^\beta$ :

$$\begin{aligned} \Gamma_k^\alpha (\varepsilon_k - \tilde{E} + \Delta) = & -\frac{J}{4N} \sum_1 (\Gamma_1^\alpha - 2\Gamma_1^\beta) \\ & - \left(\frac{J}{4N}\right)^2 \sum_{1,2} \left[ \frac{\Gamma_1^\alpha + 2\Gamma_1^\beta}{\varepsilon_k + \varepsilon_1 - \varepsilon_2 - \tilde{E} + \Delta} + \frac{2\Gamma_1^\beta}{\varepsilon_k + \varepsilon_1 - \varepsilon_2 - \tilde{E} - \Delta} \right] \\ & + \left(\frac{J}{4N}\right)^3 \sum_{1,2,3} \left[ \frac{1}{\varepsilon_k + \varepsilon_1 - \varepsilon_2 - \tilde{E} + \Delta} \left( \frac{\Gamma_3^\alpha - 2\Gamma_3^\beta}{\varepsilon_k + \varepsilon_3 - \varepsilon_2 - \tilde{E} + \Delta} \right. \right. \\ & - \frac{\Gamma_1^\alpha - 2\Gamma_1^\beta}{\varepsilon_k + \varepsilon_1 - \varepsilon_3 - \tilde{E} + \Delta} + \frac{\Gamma_1^\alpha - 2\Gamma_3^\alpha + 2\Gamma_1^\beta}{\varepsilon_1 + \varepsilon_3 - \varepsilon_2 - \tilde{E} + \Delta} + \frac{2\Gamma_3^\beta}{\varepsilon_k + \varepsilon_3 - \varepsilon_2 - \tilde{E} - \Delta} \\ & \left. \left. + \frac{2\Gamma_1^\beta}{\varepsilon_k + \varepsilon_1 - \varepsilon_3 - \tilde{E} - \Delta} + \frac{4\Gamma_1^\alpha + 2\Gamma_1^\beta - 4\Gamma_3^\beta}{\varepsilon_1 + \varepsilon_3 - \varepsilon_2 - \tilde{E} - \Delta} \right) \right] \end{aligned}$$

$$\begin{aligned}
 & + \frac{2}{\varepsilon_k + \varepsilon_1 - \varepsilon_2 - \tilde{E} - \Delta} \left( \frac{2\Gamma_3^\alpha}{\varepsilon_k + \varepsilon_3 - \varepsilon_2 - \tilde{E} + \Delta} + \frac{4\Gamma_1^\beta}{\varepsilon_k + \varepsilon_1 - \varepsilon_3 - \tilde{E} + \Delta} \right. \\
 & \left. + \frac{\Gamma_3^\beta}{\varepsilon_k + \varepsilon_3 - \varepsilon_2 - \tilde{E} - \Delta} + \frac{\Gamma_1^\beta}{\varepsilon_k + \varepsilon_1 - \varepsilon_3 - \tilde{E} - \Delta} + \frac{2\Gamma_3^\alpha - \Gamma_1^\beta}{\varepsilon_1 + \varepsilon_3 - \varepsilon_2 - \tilde{E} - \Delta} \right) \\
 & + \dots, \tag{4a}
 \end{aligned}$$

$$\Gamma_k^\beta(\varepsilon_k - \tilde{E} - \Delta) = \dots, \tag{4b}$$

where  $\tilde{E}$  which is defined by  $\tilde{E} = E - \Delta E$  represents a singular part of  $E$ .<sup>3)</sup>  $\Delta E$  consists of a regular part which is the energy shift of the normal state at  $\Delta = 0$  and correction terms which depend on  $\tilde{E}$  and  $\Delta$ , but the latter correction terms are smaller than  $-\tilde{E}$  by the order  $\rho J/4N$ , as discussed in reference 4), and thus they can be neglected. + sign in  $\pm \varepsilon_i$  in the denominators is for an electron state and - sign for a hole state, respectively. Equation (4b) for  $\Gamma_k^\beta$  is obtained by the following replacement:

$$\alpha \leftrightarrow \beta, \quad \Delta \leftrightarrow -\Delta, \tag{5}$$

in Eq. (4a). We consider the case,  $-\tilde{E} > \Delta > 0$ , so that each energy denominator of the summands is always positive. Assuming the constant density of states  $\rho$  for  $|\varepsilon| < D$ , ( $2D$  is the band width) and expanding the integrands in  $\Delta$ , we obtain the following integral equations which correspond to Eq. (2) of reference 5),

$$\begin{aligned}
 (\varepsilon - \tilde{E} + \Delta)\Gamma^\alpha(\varepsilon) & = \left(\frac{\rho J}{4N}\right) \int_0^D d\varepsilon_1 [2\Gamma^\beta(\varepsilon_1) - \Gamma^\alpha(\varepsilon_1)] \\
 & + \left(\frac{\rho J}{4N}\right)^2 \int_0^D d\varepsilon_1 \Gamma^\alpha(\varepsilon_1) \left[ \left\{ \log \frac{\varepsilon + \varepsilon_1 - \tilde{E}}{D} + \log \left( 1 + \frac{\Delta}{\varepsilon + \varepsilon_1 - \tilde{E}} \right) \right\} \right. \\
 & + \frac{\rho J}{N} \left\{ \log^2 \frac{\varepsilon + \varepsilon_1 - \tilde{E}}{D} + 2 \log \frac{\varepsilon + \varepsilon_1 - \tilde{E}}{D} \log \left( 1 + \frac{\Delta}{\varepsilon + \varepsilon_1 - \tilde{E}} \right) \right\} \\
 & + \left(\frac{\rho J}{N}\right)^2 \left\{ \log^3 \frac{\varepsilon + \varepsilon_1 - \tilde{E}}{D} + 3 \log^2 \frac{\varepsilon + \varepsilon_1 - \tilde{E}}{D} \log \left( 1 + \frac{\Delta}{\varepsilon + \varepsilon_1 - \tilde{E}} \right) \right\} \\
 & \left. + \dots \right] \\
 & + 2 \left(\frac{\rho J}{4N}\right)^2 \int_0^D d\varepsilon_1 \Gamma^\beta(\varepsilon_1) \left[ \left\{ 2 \log \frac{\varepsilon + \varepsilon_1 - \tilde{E}}{D} + \log \left( 1 - \frac{\Delta^2}{(\varepsilon + \varepsilon_1 - \tilde{E})^2} \right) \right\} \right. \\
 & + \frac{\rho J}{N} \left\{ 2 \log^2 \frac{\varepsilon + \varepsilon_1 - \tilde{E}}{D} + 2 \log \frac{\varepsilon + \varepsilon_1 - \tilde{E}}{D} \log \left( 1 - \frac{\Delta^2}{(\varepsilon + \varepsilon_1 - \tilde{E})^2} \right) \right\} \\
 & + \left(\frac{\rho J}{N}\right)^2 \left\{ 2 \log^3 \frac{\varepsilon + \varepsilon_1 - \tilde{E}}{D} + 3 \log^2 \frac{\varepsilon + \varepsilon_1 - \tilde{E}}{D} \log \left( 1 - \frac{\Delta^2}{(\varepsilon + \varepsilon_1 - \tilde{E})^2} \right) \right\} \\
 & \left. + \dots \right], \tag{6a}
 \end{aligned}$$

$$(\varepsilon - \tilde{E} - \Delta) \Gamma^\beta(\varepsilon) = \dots, \quad (6b)$$

where we retain only the logarithmic terms of the highest order for both terms dependent on and independent of  $\Delta$  explicitly under the condition

$$\left| \log \frac{-\tilde{E}}{D} \right| \gg \left| \log \left( 1 \pm \frac{\Delta}{-\tilde{E}} \right) \right|. \quad (7)$$

We find that the terms depending on  $\Delta$  explicitly are of next order in logarithmic divergence in comparison with  $\Delta$ -independent ones. In the integration kernels of Eqs. (6a, b), we calculate only the first three terms of the series, but it is natural to assume *a posteriori* the  $n$ -th order terms in these equations.\*)

Following Yoshimori's method,<sup>b)</sup> we sum up these series and introduce the functions  $G_\alpha(\varepsilon)$  and  $G_\beta(\varepsilon)$  defined by

$$G_\alpha(\varepsilon) = \int_0^\varepsilon \Gamma^\alpha(\varepsilon_1) d\varepsilon_1, \quad G_\beta(\varepsilon) = \int_0^\varepsilon \Gamma^\beta(\varepsilon_1) d\varepsilon_1; \quad (8)$$

then Eqs. (6a, b) can be written down in logarithmic accuracy, as

$$\begin{aligned} (\varepsilon - \tilde{E} + \Delta) \frac{d}{d\varepsilon} G_\alpha(\varepsilon) &= \frac{\rho J}{4N} [2G_\beta(D) - G_\alpha(D)] \\ &\quad - \left( \frac{\rho J}{4N} \right)^2 \int_\varepsilon^D d\varepsilon_1 G_\alpha(\varepsilon_1) \frac{1}{\varepsilon_1 - \tilde{E} + \Delta} \left[ 1 - \frac{\rho J}{N} \log \frac{\varepsilon_1 - \tilde{E}}{D} \right]^{-2} \\ &\quad - 2 \left( \frac{\rho J}{4N} \right)^2 \int_\varepsilon^D d\varepsilon_1 G_\beta(\varepsilon_1) \left( \frac{1}{\varepsilon_1 - \tilde{E} + \Delta} + \frac{1}{\varepsilon_1 - \tilde{E} - \Delta} \right) \left[ 1 - \frac{\rho J}{N} \log \frac{\varepsilon_1 - \tilde{E}}{D} \right]^{-2}, \end{aligned} \quad (9a)$$

$$(\varepsilon - \tilde{E} - \Delta) \frac{d}{d\varepsilon} G_\beta(\varepsilon) = \dots. \quad (9b)$$

Since Eq. (9b) is obtained by the replacement (5) applied to Eq. (9a) as before, we find the relation

$$G_\alpha(\varepsilon, \Delta) = \pm G_\beta(\varepsilon, -\Delta). \quad (10)$$

Differentiating Eq. (9a) and using Eq. (10), we obtain the following differential equation:

$$\begin{aligned} \left( 1 + \frac{\Delta}{\varepsilon - \tilde{E}} \right) \left[ (\varepsilon - \tilde{E} - \Delta)^2 \frac{d^2}{d\varepsilon^2} G_\beta(\varepsilon, \Delta) + (\varepsilon - \tilde{E} - \Delta) \frac{d}{d\varepsilon} G_\beta(\varepsilon, \Delta) \right. \\ \left. - \left( \frac{\rho J}{4N} \right)^2 \left( 1 - \frac{\rho J}{N} \log \frac{\varepsilon - \tilde{E}}{D} \right)^{-2} G_\beta(\varepsilon, \Delta) \right] = \pm 4 \left( \frac{\rho J}{4N} \right)^2 \left( 1 - \frac{\rho J}{N} \log \frac{\varepsilon - \tilde{E}}{D} \right)^{-2} G_\beta(\varepsilon, -\Delta). \end{aligned} \quad (11)$$

At  $\Delta=0$ , Eq. (11) has two singlet solutions of the form  $[1 - (\rho J/N) \log(\varepsilon - \tilde{E})/D]^r$

\*b) It will be seen from Eq. (18) that these series are convergent for any  $\varepsilon$  and  $\varepsilon_1$ .

with  $\gamma = \frac{3}{4}, \frac{1}{4}$  for  $-$  sign on the right-hand side of Eq. (11) and two triplet solutions with  $\gamma = \frac{5}{4}, -\frac{1}{4}$  for  $+$  sign.<sup>5)</sup> We solve Eq. (11) for the deviations from these solutions of  $\mathcal{A}=0$  so as to be correct in the highest order of the logarithm; for example for  $\gamma = \frac{3}{4}$ , we put

$$G(\varepsilon, \mathcal{A}) = \left(1 - \frac{\rho J}{N} \log \frac{\varepsilon - \tilde{E}}{D}\right)^{3/4} + h(\varepsilon, \mathcal{A}), \quad h(\varepsilon, 0) = 0,$$

and the equation for  $h(\varepsilon, \mathcal{A})$  reduces to

$$(\varepsilon - \tilde{E} - \mathcal{A}) \frac{d^2}{d\varepsilon^2} h(\varepsilon, \mathcal{A}) + \frac{d}{d\varepsilon} h(\varepsilon, \mathcal{A}) = \frac{3\rho J}{4N} \frac{\mathcal{A}}{(\varepsilon - \tilde{E})^2} \left(1 - \frac{\rho J}{N} \log \frac{\varepsilon - \tilde{E}}{D}\right)^{-1/4*},$$

and this can easily be solved in logarithmic accuracy. Obtained solutions can be written as

$$G_{4r}(\varepsilon, \mathcal{A}) \equiv \left(1 - \frac{\rho J}{N} \log \frac{\varepsilon - \tilde{E}}{D}\right)^r - \gamma \frac{\rho J}{N} \left(1 - \frac{\rho J}{N} \log \frac{\varepsilon - \tilde{E}}{D}\right)^{r-1} \log\left(1 - \frac{\mathcal{A}}{\varepsilon - \tilde{E}}\right), \tag{12}$$

where  $\gamma = \frac{3}{4}, \frac{1}{4}$  for  $-$  sign on the right-hand side of Eq. (11) and  $\gamma = \frac{5}{4}, -\frac{1}{4}$  for  $+$  sign. General solution for  $G_\alpha$  and  $G_\beta$  is composed by using these:

$$G_\alpha(\varepsilon, \mathcal{A}) = -A_3 G_3(\varepsilon, -\mathcal{A}) - A_1 G_1(\varepsilon, -\mathcal{A}) + A_5 G_5(\varepsilon, -\mathcal{A}) + A_{-1} G_{-1}(\varepsilon, -\mathcal{A}), \tag{13a}$$

$$G_\beta(\varepsilon, \mathcal{A}) = A_3 G_3(\varepsilon, \mathcal{A}) + A_1 G_1(\varepsilon, \mathcal{A}) + A_5 G_5(\varepsilon, \mathcal{A}) + A_{-1} G_{-1}(\varepsilon, \mathcal{A}). \tag{13b}$$

The  $\mathcal{A}$ -dependent coefficients  $A_{4r}$  are fixed by the boundary conditions of  $\varepsilon=0$  and  $D$  as follows: Substituting Eqs. (13a, b) into Eqs. (9a, b) and putting  $\varepsilon=D$ , we easily obtain

$$A_1 = A_5 = 0. \tag{14}$$

$A_3$  and  $A_{-1}$  are determined by Eqs. (8) with  $\varepsilon=0$  as

$$0 = A_3 \left[ \left(1 - \frac{\rho J}{N} \log \frac{-\tilde{E}}{D}\right)^{3/4} - 3 \frac{\rho J}{4N} \left(1 - \frac{\rho J}{N} \log \frac{-\tilde{E}}{D}\right)^{-1/4} \log\left(1 - \frac{\mathcal{A}}{-\tilde{E}}\right) \right] + A_{-1} \left[ \left(1 - \frac{\rho J}{N} \log \frac{-\tilde{E}}{D}\right)^{-1/4} + \frac{\rho J}{4N} \left(1 - \frac{\rho J}{N} \log \frac{-\tilde{E}}{D}\right)^{-5/4} \log\left(1 - \frac{\mathcal{A}}{-\tilde{E}}\right) \right], \tag{15a}$$

$$0 = -A_3 \left[ \left(1 - \frac{\rho J}{N} \log \frac{-\tilde{E}}{D}\right)^{3/4} - 3 \frac{\rho J}{4N} \left(1 - \frac{\rho J}{N} \log \frac{-\tilde{E}}{D}\right)^{-1/4} \log\left(1 + \frac{\mathcal{A}}{-\tilde{E}}\right) \right] + A_{-1} \left[ \left(1 - \frac{\rho J}{N} \log \frac{-\tilde{E}}{D}\right)^{-1/4} + \frac{\rho J}{4N} \left(1 - \frac{\rho J}{N} \log \frac{-\tilde{E}}{D}\right)^{-5/4} \log\left(1 + \frac{\mathcal{A}}{-\tilde{E}}\right) \right]. \tag{15b}$$

\*) Although there is another inhomogeneous term proportional to  $(\rho J/N)^2$  in this equation, the contribution from this to the solution can be neglected by the condition (7).

By the condition that Eqs. (15a, b) have a non-trivial solution, we obtain within logarithmic accuracy

$$\left(1 - \frac{\rho J}{N} \log \frac{-\tilde{E}}{D}\right)^{1/2} = \frac{\rho J}{4N} \left(1 - \frac{\rho J}{N} \log \frac{-\tilde{E}}{D}\right)^{-1/2} \log \left(1 - \frac{A^2}{\tilde{E}^2}\right), \quad (16)$$

or

$$\begin{aligned} \left(1 - \frac{\rho J}{N} \log \frac{-\tilde{E}_0}{D}\right)^{1/2} - \frac{\rho J}{2N} \left(1 - \frac{\rho J}{N} \log \frac{-\tilde{E}_0}{D}\right)^{-1/2} \log \frac{\tilde{E}}{\tilde{E}_0} \\ = \frac{\rho J}{4N} \left(1 - \frac{\rho J}{N} \log \frac{-\tilde{E}_0}{D}\right)^{-1/2} \log \left(1 - \frac{A^2}{\tilde{E}^2}\right), \end{aligned} \quad (17)$$

where  $\tilde{E}_0$  is the binding energy of  $A=0$  for  $J < 0$ ,<sup>5),6)</sup>

$$\tilde{E}_0 = -D \exp[N/\rho J].$$

Comparing the coefficients of  $\rho J/N$  in Eq. (17), we obtain the result

$$\tilde{E} = -(\tilde{E}_0^2 + A^2)^{1/2}. \quad (18)$$

As the ratio of  $A_3$  and  $A_{-1}$  is determined by Eq. (18), the wave functions  $\Gamma^\alpha(\varepsilon)$  and  $\Gamma^\beta(\varepsilon)$  are expressed as

$$\Gamma^\alpha(\varepsilon) = -A \frac{1}{\varepsilon - \tilde{E} + A} \left[1 - \frac{\rho J}{N} \log \frac{\varepsilon - \tilde{E}_0}{D}\right]^{-1/4}, \quad (19a)$$

$$\Gamma^\beta(\varepsilon) = A \frac{1}{\varepsilon - \tilde{E} - A} \left[1 - \frac{\rho J}{N} \log \frac{\varepsilon - \tilde{E}_0}{D}\right]^{-1/4}, \quad (19b)$$

where  $A$  is the normalization constant. From Eq. (18), we obtain the magnitude of the localized spin induced by the magnetic field as

$$\langle S_z \rangle = -\frac{d\tilde{E}}{dA} = \frac{1}{2} \frac{A}{(\tilde{E}_0^2 + A^2)^{1/2}}. \quad (20)$$

After subtracting the Zeeman energy of the induced localized moment  $\langle S_z \rangle$  from  $\tilde{E}$ , we obtain the effective binding energy  $E_b$  as

$$\tilde{E}_b = -\frac{\tilde{E}_0^2}{(\tilde{E}_0^2 + A^2)^{1/2}}. \quad (21)$$

$A$ -dependences of  $\langle S_z \rangle$  and  $\tilde{E}_b$  given by Eqs. (20) and (21) are shown in Figs. 1 and 2, respectively. The susceptibility at weak field is obtained by Eq. (20):

$$\chi = \frac{1}{-\tilde{E}_0} \left(\frac{1}{2} g \mu_B\right)^2, \quad (22)$$

and this is just the same expression as that derived in the previous paper.<sup>4)</sup>

So far the calculations have been carried out under the condition of (7),  $1 \gg \log(1 + A/\tilde{E})/\log(-\tilde{E}/D)$ . Considering Eq. (18), we find that the right-hand side of this expression has the order of  $\rho J/N$  at  $A' = |\tilde{E}_0|$  and the order of unity

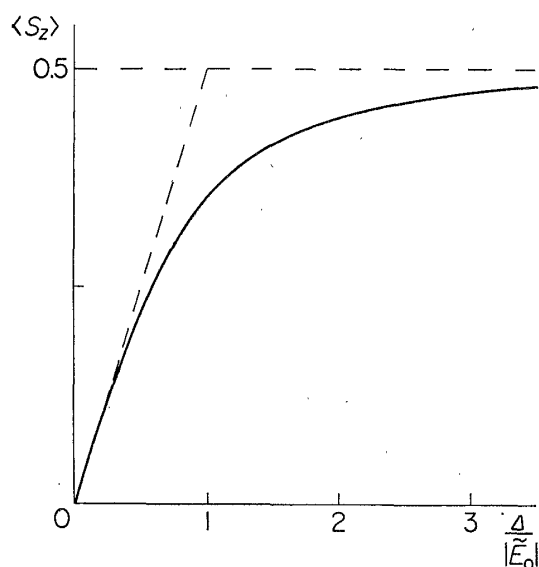


Fig. 1. The magnitude of the localized spin induced by the magnetic field.

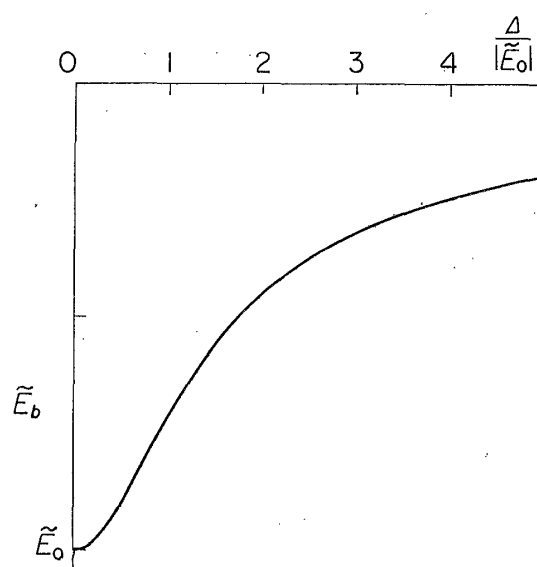


Fig. 2. The effective binding energy as a function of the applied field.

for  $\Delta'' = D \exp[2N/3\rho J]$ , where the present calculation is useless. In the weak coupling limit,  $\Delta''/\Delta'$  tends to infinity and, therefore, our result is valid even for high field compared with the binding energy at  $\Delta=0$ .

### § 3. Summary and conclusions

In this paper we have obtained the binding energy of the ground state which is a singlet state at  $H=0$  for  $J<0$  as a function of the applied field in the weak coupling limit by collecting the most divergent terms both for field-dependent and field-independent terms. The obtained field-dependence of the binding energy is expressed by the hyperbola,  $\tilde{E}^2 = \tilde{E}_0^2 + \Delta^2$ . It will be shown in the Appendix that this expression is also obtained in each stage of approximation of iteration if one uses the value of  $\tilde{E}_0$  in its approximation. Thus it can be said that a qualitative feature of the magnetic-field dependence of the system is already included correctly even in the zeroth approximation as discussed in reference 6). Thus, the result for the susceptibility obtained by iteration method in the previous paper is confirmed. From the expression for the energy we obtained the induced localized moment. As field is increased beyond the zero-field value of the binding energy, the localized spin is still quenched partially and asymptotically approaches the unquenched value, one half, at high field. The effective binding energy which is obtained by subtracting the Zeeman energy of the induced localized spin from the energy  $\tilde{E}$  approaches zero gradually as the field is increased. That is, within the weak coupling limit, it is concluded that the bound state does not disappear at a finite value of magnetic field, but approaches the 'normal' state asymptotically.

According to the usual perturbation theory in the presence of the field at 0°K,<sup>7)</sup> the magnitude of the localized spin is expressed by the geometric series (in our notation)

$$\langle S_z \rangle = S \left[ 1 + \frac{\rho J}{2N} \left\{ \frac{\rho J}{N} \log \frac{2A}{D} + \left( \frac{\rho J}{N} \log \frac{2A}{D} \right)^2 + \left( \frac{\rho J}{N} \log \frac{2A}{D} \right)^3 + \dots \right\} \right],$$

which is convergent for  $A$  well above  $A_c = (D/2) \exp[N/\rho J]$ , but diverges below  $A_c$  for the antiferromagnetic exchange interaction  $J < 0$ . It can be shown that since the energy of the normal state is higher than that of the bound state at high field  $A > A_c$  in which the above series is convergent, the bound state is always stable.

Recently, Nam and Woo<sup>8)</sup> have calculated the binding energy of the present system on the basis of the zeroth approximation of our treatment, neglecting the effect of electron-hole pairs. Their binding energy of the zero-field case is, therefore, given by  $-D \exp[4N/3\rho J]$  instead of our binding energy  $-D \exp[N/\rho J]$ . Moreover, in their calculation there is an error; the last term in Eq. (4) of their paper,  $+\frac{1}{4}a_k a_q f_k f_q$ , should be corrected as  $-\frac{1}{4}a_k a_q f_k f_q$ . This error makes their conclusion incorrect, particularly at high field; the right-hand side of the fourth equation of (7) of their paper,  $(4\delta - 3\delta^2)/(2 - 11\delta + 6\delta^2)$ , should be corrected as  $(4\delta - 3\delta^2)/(2 - 3\delta)$ . After this error is corrected, the secular equation becomes identical to the zeroth approximation of Eq. (24) given in the previous paper.<sup>4)</sup>

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### Appendix

In this Appendix we shall show that the same result as Eq. (18) is obtained at each stage of the approximation of the iteration method. In the previous paper the energy eigen-value is determined, in so far as the logarithmic terms of the highest order are retained, by the secular equation,

$$F(x, y) = 0, \quad (\text{A}\cdot\text{1})$$

where  $F(x, y)$  is the symmetric polynomial of  $x$  and  $y$ ,

$$x = \frac{\rho J}{4N} \log \frac{-\tilde{E} + A}{D}, \quad y = \frac{\rho J}{4N} \log \frac{-\tilde{E} - A}{D}. \quad (\text{A}\cdot\text{2})$$

Though we derived the susceptibility from Eq. (A·1) on the assumption of an infinitesimal field, Eq. (A·1) can also be solved so as to be valid for a finite



field by retaining the most divergent terms for the field-dependent as well as for the field-independent terms as in the text. We divide  $x$  and  $y$  in Eq. (A·2) into three terms in the following way:

$$\begin{aligned} x &= \frac{\rho J}{4N} \left[ \log \frac{-\tilde{E}_0}{D} + \log \frac{\tilde{E}}{\tilde{E}_0} + \log \left( 1 - \frac{\Delta}{\tilde{E}} \right) \right], \\ y &= \frac{\rho J}{4N} \left[ \log \frac{-\tilde{E}_0}{D} + \log \frac{\tilde{E}}{\tilde{E}_0} + \log \left( 1 + \frac{\Delta}{\tilde{E}} \right) \right], \end{aligned} \quad (\text{A}\cdot\text{3})$$

where  $\tilde{E}_0$  is the energy in the absence of the field at each stage of approximation. The second and third terms on the right-hand side of (A·3) are of the next order compared with the first by the condition (7). Expanding  $F(x, y)$  about  $x=y=x_0 \equiv (\rho J/4N) \log(-\tilde{E}_0/D)$  and using the fact that  $F(x_0, x_0) = 0$  and  $(d/dx_0)F(x_0, x_0) \neq 0$ , we obtained the result  $\tilde{E}^2 = \tilde{E}_0^2 + \Delta^2$ .

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