

Anomalies and Bound State Due to the Anisotropic s - d Exchange Interaction

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(Received November 22, 1969)

The Kondo problem for the anisotropic s - d exchange interaction is investigated in detail. The scattering amplitude of a conduction electron is calculated in the most divergent approximation (Abrikosov's approximation). The importance of some types of terms overlooked in the previous work by Miwa and Nagaoka is pointed out. By changing the degree of anisotropy of the exchange integral the behaviors of the obtained scattering amplitude—especially the divergence difficulties—are examined. To see physical meaning of the divergence difficulties the problem of the existence of the bound state realized as the ground state of this coupled many-body system is discussed by extending the Yosida-Okiji-Yoshimori theory to the anisotropic case. It is shown that the exact solution of the bound state can be obtained also for the anisotropic s - d interaction, and that the divergence difficulties stated above are closely connected with the existence of the bound state.

§ 1. Introduction

Since Kondo's work¹⁾ on the resistance minimum of dilute alloys which has revealed an important many-body effect brought about by quantum mechanical fluctuations of a localized spin, a new stage has come in the investigation of the properties of alloys containing magnetic impurities. Owing to considerable theoretical and experimental studies directed toward understanding the physical origin of the many-body scattering as well as toward a determination of the ground state of this coupled many-body system, some aspects of the problem have already been clarified.²⁾ Nevertheless we still have many problems left unsolved.

Most of previous theoretical researches on dilute alloys with magnetic impurities have been performed on the basis of the following model: Conduction electrons are scattered by a magnetic impurity with its spin S . The interaction between conduction electrons and a localized spin is the *isotropic* s - d exchange interaction

$$H' = -\frac{J}{N} \sum_{\mathbf{k}\mathbf{k}'} \sum_{\alpha\alpha'} \mathbf{S} \cdot a_{\mathbf{k}\alpha}^+ \boldsymbol{\sigma}_{\alpha\alpha'} a_{\mathbf{k}'\alpha'}, \quad (1.1)$$

where $a_{\mathbf{k}\alpha}$ and $a_{\mathbf{k}\alpha}^+$ are annihilation and creation operators of a conduction electron with wave vector \mathbf{k} and spin α , and $\boldsymbol{\sigma}$ is the Pauli spin operator.

In this paper we investigate the Kondo problem of a more general model—the *anisotropic* s - d exchange interaction

$$H' = -\frac{1}{N} \sum_{\substack{\mathbf{k}\mathbf{k}' \\ \alpha\alpha'}} \mathbf{S} \cdot \mathbf{J} \cdot a_{\mathbf{k}\alpha}^{\dagger} \boldsymbol{\sigma}_{\alpha\alpha'} a_{\mathbf{k}'\alpha'} , \quad (1.2)$$

where the exchange integral \mathbf{J} is a tensor. Diagonalizing the tensor \mathbf{J} , we have from (1.2)

$$H' = -\frac{1}{N} \sum_{i=x,y,z} \sum_{\substack{\mathbf{k}\mathbf{k}' \\ \alpha\alpha'}} J_i S^i a_{\mathbf{k}\alpha}^{\dagger} \sigma_{\alpha\alpha'}^i a_{\mathbf{k}'\alpha'} . \quad (1.3)$$

The anisotropic s - d interaction is interesting for several reasons, in particular, from purely theoretical viewpoints. This is more general than the isotropic s - d interaction (1.1) and includes the isotropic case as one of special cases. Even the Ising case (or classical limit), in which only one of J_x , J_y and J_z is different from zero, is also one of limiting cases of (1.3). The isotropic case has been studied by many authors. On the other hand, for the Ising case, the s - d interaction is equivalent to a potential scattering without internal degrees of freedom, and the exact solution can be obtained easily. Therefore, if we succeed in solving the problem of the anisotropic s - d exchange interaction, we can further extend our understandings of the Kondo problem. In fact, taking the degree of anisotropy of the exchange integral as a controllable parameter, we can examine the importance of quantum effects due to a localized spin in detail.

It is worthwhile to notice that the anisotropic s - d exchange interaction is not an artifact. If a magnetic impurity ion is subjected to a strong crystal field and the crystal field splitting is so large that we can safely restrict our discussions within the ground multiplet, the s - d (or s - f) exchange interaction in this case has the same form as (1.2), where \mathbf{S} is regarded as an effective spin of the ground multiplet.

The purpose of this paper is first to calculate the scattering amplitude of a conduction electron interacting with a localized spin by the anisotropic s - d interaction in the most divergent approximation (i.e. in the logarithmic accuracy). This is a natural extension of the calculation done for the isotropic s - d interaction.³⁾ Then we study the behavior of the scattering amplitude and discuss in which case the scattering amplitude is divergent, changing the degree of anisotropy. Such a kind of analysis has been performed previously by Miwa and Nagaoka.⁴⁾ But unfortunately, contrary to the assertions of the authors, they overlooked some types of terms which should be taken into account within the logarithmic accuracy, as we will show later. This is the reason why we attack this problem anew.

The second purpose is to study the ground state of conduction electrons coupled with a localized spin by the anisotropic s - d exchange interaction. The isotropic limit has been investigated by Yosida, Okiji and Yoshimori.^{5)~8)} In particular Yoshimori⁷⁾ has obtained the exact solution in the weak coupling limit, which shows that there exists singlet many-body bound state for the antifer-

romagnetic exchange interaction and no bound state for the ferromagnetic case. If we change continuously the degree of anisotropy of the exchange integral in the anisotropic s - d interaction, we have a variety of cases including the antiferromagnetic and ferromagnetic isotropic limits. Here arises a question we wish to answer in this paper: How does the existence of the bound state depend on the degree of anisotropy? For this purpose we extend the Yosida-Okiji-Yoshimori theory to the more general case—the anisotropic s - d exchange interaction.

In § 2 the scattering amplitude is calculated in the perturbation expansion based on Doniach's method.⁹⁾ Here we confine ourselves to the calculations in logarithmic accuracy. The result is compared with that obtained by Miwa and Nagaoka.⁴⁾

In § 3 we sum up all the most divergent terms in order to examine in detail in which case the obtained expression for the scattering amplitude is divergent.

Section 4 is devoted to investigation of the bound state due to the anisotropic s - d interaction. For simplicity we assume in this section that the exchange integral is axially symmetric (at least two of J_x , J_y and J_z are equal). It is shown that the bound state is determined by the extended Yosida-Yoshimori equation, which can be solved exactly.

Conclusions are given in § 5. Relations of the results obtained in this paper with the recent paper by Anderson et al.¹⁰⁾ are also discussed briefly.

§ 2. Perturbation expansion of the scattering amplitude

The importance of higher order terms in the perturbation expansion of the s - d problem comes mainly from quantum mechanical fluctuations of a localized spin. For this reason it is quite natural to expect that important terms in the perturbation expansion can be selected successfully by certain kinds of commutator expansion of a localized spin. In fact, Doniach⁹⁾ has given a formulation of the linked cluster expansion of the s - d interaction, which is in line with the spirit stated above. His method is effective even in the anisotropic s - d interaction. According to Doniach the t -matrix of the scattering of a conduction electron by a localized spin can be written in the form

$$t(\omega) = N^{-1} V_{\text{eff}}(\omega) [1 - F(\omega) V_{\text{eff}}(\omega)]^{-1}, \quad (2.1)$$

$$F(\omega) = N^{-1} \sum_{\mathbf{k}} (\omega - \varepsilon_{\mathbf{k}} + i\delta)^{-1} \simeq -i\pi\rho, \quad (\delta \rightarrow +0)$$

where ρ is the density of states of conduction electrons and $V_{\text{eff}}(\omega)$ is the “effective potential”, which corresponds to the sum of all “irreducible” diagrams. Complicated problems of the Kondo effects are contained in $V_{\text{eff}}(\omega)$. Now we calculate $V_{\text{eff}}(\omega)$ in the perturbation expansion of the anisotropic s - d interaction, following the prescription given by Doniach. Here we confine ourselves to calculations within the logarithmic accuracy. In other words we retain only the

most divergent terms in each order of the exchange integral. In Doniach's method the most divergent terms in the n -th order of the exchange interaction come from those which contain the $(n-1)$ commutators of spin operators of an impurity. Without repeating details of the Doniach's method, we show the evaluation of $V_{\text{eff}}(\omega)$ up to fourth order.

(i) 1st order

There is only one first-order term of V_{eff} , which is shown in Fig. 1 (a).

$$V_{\text{eff}}^{(1)}(\omega) = -(J_x S^x \sigma^x + J_y S^y \sigma^y + J_z S^z \sigma^z). \tag{2.2}$$

(ii) 2nd order

The second-order term of V_{eff} is also only one shown in Fig. 1 (b):

$$V_{\text{eff}}^{(2)}(\omega) = \sum_{i,j} \int_{-\infty}^{\infty} dt e^{i\omega t} \theta(-t) G_0(t) (-J_i) (-J_j) \sigma^i \sigma^j [S^j, S^i], \tag{2.3}$$

where $\theta(t)$ is a step function defined by

$$\theta(t) = \begin{cases} 1 & \text{for } t > 0 \\ 0 & \text{for } t < 0 \end{cases}$$

and $G_0(t)$ is the free propagator of a conduction electron

$$G_0(t) = \frac{i}{N} \sum_{\mathbf{k}} \exp(-i\varepsilon_{\mathbf{k}} t) \times [(1-f_{\mathbf{k}})\theta(t) - f_{\mathbf{k}}\theta(-t)]. \tag{2.4}$$

Performing integrations over t and \mathbf{k} , we have from (2.3)

$$V_{\text{eff}}^{(2)}(\omega) = -\left(\rho \ln \frac{|\omega|}{D}\right) (2J_y J_z S^x \sigma^x + 2J_z J_x S^y \sigma^y + 2J_x J_y S^z \sigma^z). \tag{2.5}$$

Here we have assumed for simplicity that the temperature is 0°K , and that the density of states of conduction electrons has the form

$$\rho(\varepsilon) = \begin{cases} \rho & \text{for } -D < \varepsilon < D \\ 0 & \text{otherwise.} \end{cases}$$

(iii) 3rd order

There are two types of graphs in this order, i.e. Figs. 1 (c) and (d). But (d) can be neglected in the most divergent approximation. The contribution of Fig. 1

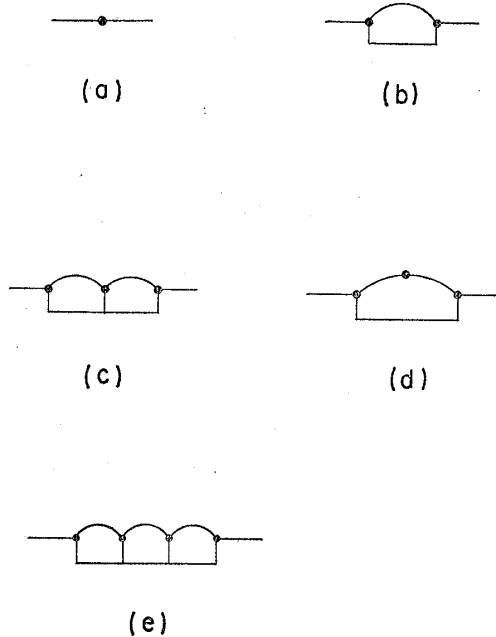


Fig. 1. Some diagrams of the effective potential $V_{\text{eff}}(\omega)$ according to Doniach.⁹⁾ (a): 1st order of the exchange integral, (b): 2nd order, (c) and (d): 3rd order, (e): 4th order. Diagrams (a), (b), (c) and (e) should be taken into account in the logarithmic accuracy, and the contribution of the third order term corresponding to (d) can be neglected in this approximation.

(c) is of the form

$$V_{\text{eff}}^{(3)}(\omega) = \int_{-\infty}^{\infty} dt e^{i\omega t} \int_{-\infty}^{\infty} dt_1 G_0(t-t_1) G_0(t_1) \sum_{ijk} (-J_i) (-J_j) (-J_k) \\ \times \sigma^i \sigma^j \sigma^k [\theta(-t_1) \theta(t_1-t) [[S^k, S^j], S^i] \\ + \theta(-t) \theta(t-t_1) [[S^k, S^i], S^j]]. \quad (2.6)$$

It should be noted here that the second term in the parenthesis vanishes because of the relation

$$\sum_{ijk} J_i J_j J_k \sigma^i \sigma^j \sigma^k [[S^k, S^i], S^j] = 0.$$

Thus integrations over t and t_1 lead to

$$V_{\text{eff}}^{(3)}(\omega) \simeq - \sum_{ijk} J_i J_j J_k \sigma^i \sigma^j \sigma^k \left(\rho \ln \frac{|\omega|}{D} \right)^2 [[S^k, S^j], S^i] \\ = - \left(\rho \ln \frac{|\omega|}{D} \right)^2 [2J_x (J_y^2 + J_z^2) S^x \sigma^x \\ + 2J_y (J_z^2 + J_x^2) S^y \sigma^y + 2J_z (J_x^2 + J_y^2) S^z \sigma^z] \quad (2.7)$$

for $T=0^\circ\text{K}$.

Up to this order the situation is rather simple, but terms higher than the fourth order are quite complicated, as shown below.

(iv) 4th order

In the most divergent approximation it is sufficient to take into account only the diagram shown in Fig. 1 (e), which corresponds to the contribution

$$V_{\text{eff}}^{(4)}(\omega) = \int_{-\infty}^{\infty} dt e^{i\omega t} \int \int_{-\infty}^{\infty} dt_1 dt_2 G_0(t-t_1) G_0(t_1-t_2) G_0(t_2) \\ \times \sum_{ijkl} (-J_i) (-J_j) (-J_k) (-J_l) \sigma^i \sigma^j \sigma^k \sigma^l \\ \times [\theta(-t_2) \theta(t_2-t_1) \theta(t_1-t) [[S^l, S^k], S^j], S^i] \\ + \theta(-t_2) \theta(t_2-t) \theta(t-t_1) [[S^l, S^k], S^i], S^j \\ + \theta(-t_1) \theta(t_1-t_2) \theta(t_2-t) [[S^l, S^j], S^k], S^i \\ + \theta(-t_1) \theta(t_1-t) \theta(t-t_2) [[S^l, S^j], S^i], S^k \\ + \theta(-t) \theta(t-t_1) \theta(t_1-t_2) [[S^l, S^i], S^j], S^k \\ + \theta(-t) \theta(t-t_2) \theta(t_2-t_1) [[S^l, S^i], S^k], S^j]. \quad (2.8)$$

As the third term in the parenthesis is identically equal to zero, we perform integrations over t , t_1 and t_2 in five terms except the third. After elementary calculations we find that at $T=0^\circ\text{K}$

$$V_{\text{eff}}^{(4)}(\omega) \simeq \sum_{ijkl} J_i J_j J_k J_l \sigma^i \sigma^j \sigma^k \sigma^l \\ \times \left[- \left(\rho \ln \frac{|\omega|}{D} \right)^3 [[S^l, S^k], S^j], S^i \right]$$

$$\begin{aligned}
& + \frac{1}{2} \left(\rho \ln \frac{|\omega|}{D} \right)^3 [[[S^l, S^k], S^i], S^j] \\
& + \frac{1}{6} \left(\rho \ln \frac{|\omega|}{D} \right)^3 [[[S^l, S^j], S^i], S^k] \\
& - \frac{1}{3} \left(\rho \ln \frac{|\omega|}{D} \right)^3 [[[S^l, S^i], S^j], S^k] \\
& + \frac{1}{6} \left(\rho \ln \frac{|\omega|}{D} \right)^3 [[[S^l, S^i], S^k], S^j], \quad (2.9a)
\end{aligned}$$

which is equal to

$$\begin{aligned}
V_{\text{eff}}^{(4)}(\omega) = & \left(\rho \ln \frac{|\omega|}{D} \right)^3 \left[-J_y J_z (4J_x^2 + 2J_y^2 + 2J_z^2) + \frac{1}{2} J_y J_z (-4J_x^2 + 2J_y^2 + 2J_z^2) \right. \\
& + \frac{1}{6} \cdot 4J_y J_z J_x^2 - \frac{1}{3} \cdot 2J_y J_z (J_y^2 + J_z^2) \\
& \left. + \frac{1}{6} \cdot 2J_y J_z (J_y^2 + J_z^2) \right] S^x \sigma^x \\
& + (\text{terms in which } x, y \text{ and } z \text{ are changed cyclically}). \quad (2.9b)
\end{aligned}$$

Arranging terms, we obtain

$$\begin{aligned}
V_{\text{eff}}^{(4)}(\omega) = & \left(\rho \ln \frac{|\omega|}{D} \right)^3 \left[-\frac{4}{3} J_y J_z (4J_x^2 + J_y^2 + J_z^2) S^x \sigma^x \right. \\
& \left. + (\text{terms in which } x, y \text{ and } z \text{ are changed cyclically}) \right]. \quad (2.9c)
\end{aligned}$$

Here a comment on the complex situation in the anisotropic s - d interaction may be useful. One may notice at once that for the isotropic case, $J_x = J_y = J_z$, all the terms except for the first in (2.9a) or (2.9b) are cancelled out. This makes circumstances in the isotropic case quite simple, because it is only the same type of terms as the first term in the parenthesis of (2.9a) that should be taken into account in the most divergent approximation. According to this observation Doniach⁹⁾ has summed up all the most divergent terms of $V_{\text{eff}}(\omega)$ for the isotropic s - d interaction, which is found to be a geometrical series. On the other hand, for the anisotropic case, four terms in (2.9a) (from the second to the fifth term) different from the first term in the type of spin commutators does contribute, as seen above. In this connection we recall the work by Miwa and Nagaoka,⁴⁾ who have calculated the effective potential $V_{\text{eff}}(\omega)$ for the anisotropic s - d interaction in the most divergent approximation. But they have taken into account only the terms, the type of which is the same as the first term in (2.9a), and overlooked many other terms that cannot be neglected in the logarithmic accuracy. Up to third order their results and ours are the same. But terms higher than the fourth order are different between these.

Summing up (2.2), (2.5), (2.7) and (2.9c), we find that

$$V_{\text{eff}}(\omega) \simeq -S^x \sigma^x \left[J_x + 2J_y J_z \left(\rho \ln \frac{|\omega|}{D} \right) + 2J_x (J_y^2 + J_z^2) \left(\rho \ln \frac{|\omega|}{D} \right)^2 + \frac{4}{3} J_y J_z (4J_x^2 + J_y^2 + J_z^2) \left(\rho \ln \frac{|\omega|}{D} \right)^3 + \dots \right] + (\text{terms in which } x, y, \text{ and } z \text{ are changed cyclically}). \quad (2.10)$$

From (2.1) and (2.10) the t -matrix in the most divergent approximation averaged over the direction of the localized spin is given by

$$t(\omega) \simeq -\frac{i\pi\rho}{N} \langle [V_{\text{eff}}(\omega)]^2 \rangle_{AV}, \quad (2.11)$$

where Eq. (2.10) should be substituted for $V_{\text{eff}}(\omega)$. The symbol $\langle \dots \rangle_{AV}$ denotes the average over the direction of a localized spin. In the isotropic limit of the exchange integral Eq. (2.11) is nothing but the expression for the t -matrix obtained by Abrikosov⁹⁾ and Doniach.⁹⁾

Here one may ask the following question: What is the closed-form expression for the effective potential $V_{\text{eff}}(\omega)$ in (2.10)? Our answer will be given in the following section.

§ 3. Summation of the most divergent terms for the scattering amplitude

In order to sum up all the most divergent terms for the anisotropic s - d interaction and to obtain the expression of the closed form, Abrikosov's method⁹⁾ is more convenient than Doniach's in the previous section, although both give the same final results. In his original paper Abrikosov has performed an analysis of the scattering amplitude due to the isotropic s - d interaction in the most divergent approximation. If we make a close examination of his analysis, we find that a greater part of his discussions are applicable also to the anisotropic s - d interaction only with slight modifications.

In accordance with Abrikosov, let us calculate the vertex function $\tau_{\alpha\beta, \alpha'\beta'}(\omega)$ ($\Gamma_{\alpha\beta, \alpha'\beta'}(\omega)$ in Abrikosov's original notation) in the logarithmic accuracy. The vertex function $\tau_{\alpha\beta, \alpha'\beta'}(\omega)$ is nothing but the scattering amplitude of the scattering process, in which a conduction electron with energy ω and spin α is scattered elastically into the state with spin α' and at the same time a localized spin is flipped from β to β' . In the most divergent approximation, $\tau_{\alpha\beta, \alpha'\beta'}(\omega)$ is equivalent to the effective potential $V_{\text{eff}}(\omega)$ defined in the previous section. For the anisotropic s - d interaction $\tau_{\alpha\beta, \alpha'\beta'}$ is given, in the most divergent approximation, as the solution of the integral equation

$$\begin{aligned} \tau_{\alpha\beta, \alpha'\beta'}(t) = & - \sum_{i=x,y,z} J_i \sigma_{\alpha\alpha'}^i S_{\beta\beta'}^i \\ & - \int_0^t ds \sum_{\alpha''\beta''} [\tau_{\alpha\beta, \alpha''\beta''}(s) \tau_{\alpha''\beta'', \alpha'\beta'}(s) - \tau_{\alpha\beta, \alpha''\beta'}(s) \tau_{\alpha''\beta, \alpha'\beta''}(s)], \end{aligned} \quad (3.1)$$

where $t = \rho \ln(D/|\omega|)$. Solving Eq. (3.1) by the iteration method up to the fourth order of the exchange integral, we find that $\tau_{\alpha\beta, \alpha'\beta'}$ is the same as Eq. (2.10). Here we solve Eq. (3.1) exactly. For this purpose we put

$$\tau_{\alpha\beta, \alpha'\beta'} = \tau_0 \delta_{\alpha\alpha'} \delta_{\beta\beta'} + \sum_{i=x,y,z} \tau_i \sigma_{\alpha\alpha'}^i S_{\beta\beta'}^i. \quad (3.2)$$

Substituting (3.2) into (3.1), we easily obtain

$$\begin{cases} \tau_0 = 0, \\ \tau_x(t) = -J_x + 2 \int_0^t ds \tau_y(s) \tau_z(s), \\ \tau_y(t) = -J_y + 2 \int_0^t ds \tau_z(s) \tau_x(s), \\ \tau_z(t) = -J_z + 2 \int_0^t ds \tau_x(s) \tau_y(s). \end{cases} \quad (3.3)$$

Equation (3.3) can be transformed into differential equations

$$\begin{cases} \frac{d\tau_x(t)}{dt} = 2\tau_y(t) \tau_z(t), \\ \frac{d\tau_y(t)}{dt} = 2\tau_z(t) \tau_x(t), \\ \frac{d\tau_z(t)}{dt} = 2\tau_x(t) \tau_y(t) \end{cases} \quad (3.4)$$

with the initial conditions $\tau_i(0) = -J_i$ ($i = x, y, z$). First we note that the relation

$$\begin{aligned} [\tau_x(t)]^2 - J_x^2 &= [\tau_y(t)]^2 - J_y^2 \\ &= [\tau_z(t)]^2 - J_z^2 \end{aligned} \quad (3.5)$$

holds. Thus it is sufficient only to solve a differential equation for the quantity $f(t)$ defined by

$$\begin{aligned} f(t) &= \frac{1}{3} \{ [\tau_x(t)]^2 + [\tau_y(t)]^2 + [\tau_z(t)]^2 \} \\ &\quad - \frac{1}{3} (J_x^2 + J_y^2 + J_z^2). \end{aligned} \quad (3.6)$$

The differential equation for $f(t)$ has the form

$$\left(\frac{df}{dt} \right)^2 = 16(f - e_1)(f - e_2)(f - e_3), \quad (3.7)$$

where the definitions of parameters e_1 , e_2 and e_3 are

$$\begin{cases} e_1 = \frac{1}{3}(-2J_x^2 + J_y^2 + J_z^2), \\ e_2 = \frac{1}{3}(J_x^2 - 2J_y^2 + J_z^2), \\ e_3 = \frac{1}{3}(J_x^2 + J_y^2 - 2J_z^2). \end{cases} \quad (3.8)$$

The initial condition for Eq. (3.7) is $f(0) = 0$, as can be seen from Eq. (3.6). The solution of the differential Equation (3.7), which satisfies this initial condition, is given by

$$f(t) = \mathcal{P}(2(t - t_c)), \quad (3.9)$$

where $\mathcal{P}(z)$ is the Weierstrassian elliptic function,¹¹⁾ and t_c is defined as

$$t_c = \pm \int_{f_0}^{\infty} \frac{df}{4\sqrt{(f - e_1)(f - e_2)(f - e_3)}}, \quad (3.10)$$

$$f_0 = \frac{1}{3}(J_x^2 + J_y^2 + J_z^2).$$

Here the sign \pm means that of $(-J_x J_y J_z)$. Thus the mathematical properties of $f(t)$ as a function of t is completely determined from those of $\mathcal{P}(z)$. Important properties of $\mathcal{P}(z)$ for later discussions are as follows.

(i) $\mathcal{P}(z)$ is a doubly periodic function with periods $2\omega_1$ and $2\omega_2$, and has double poles at the points $z = \Omega_{mn} = 2m\omega_1 + 2n\omega_2$ (m, n : integer) as

$$\mathcal{P}(z) = \frac{1}{z^2} + \sum'_{m,n} \left[\frac{1}{(z - \Omega_{mn})^2} - \frac{1}{\Omega_{mn}^2} \right], \quad (3.11)$$

where \sum'_{mn} means that in the summation the term corresponding to $m = n = 0$ is omitted.

(ii) If e_1, e_2 and e_3 are real as in our case, we can take ω_1 as real and ω_2 as imaginary in the form

$$\begin{cases} 2\omega_1 = \int_{e_M}^{\infty} \frac{du}{\sqrt{(u - e_1)(u - e_2)(u - e_3)}}, \\ 2\omega_2 = i \int_{-\infty}^{e_m} \frac{du}{\sqrt{-(u - e_1)(u - e_2)(u - e_3)}}, \end{cases} \quad (3.12)$$

where $e_M(e_m)$ is the maximum (minimum) of e_1, e_2 and e_3 .

(iii) The Weierstrassian elliptic function $\mathcal{P}(z)$ is related with the Jacobian elliptic function, for instance, $\text{sn}(z, k)$ by

$$\mathcal{P}(z) = e_1 + \frac{e_3 - e_1}{\text{sn}^2(z\sqrt{e_3 - e_1}, k)}, \quad (3.13)$$

where $k = \sqrt{(e_2 - e_1)/(e_3 - e_1)}$.

Making use of these relations, we can discuss the behavior of the scattering amplitude for the anisotropic *s-d* interaction. First we study in which case the scattering amplitude in the logarithmic accuracy is divergent. The conditions for $f(t)$ not to have poles on positive real axis of $t (= \rho \ln(D/|\omega|))$, $+\infty > t > 0$,

are the following: (1) The real period ω_1 goes to infinity and (2) $t_c < 0$. From (3.10) and (3.12) these conditions mean that $f(t)$ has no pole on the positive real axis of t , when (1) one of

$$J_x^2 \geq J_y^2 = J_z^2,$$

$$J_y^2 \geq J_x^2 = J_z^2$$

and

$$J_z^2 \geq J_x^2 = J_y^2$$

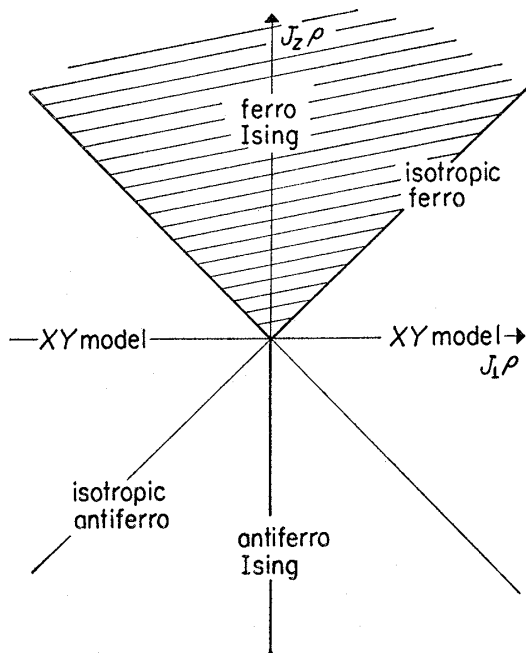


Fig. 2. Behaviors of the scattering amplitude for the axially symmetric s - d exchange interaction ($J_x = J_y = J_{\perp}$). The scattering amplitude in the most divergent approximation has poles on the positive real axis of $t (= \rho \ln(D/|\omega|))$ except in the hatched region, where $J_z \geq |J_{\perp}|$ is satisfied, and in the antiferromagnetic Ising case.

The energies given by (3.14a) and (3.14b) are equal to the binding energy of the collective bound state realized as the ground state of our system.

Before we discuss some limiting cases, we will give expressions for the scattering amplitude in terms of the Jacobian elliptic functions, which may be convenient for later purposes. Using the relation (3.13) and the definition of e_i , (3.8), we have

$$\tau_x^2 = (J_x^2 - J_z^2) \frac{1}{\text{sn}^2(2(t - t_c) \sqrt{J_x^2 - J_z^2}, k)},$$

is satisfied and (2) $J_x J_y J_z \geq 0$. In particular, for the axially symmetric case $J_x = J_y = J_{\perp}$, $f(t)$ has no pole on the positive real axis of t , when both $J_z^2 \geq J_{\perp}^2$ and $J_z \geq 0$ are satisfied, or when $J_z < 0$ and $J_{\perp} = 0$ are satisfied. Otherwise $f(t)$ has poles. This result is shown in Fig. 2.

If at least one of the two conditions is not satisfied, $f(t)$ has double poles on the positive real axis of t . From the definition of t and Eq. (3.11) we find that the largest energy, at which the scattering amplitude diverges, is given by

$$|\omega| = D e^{-t_c/\rho} \quad \text{for } J_x J_y J_z < 0 \tag{3.14a}$$

and

$$|\omega| = D e^{-(\omega_1 + t_c)/\rho} \quad \text{for } J_x J_y J_z > 0, \tag{3.14b}$$

where ω_1 is defined by (3.12). The quantities t_c and ω_1 are expressed, in general, in terms of elliptic integral. It will be shown in the following section that the

$$\begin{cases} \tau_y^2 = (J_x^2 - J_z^2) \frac{\operatorname{dn}^2(2(t-t_c) \sqrt{J_x^2 - J_z^2}, k)}{\operatorname{sn}^2(2(t-t_c) \sqrt{J_x^2 - J_z^2}, k)}, \\ \tau_z^2 = (J_x^2 - J_z^2) \frac{\operatorname{cn}^2(2(t-t_c) \sqrt{J_x^2 - J_z^2}, k)}{\operatorname{sn}^2(2(t-t_c) \sqrt{J_x^2 - J_z^2}, k)}, \end{cases} \quad (3.15)$$

where $k = \sqrt{(J_x^2 - J_y^2)/(J_x^2 - J_z^2)}$. Here use has been made of the definitions of $\operatorname{cn}(z, k)$ and $\operatorname{dn}(z, k)$

$$\begin{cases} \operatorname{cn}^2(z, k) = 1 - \operatorname{sn}^2(z, k), \\ \operatorname{dn}^2(z, k) = 1 - k^2 \operatorname{sn}^2(z, k). \end{cases} \quad (3.16)$$

Of course it should be noted that there exist other ways of expressing τ_i in terms of the Jacobian elliptic functions. Now we will turn to the study of limiting cases.

(1) *the axially symmetric case* ($J_x = J_y = J_\perp$)

In this case the modulus k in (3.14) is equal to zero. Thus, noting the properties

$$\begin{aligned} \operatorname{sn}(z, 0) &= \sin z, & \operatorname{cn}(z, 0) &= \cos z, \\ \operatorname{dn}(z, 0) &= 1 \end{aligned} \quad (3.17)$$

and calculating t_c from Eq. (3.10) explicitly, we have

$$\begin{cases} \tau_x(t) = \tau_y(t) = \tau_\perp(t) \\ \quad = \sqrt{J_\perp^2 - J_z^2} \frac{\operatorname{sgn}(J_\perp J_z)}{\sin(\tan^{-1}(\sqrt{J_\perp^2 - J_z^2}/-J_z) - 2\sqrt{J_\perp^2 - J_z^2}t)} \\ \tau_z(t) = \sqrt{J_\perp^2 - J_z^2} \cot\left(\tan^{-1} \frac{\sqrt{J_\perp^2 - J_z^2}}{-J_z} - 2\sqrt{J_\perp^2 - J_z^2}t\right) \end{cases} \quad (3.18)$$

for $J_\perp^2 \geq J_z^2$, and

$$\begin{cases} \tau_x(t) = \tau_y(t) = \tau_\perp(t) \\ \quad = \sqrt{J_z^2 - J_\perp^2} \frac{\operatorname{sgn}(J_\perp J_z)}{\sinh(\tanh^{-1}(\sqrt{J_z^2 - J_\perp^2}/-J_z) - 2\sqrt{J_z^2 - J_\perp^2}t)} \\ \tau_z(t) = \sqrt{J_z^2 - J_\perp^2} \coth\left(\tanh^{-1} \frac{\sqrt{J_z^2 - J_\perp^2}}{-J_z} - 2\sqrt{J_z^2 - J_\perp^2}t\right) \end{cases} \quad (3.19)$$

for $J_z^2 \geq J_\perp^2$. In (3.18) \tan^{-1} means the principal value, i.e. $-\pi/2 < \tan^{-1}x < \pi/2$. From (3.18) and (3.19) one may notice the difference between the two cases $J_\perp^2 \geq J_z^2$ and $J_z^2 \geq J_\perp^2$.

(2) *the isotropic case* ($J_\perp = J_z = J$)

This is a special case of the axially symmetric exchange interaction. We can easily obtain from (3.18) or (3.19)

$$\tau_{\perp}(t) = \tau_z(t) = \frac{1}{-1/J - 2t}, \quad (3.20)$$

which is nothing but the result found by Abrikosov.³⁾

(3) *the Ising case* ($J_{\perp} = 0$)

Setting $J_{\perp} \rightarrow 0$ in (3.19), we have

$$\begin{cases} \tau_{\perp}(t) = 0, \\ \tau_z(t) = -J_z. \end{cases} \quad (3.21)$$

Divergence difficulties of the scattering amplitude for the positive real value of t ($+\infty > t > 0$) suggest that something real and physical must occur. In the next section we will study the ground state of conduction electrons and a localized spin coupled by the anisotropic s - d interaction and find the intimate connections between the divergence difficulties and the many-body bound state realized as the ground state of this system.

§ 4. Bound state

To consider the physical meaning of the divergence of the scattering amplitude found in the previous section and what it suggests, we study the ground state—the collective bound state due to the anisotropic s - d exchange interaction—following the formulation of Yosida, Okiji and Yoshimori.^{5)~8)} The wave function of the ground state Ψ is expanded as

$$\begin{aligned} \Psi = \sum_{\beta} [\sum_{k\alpha} \Gamma_{\alpha\beta}(\epsilon_k) a_{k\alpha}^{\dagger} \\ + \sum_{\substack{k_1, k_2, k_3 \\ \alpha_1, \alpha_2, \alpha_3}} \Gamma_{\alpha_1\alpha_2\alpha_3\beta}(\epsilon_{k_1}, \epsilon_{k_2}, \epsilon_{k_3}) a_{k_1\alpha_1}^{\dagger} a_{k_2\alpha_2}^{\dagger} a_{k_3\alpha_3}^{\dagger} + \dots] \chi_{\beta} \Phi_0, \end{aligned} \quad (4.1)$$

where χ_{β} is the eigenfunction of the impurity spin, and Φ_0 denotes the Fermi vacuum. The coefficients $\Gamma_{\alpha\beta}, \Gamma_{\alpha_1\alpha_2\alpha_3\beta}, \dots$ are determined from the Schrödinger equation. Eliminating higher order coefficients $\Gamma_{\alpha_1\alpha_2\alpha_3\beta}, \Gamma_{\alpha_1\alpha_2\alpha_3\alpha_4\beta}, \dots$ by iteration with the use of the relations derived by the Schrödinger equation, we can reduce the equation for $\Gamma_{\alpha\beta}(\epsilon)$ to the integral equation

$$\begin{aligned} (\epsilon - \tilde{E}) \Gamma_{\alpha\beta}(\epsilon) - \sum_i \sum_{\alpha'\beta'} J_i \sigma_{\alpha\alpha'}^i S_{\beta\beta'}^i \rho \int_0^D d\epsilon' \Gamma_{\alpha'\beta'}(\epsilon') \\ + \sum_{\alpha'\beta'} \rho \int_0^D d\epsilon' K_{\alpha\beta, \alpha'\beta'}(\epsilon + \epsilon' - \tilde{E}) \Gamma_{\alpha'\beta'}(\epsilon') = 0, \end{aligned} \quad (4.2)$$

where \tilde{E} is the anomalous part of the ground state energy E (the binding energy): $E = \Delta E + \tilde{E}$ with the normal part ΔE , which can be obtained by the ordinary perturbation expansion. We calculate the kernel $K_{\alpha\beta, \alpha'\beta'}(\epsilon)$ in the logarithmic accuracy. One way is to perform iteration directly. The other is based on Nakajima's observation¹²⁾ that the kernel $K_{\alpha\beta, \alpha'\beta'}(\epsilon)$ is tightly connected with

the scattering amplitude calculated by Abrikosov.⁹⁾ The latter is more convenient than the former for the present purpose. Nakajima's arguments have been done for the isotropic s - d interaction. But close examinations show that an analogous relation

$$K_{\alpha\beta, \alpha'\beta'}(\epsilon) = -A_{\alpha\beta, \alpha'\beta'}^{(2)}(t), \tag{4.3}$$

$$t = \rho \ln \frac{D}{\epsilon}$$

holds for the anisotropic s - d interaction, where $A_{\alpha\beta, \alpha'\beta'}^{(2)}(t)$ is a quantity corresponding to $A^{(2)}$ in Abrikosov's paper.⁹⁾

$$A_{\alpha\beta, \alpha'\beta'}^{(2)}(t) = - \int_0^t dt' \sum_{i,j} \tau_i(t') \tau_j(t') \langle \alpha | \sigma^i \sigma^j | \alpha' \rangle \langle \beta | S^j S^i | \beta' \rangle. \tag{4.4}$$

Here $\tau_i(t)$ is the vertex function calculated in the previous section in the logarithmic accuracy.

To solve the integral Equation (4.2) we transform it into a differential equation.⁷⁾ This procedure is found to be powerful not only for the isotropic s - d interaction, but also for the anisotropic one. For this purpose let us introduce the function $G_{\alpha\beta}(\epsilon)$ defined as

$$G_{\alpha\beta}(\epsilon) = \int_0^\epsilon d\epsilon' \Gamma_{\alpha\beta}(\epsilon'). \tag{4.5}$$

Then we can reduce Eq. (4.2) to a differential equation for $G_{\alpha\beta}(\epsilon)$. First we note that within the logarithmic accuracy the term with the kernel $K_{\alpha\beta, \alpha'\beta'}$ can be approximated as follows:^{7),8)}

$$\int_0^D d\epsilon' K_{\alpha\beta, \alpha'\beta'}(\epsilon + \epsilon' - \tilde{E}) \Gamma_{\alpha'\beta'}(\epsilon') \simeq - \int_\epsilon^D d\epsilon' \frac{dK_{\alpha\beta, \alpha'\beta'}(\epsilon' - \tilde{E})}{d\epsilon'} \cdot G_{\alpha'\beta'}(\epsilon'). \tag{4.6}$$

Substituting (4.5) and (4.6) into (4.2) and differentiating both sides of (4.2) with respect to ϵ , we have a differential equation for $G_{\alpha\beta}(\epsilon)$:

$$(\epsilon - \tilde{E})^2 \frac{d^2 G_{\alpha\beta}(\epsilon)}{d\epsilon^2} + (\epsilon - \tilde{E}) \frac{dG_{\alpha\beta}(\epsilon)}{d\epsilon} - \rho^2 \sum_{\alpha'\beta'} \sum_{i,j} \tau_i(u) \tau_j(u) \langle \alpha | \sigma^i \sigma^j | \alpha' \rangle \langle \beta | S^j S^i | \beta' \rangle G_{\alpha'\beta'}(\epsilon) = 0, \tag{4.7}$$

where $u = \rho \ln(D/(\epsilon - \tilde{E}))$. Boundary conditions for (4.7) are

$$G_{\alpha\beta}(0) = 0 \tag{4.8a}$$

and

$$(\epsilon - \tilde{E}) \left. \frac{dG_{\alpha\beta}(\epsilon)}{d\epsilon} \right|_{\epsilon=D} = \sum_i \sum_{\alpha'\beta'} J_i \sigma_{\alpha\alpha'}^i S_{\beta\beta'}^i \rho G_{\alpha'\beta'}(D). \tag{4.8b}$$

Now we change the variable from ϵ to $u = \rho \ln(D/(\epsilon - \tilde{E}))$. Equations (4.7),

(4.8a) and (4.8b) are transformed into the equations for $g_{\alpha\beta}(u)$ defined as $g_{\alpha\beta}(u) = G_{\alpha\beta}(\epsilon)$, i.e.

$$\frac{d^2 g_{\alpha\beta}(u)}{du^2} - \sum_{i,j} \sum_{\alpha'\beta'} \tau_i(u) \tau_j(u) \langle \alpha | \sigma^i \sigma^j | \alpha' \rangle \langle \beta | S^j S^i | \beta' \rangle g_{\alpha'\beta'}(u) = 0 \quad (4.9)$$

with the boundary conditions

$$\begin{cases} g_{\alpha\beta}(\tilde{u}) = 0, \\ \left. \frac{dg_{\alpha\beta}(u)}{du} \right|_{u=0} = - \sum_i \sum_{\alpha'\beta'} J_i \sigma_{\alpha\alpha'}^i S_{\beta\beta'}^i g_{\alpha'\beta'}(0) \end{cases} \quad (4.10)$$

where

$$\tilde{u} = \rho \ln \frac{D}{-\tilde{E}}.$$

So far our discussions are applicable quite generally for the anisotropic s - d interaction. Hereafter we assume for simplicity that the exchange integral is axially symmetric, i.e. $J_x = J_y = J_\perp$ and that the spin of the impurity atom S is equal to $1/2$. Under these assumptions the coupled equations (4.9) are separated into the following:

$$\left\{ \frac{d^2 g_{\uparrow\uparrow}}{du^2} - \left(\tau_\perp^2(u) + \frac{1}{4} \tau_z^2(u) \right) g_{\uparrow\uparrow} = 0, \right. \quad (4.11a)$$

$$\left. \frac{d^2 (g_{\uparrow\downarrow} \pm g_{\downarrow\uparrow})}{du^2} - \left(\pm \tau_\perp(u) \tau_z(u) + \frac{1}{4} \tau_z^2(u) \right) (g_{\uparrow\downarrow} \pm g_{\downarrow\uparrow}) = 0, \right. \quad (4.11b)$$

$$(4.11c)$$

where $g_{\uparrow\uparrow}$, $g_{\uparrow\downarrow} + g_{\downarrow\uparrow}$ and $g_{\downarrow\downarrow}$ correspond to the states with the total spin $S_{\text{total}} = 1$ and its z -component $S_{\text{total}}^z = 1, 0, -1$, $g_{\uparrow\downarrow} - g_{\downarrow\uparrow}$ a singlet with $S_{\text{total}} = 0$. As the wave function $g_{\downarrow\downarrow}$ obeys the same equation as (4.11a), we omit it. The quantities $\tau_\perp(u)$ and $\tau_z(u)$ in (4.11a) ~ (4.11c) have already been obtained in the previous section ((3.18) or (3.19)).

First we will study the case $J_\perp^2 \geq J_z^2$. To simplify the differential equations (4.11a) ~ (4.11c) let us introduce a new variable x defined by $x = \cos(y - y_0)$, where

$$y = 2u \sqrt{J_\perp^2 - J_z^2} \quad (4.12)$$

and

$$y_0 = \tan^{-1} \frac{\sqrt{J_\perp^2 - J_z^2}}{-J_z}. \quad (4.13)$$

Substituting the expressions for $\tau_\perp(u)$ and $\tau_z(u)$, (3.18), into Eqs. (4.11a) ~ (4.11c), we can rewrite these in terms of a new variable in the form

$$\left\{ \begin{aligned} & \left[\frac{d^2}{dx^2} + \frac{x}{x^2-1} \frac{d}{dx} - \frac{x^2+4}{16(x^2-1)^2} \right] g_{\uparrow\uparrow} = 0, & (4.14a) \\ & \left[\frac{d^2}{dx^2} + \frac{x}{x^2-1} \frac{d}{dx} - \frac{x^2 \pm 4x \operatorname{sgn}(J_{\perp}J_z)}{16(x^2-1)^2} \right] (g_{\uparrow\downarrow} \pm g_{\downarrow\uparrow}) = 0. & (4.14b) \\ & & (4.14c) \end{aligned} \right.$$

Solutions of these equations can easily be found. From Eq. (4.14a) we have

$$g_{\uparrow\uparrow} = \frac{1}{(1-x)^{1/8}(1+x)^{1/8}} \left[A_1 + B_1 \int^x \frac{dx'}{(1-x')^{1/4}(1+x')^{1/4}} \right] \quad (4.15a)$$

and from (4.14b) and (4.14c)

$$g_{\uparrow\downarrow} + g_{\downarrow\uparrow} = \frac{(1+x)^{3/8}}{(1-x)^{1/8}} \left[A_2 + B_2 \int^x \frac{dx'}{(1-x')^{1/4}(1+x)^{5/4}} \right], \quad (4.15b)$$

$$g_{\uparrow\downarrow} - g_{\downarrow\uparrow} = \frac{(1-x)^{3/8}}{(1+x)^{1/8}} \left[A_3 + B_3 \int^x \frac{dx'}{(1-x')^{5/4}(1+x')^{1/4}} \right] \quad (4.15c)$$

for the case $\operatorname{sgn}(J_{\perp}J_z) > 0$. For $\operatorname{sgn}(J_{\perp}J_z) < 0$, $g_{\uparrow\downarrow} + g_{\downarrow\uparrow}$ and $g_{\uparrow\downarrow} - g_{\downarrow\uparrow}$ should be interchanged. In (4.15a) ~ (4.15c) the constants A_1, B_1, \dots, B_3 are determined from the boundary conditions (4.10). Eliminating these constants A_1, B_1, \dots, B_3 in this way, we obtain our final results for the case $\operatorname{sgn}(J_{\perp}J_z) > 0$ as follows:

$$\left\{ \begin{aligned} & g_{\uparrow\uparrow}(x) = g_{\uparrow\uparrow}(x_0) \\ & \times \frac{\frac{x_0}{4(1-x_0^2)} \frac{1}{(1-x)^{1/8}(1+x)^{1/8}} \int_{\tilde{x}}^x \frac{dx'}{(1-x')^{1/4}(1+x')^{1/4}}}{\frac{1}{(1-x_0)^{3/8}(1+x_0)^{3/8}} + \frac{x_0}{4(1-x_0^2)} \frac{1}{(1-x_0)^{1/8}(1+x_0)^{1/8}} \int_{\tilde{x}}^{x_0} \frac{dx'}{(1-x')^{1/4}(1+x')^{1/4}}}, & (4.16a) \end{aligned} \right.$$

$$\left\{ \begin{aligned} & (g_{\uparrow\downarrow} + g_{\downarrow\uparrow})(x) = (g_{\uparrow\downarrow} + g_{\downarrow\uparrow})(x_0) \\ & \times \frac{\frac{2-x_0}{4(1-x_0^2)} \frac{(1+x)^{3/8}}{(1-x)^{1/8}} \int_{\tilde{x}}^x \frac{dx'}{(1-x')^{1/4}(1+x')^{5/4}}}{\frac{1}{(1-x_0)^{3/8}(1+x_0)^{3/8}} + \frac{2-x_0}{4(1-x_0^2)} \frac{(1+x_0)^{3/8}}{(1-x_0)^{1/8}} \int_{\tilde{x}}^{x_0} \frac{dx'}{(1-x')^{1/4}(1+x')^{5/4}}}, & (4.16b) \end{aligned} \right.$$

$$\left\{ \begin{aligned} & (g_{\uparrow\downarrow} - g_{\downarrow\uparrow})(x) = (g_{\uparrow\downarrow} - g_{\downarrow\uparrow})(x_0) \\ & \times \frac{\frac{-2-x_0}{4(1-x_0^2)} \frac{(1-x)^{3/8}}{(1+x)^{1/8}} \int_{\tilde{x}}^x \frac{dx'}{(1-x')^{5/4}(1+x')^{1/4}}}{\frac{1}{(1-x_0)^{7/8}(1+x_0)^{3/8}} + \frac{-2-x_0}{4(1-x_0^2)} \frac{(1-x_0)^{3/8}}{(1+x_0)^{1/8}} \int_{\tilde{x}}^{x_0} \frac{dx'}{(1-x')^{5/4}(1+x')^{1/4}}}, & (4.16c) \end{aligned} \right.$$

where x_0 and \tilde{x} are defined by

$$\begin{cases} x_0 = \cos y_0 = |J_z/J_\perp|, & (4.17) \\ \tilde{x} = \cos(\tilde{y} - y_0) = \cos\left(2\tilde{u} \sqrt{J_\perp^2 - J_z^2} - \tan^{-1} \frac{\sqrt{J_\perp^2 - J_z^2}}{-J_z}\right) \\ = \cos\left(2\sqrt{J_\perp^2 - J_z^2} \rho \ln \frac{D}{-\tilde{E}} - \tan^{-1} \frac{\sqrt{J_\perp^2 - J_z^2}}{-J_z}\right). & (4.18) \end{cases}$$

Setting $x = x_0$ in (4.16a) ~ (4.16c), we find the equations to determine the binding energy \tilde{E} :

$$1 = \frac{\frac{x_0}{4(1-x_0^2)} \frac{1}{(1-x_0)^{1/8} (1+x_0)^{1/8}} \int_{\tilde{x}}^{x_0} \frac{dx'}{(1-x')^{1/4} (1+x')^{1/4}}}{\frac{1}{(1-x_0)^{3/8} (1+x_0)^{3/8}} + \frac{x_0}{4(1-x_0^2)} \frac{1}{(1-x_0)^{1/8} (1+x_0)^{1/8}} \int_{\tilde{x}}^{x_0} \frac{dx'}{(1-x')^{1/4} (1+x')^{1/4}}} \quad (4.19a)$$

for $g_{\uparrow\uparrow}(x)$,

$$1 = \frac{\frac{2-x_0}{4(1-x_0^2)} \frac{(1+x_0)^{3/8}}{(1-x_0)^{1/8}} \int_{\tilde{x}}^{x_0} \frac{dx'}{(1-x')^{1/4} (1+x')^{5/4}}}{\frac{1}{(1-x_0)^{3/8} (1+x_0)^{7/8}} + \frac{2-x_0}{4(1-x_0^2)} \frac{(1+x_0)^{3/8}}{(1-x_0)^{1/8}} \int_{\tilde{x}}^{x_0} \frac{dx'}{(1-x')^{1/4} (1+x')^{5/4}}} \quad (4.19b)$$

for $g_{\uparrow\downarrow}(x) + g_{\downarrow\uparrow}(x)$,

$$1 = \frac{\frac{-2-x_0}{4(1-x_0^2)} \frac{(1-x_0)^{3/8}}{(1+x_0)^{1/8}} \int_{\tilde{x}}^{x_0} \frac{dx'}{(1+x')^{1/4} (1-x')^{5/4}}}{\frac{1}{(1-x_0)^{7/8} (1+x_0)^{3/8}} + \frac{-2-x_0}{4(1-x_0^2)} \frac{(1-x_0)^{3/8}}{(1+x_0)^{1/8}} \int_{\tilde{x}}^{x_0} \frac{dx'}{(1+x')^{1/4} (1-x')^{5/4}}} \quad (4.19c)$$

for $g_{\uparrow\downarrow}(x) - g_{\downarrow\uparrow}(x)$. Equations (4.19a) ~ (4.19c) have solutions, only when the integral in each equation diverges. Thus we come to the following conclusions:

- i) Equation (4.19a) has no solution.
- ii) The solution of Eq. (4.19b) is $\tilde{x} = -1$, i.e.

$$\cos\left(2\sqrt{J_\perp^2 - J_z^2} \rho \ln \frac{D}{-\tilde{E}} - \tan^{-1} \frac{\sqrt{J_\perp^2 - J_z^2}}{-J_z}\right) = -1 \quad (4.20a)$$

or

$$\tilde{E} = -D \exp\left[-\frac{1}{2\sqrt{J_\perp^2 - J_z^2} \rho} \left((2n+1)\pi + \tan^{-1} \frac{\sqrt{J_\perp^2 - J_z^2}}{-J_z}\right)\right]. \quad (4.20b)$$

($n = \text{integer}$)

Deriving the integral equation for the bound state, (4.2) and (4.3), we assumed that the s - d exchange interaction is so weak that $J_\perp \rho, J_z \rho \ll 1$ and $|\tilde{E}|/D \ll 1$. Further the kernel $K(\epsilon + \epsilon' - \tilde{E})$ should not be divergent for positive values of ϵ and ϵ' . From these conditions the following is found to be the only one that may be allowed as a bound state in (4.20b):

$$\tilde{E} = -D \exp \left[-\frac{1}{2\sqrt{J_{\perp}^2 - J_z^2} \rho} \left(\pi + \tan^{-1} \frac{\sqrt{J_{\perp}^2 - J_z^2}}{-J_z} \right) \right] \quad (4.21)$$

for $J_z > 0$.

iii) The solution of Eq. (4.19c) is $\tilde{x} = 1$, i.e.

$$\cos \left(2\sqrt{J_{\perp}^2 - J_z^2} \rho \ln \frac{D}{-\tilde{E}} - \tan^{-1} \frac{\sqrt{J_{\perp}^2 - J_z^2}}{-J_z} \right) = 1, \quad (4.22a)$$

or

$$\tilde{E} = -D \exp \left[-\frac{1}{2\sqrt{J_{\perp}^2 - J_z^2} \rho} \left(2n\pi + \tan^{-1} \frac{\sqrt{J_{\perp}^2 - J_z^2}}{-J_z} \right) \right]. \quad (4.22b)$$

($n = \text{integer}$)

From the same reason as in ii) the solution that may be allowed in (4.22b) is the following:

$$\tilde{E} = -D \exp \left[-\frac{1}{2\sqrt{J_{\perp}^2 - J_z^2} \rho} \tan^{-1} \frac{\sqrt{J_{\perp}^2 - J_z^2}}{-J_z} \right] \quad (4.23)$$

for $J_z < 0$.

For the solutions with $n \geq 1$ in (4.20b) and (4.22b) the kernel $K(\epsilon + \epsilon' - \tilde{E})$ calculated in the most divergent approximation diverges at a certain value of ϵ and ϵ' . Thus the energies with $n \geq 1$ may suggest possible existence of the excited resonance state for $|J_{\perp}| > |J_z|$, although it is not known for certain because of our approximation for the integral kernel.

So far we have discussed in detail bound states for the case of $\text{sgn}(J_{\perp}J_z) > 0$. If $\text{sgn}(J_{\perp}J_z) < 0$, it is sufficient only to interchange $g_{\uparrow\downarrow} + g_{\downarrow\uparrow}$ and $g_{\uparrow\downarrow} - g_{\downarrow\uparrow}$ in the above results.

Now we will turn to the case $J_z^2 \geq J_{\perp}^2$. In this case we substitute into the differential equations (4.11a) ~ (4.11c) the expressions for $\tau_{\perp}(t)$ and $\tau_z(t)$ (3.18) instead of (3.17) and solve them in the same way as for $J_{\perp}^2 \geq J_z^2$. Analogous calculations lead to the following equations to determine the binding energy \tilde{E} for this case with the definition of x_0 and \tilde{x} ,

$$\left\{ \begin{aligned} x_0 &= |J_{\perp}/J_z| \geq 1, & (4.24) \\ \tilde{x} &= \cosh \left(2\sqrt{J_z^2 - J_{\perp}^2} \rho \ln \frac{D}{-\tilde{E}} - \tanh^{-1} \frac{\sqrt{J_z^2 - J_{\perp}^2}}{-J_z} \right), & (4.25) \end{aligned} \right.$$

$$1 = \frac{\frac{x_0}{4(x_0^2 - 1)} \frac{1}{(x_0 - 1)^{1/8} (x_0 + 1)^{1/8}} \int_{\tilde{x}}^{x_0} \frac{dx'}{(x' - 1)^{1/4} (x' + 1)^{1/4}}}{\frac{1}{(x_0 - 1)^{3/8} (x_0 + 1)^{3/8}} - \frac{x_0}{4(x_0^2 - 1)} \frac{1}{(x_0 - 1)^{1/8} (x_0 + 1)^{1/8}} \int_{\tilde{x}}^{x_0} \frac{dx'}{(x' - 1)^{1/4} (x' + 1)^{1/4}}} \quad (4.26a)$$

for $g_{\uparrow\uparrow}(x)$,

$$1 = \frac{\frac{2-x_0}{4(x_0^2-1)} \frac{(x_0+1)^{3/8}}{(x_0-1)^{1/8}} \int_{\tilde{x}}^{x_0} \frac{dx'}{(x'-1)^{1/4}(x'+1)^{5/4}}}{\frac{1}{(x_0-1)^{3/8}(x_0+1)^{7/8}} - \frac{2-x_0}{4(x_0^2-1)} \frac{(x_0+1)^{3/8}}{(x_0-1)^{1/8}} \int_{\tilde{x}}^{x_0} \frac{dx'}{(x'-1)^{1/4}(x'+1)^{5/4}}} \quad (4.26b)$$

for $g_{\uparrow\downarrow}(x) + g_{\downarrow\uparrow}(x)$,

$$1 = \frac{\frac{2+x_0}{4(x_0^2-1)} \frac{(x_0-1)^{3/8}}{(x_0+1)^{1/8}} \int_{\tilde{x}}^{x_0} \frac{dx'}{(x'+1)^{1/4}(x'-1)^{5/4}}}{\frac{1}{(x_0-1)^{7/8}(x_0+1)^{3/8}} + \frac{2+x_0}{4(x_0^2-1)} \frac{(x_0-1)^{3/8}}{(x_0+1)^{1/8}} \int_{\tilde{x}}^{x_0} \frac{dx'}{(x'+1)^{1/4}(x'-1)^{5/4}}} \quad (4.26c)$$

for $g_{\uparrow\downarrow}(x) - g_{\downarrow\uparrow}(x)$. Here we have made the assumption of $\text{sgn}(J_{\perp}J_z) > 0$. For the case $\text{sgn}(J_{\perp}J_z) < 0$, $g_{\uparrow\downarrow} + g_{\downarrow\uparrow}$ and $g_{\uparrow\downarrow} - g_{\downarrow\uparrow}$ should be changed with each other. The solutions of equations (4.26a) ~ (4.26c) can be found easily.

- i) Equations (4.26a) and (4.26b) have no solution.
- ii) The solution of (4.26c) is $\tilde{x}=1$, i.e.

$$\tilde{E} = -D \exp \left[-\frac{1}{2\sqrt{J_z^2 - J_{\perp}^2}} \tanh^{-1} \frac{\sqrt{J_z^2 - J_{\perp}^2}}{-J_z} \right] \quad (4.27)$$

for $J_z < 0$. When $J_z > 0$, we are faced with an apparently unphysical situation $|\tilde{E}|/D \gg 1$. Therefore for the case $J_z > 0$ it should be omitted.

Thus we have obtained the exact solutions of collective bound states for the anisotropic (axially symmetric) s - d interaction, which are summarized in Table I for convenience. The sign of J_{\perp} is not important, because it changes

Table I. Binding energy \tilde{E} for the anisotropic s - d interaction. The bound state with the binding energy given below is the solution of $g_{\uparrow\downarrow} + g_{\downarrow\uparrow}$ when $J_{\perp} > 0$ and $g_{\uparrow\downarrow} - g_{\downarrow\uparrow}$ when $J_{\perp} < 0$.

	$J_z < 0$	$J_z > 0$
$ J_{\perp} \geq J_z $	$D \exp \left[-\frac{1}{2\sqrt{J_{\perp}^2 - J_z^2} \rho} \tan^{-1} \frac{\sqrt{J_{\perp}^2 - J_z^2}}{-J_z} \right]$	$D \exp \left[-\frac{1}{2\sqrt{J_{\perp}^2 - J_z^2} \rho} \left(\pi + \tan^{-1} \frac{\sqrt{J_{\perp}^2 - J_z^2}}{-J_z} \right) \right]$
$ J_{\perp} \leq J_z $	$D \exp \left[-\frac{1}{2\sqrt{J_z^2 - J_{\perp}^2} \rho} \tanh^{-1} \frac{\sqrt{J_z^2 - J_{\perp}^2}}{-J_z} \right]$	0

only the phase factor of the wave function. These results may be regarded as an extension of the calculations by Yosida, Okiji and Yoshimori^{5)~8)} to the anisotropic case, and show that the binding energy is tightly connected with the divergence of the scattering amplitude obtained in the previous section.

Let us examine some limiting cases.

i) *the isotropic limit* ($J_{\perp} = J_z = J$)

This case can be obtained either from $J_{\perp}^2 \geq J_z^2$ or from $J_z^2 \geq J_{\perp}^2$ by a limiting procedure. Both calculations give the same result, as a matter of course: a singlet bound state for the antiferromagnetic exchange ($J < 0$) with the binding energy

$$\tilde{E} = -D \exp\left[-\frac{1}{2|J|\rho}\right] \quad (4.28)$$

and no bound state for the ferromagnetic coupling. This is nothing but the result previously obtained by Yoshimori.⁷⁾ In fact, for the isotropic case the quantities x_0 and \tilde{x} in (4.19a) ~ (4.19c) or (4.26a) ~ (4.26c) are nearly equal to unity and integrations can be performed explicitly. Then these equations are found to be the same as those obtained by Yoshimori as equations, which determine the binding energy of the bound state due to isotropic s - d interaction.

ii) *the XY model* ($J_z = 0$)

This is obtained from the case $J_{\perp}^2 \geq J_z^2$ by setting $J_z \rightarrow 0$. The binding energy is given by

$$\tilde{E} = -D \exp\left[-\frac{\pi}{4|J_{\perp}|\rho}\right] \quad (4.29)$$

irrespective of the sign of J_{\perp} .

iii) *the Ising limit* ($J_{\perp} = 0$)

This is a limiting case of the calculation for $J_z^2 \geq J_{\perp}^2$. There exists no bound state. This is quite natural because of nonexistence of quantum effects.

§ 5. Conclusions

In this paper we have investigated the scattering amplitude in the most divergent approximation and the many-body bound state due to the *anisotropic* s - d interaction in order to extend our knowledge on the Kondo problem. We have succeeded in obtaining the exact solution of the bound state for the anisotropic s - d interaction, and have found that the divergence difficulty of the scattering amplitude calculated in the logarithmic accuracy and the collective bound state of the coupled system of conduction electrons and a localized spin are closely connected even in the anisotropic s - d exchange model as in the isotropic case. One of the important conclusions of this paper we wish to emphasize is that from a viewpoint such as that of the Kondo problem the anisotropic (axially symmetric) s - d interaction can be separated into three cases:

- i) $|J_{\perp}| \geq |J_z|$,
- ii) $|J_z| \geq |J_{\perp}|$ and $J_z > 0$,
- iii) $|J_z| \geq |J_{\perp}|$ and $J_z < 0$

as shown in Fig. 2. Within each case the difference of the degree of anisotropy does not change the essential properties of solutions. But between two cases, for example i) and ii), the behaviors of the scattering amplitude and the bound state are qualitatively different. This result is analogous to that of the recent paper by Anderson et al,¹⁰⁾ in which it is proved that a scaling law holds in each region of Fig. 2. Detailed discussions of the relation between our calculations and the theory by Anderson et al. will be left for a future study.

Acknowledgements

The author would like to express his sincere thanks to Professor H. Miwa for helpful discussions during the course of this work and a careful reading of the manuscript. He is also indebted to Professor J. Kanamori for valuable comments, and to Sakkokai Foundation for financial support.

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