Ground State of the Asymmetric Anderson Model
—Perturbation Approach with Respect to the s-d Mixing Integral—

Satoru INAGAKI

The Institute for Solid State Physics
The University of Tokyo, Tokyo 106

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The ground state of the asymmetric Anderson model is investigated in the limit of strong d-electron correlation. The secular equation for the ground state energy is expanded into the perturbation series with respect to s-d mixing integral, $V$, or the width of the d-level, $\Delta$. When the energy level of the localized d-state is near the Fermi level, $E_F \approx 0$, it is shown that this secular equation is equivalent, up to the third dominant order, to the coupled integral equations for two self-energies $\Sigma_d(\omega)$ and $\Sigma_1(\omega)$ which are introduced for the d-unoccupied state and for the d-occupied state, respectively.

The ground state energy and other physical quantities such as the d-electron number and spin- and charge-susceptibilities can be expressed in terms of $\Sigma_d$ and $\Sigma_1$. By solving the integral equations, these quantities are calculated numerically as a function of $D$ and $\Delta$, and also analytically in the limit of small values of $\Delta/D$, $D$ being the width of the conduction band.

§1. Introduction

Recently the asymmetric Anderson model\(^1\) has been discussed by several authors\(^2-8\) in connection with the valence fluctuating state of certain rare-earth compounds. In particular Krishna-murthy et al.\(^3\) calculated the temperature dependence of the spin susceptibility by using the numerical renormalization group technique, and Haldane\(^5\) argued the scaling properties of the model. Yosida and Sakurai\(^6\) recently discussed the general feature of the ground state on the basis of Anderson's orthogonality theorem.\(^9\) In this paper we perform more direct calculations for the ground state. We investigate the ground state in the case of strong d-electron correlation by the perturbation approach with respect to the s-d mixing integral which follows the approach developed by Yosida\(^10\) for the ground state of the s-d exchange model. The ground state energy is evaluated and it is given as an explicit function of the d-level, $E_d$, the width of the d-level, $\Delta$, the width of the conduction band, $D$, and the applied magnetic field, $H$. The physical quantities of the ground state such as the number of localized d-electrons, spin- and charge-susceptibilities are also evaluated.

The outline of this paper is as follows. In §2 the perturbation expansion for the ground state energy is performed. An expression for the energy is derived which includes exactly all terms up to the third dominant order in the perturbation
series for $E_a=0$. This expression is generalized for non-zero values of $E_a$ and $H$, and then it is transformed into coupled integral equations for two self-energies of $d$-unoccupied state and $d$-occupied state. In § 3 the equations are solved, and the ground state energy is calculated. The number of the $d$-electrons, the spin- and charge-susceptibilities are calculated in § 4. The specific heat is also discussed. Conclusion and discussion are given in § 5.

At the end of § 2 it is commented that the present approach reproduces correctly the leading terms of the known results for the case without electron interactions.

§ 2. Perturbation expansion with respect to the s-d mixing integral $V$

The Anderson Hamiltonian is written as:  

$$H = H_0 + H',$$

$$H_0 = \sum_{k,\sigma} \varepsilon_k a_k^{\dagger} a_k + E_d (n_{d\uparrow} + n_{d\downarrow}) + U n_{d\uparrow} n_{d\downarrow},$$

$$H' = V \sum_{k,\sigma} (a_k^{\dagger} d_{\sigma} + d_{\sigma}^{\dagger} a_k).$$

(2.1)

In this paper we confine our considerations to the case of infinite $U$. Then, in the perturbation method with respect to the s-d mixing integral $V$ which has been developed by Yosida\textsuperscript{10} for the ground state of the s-d exchange model, the wave function of the ground state is given as follows:

$$\psi = \psi_0 + \psi_1 + \psi_2,$$

$$\psi_0 = \{ \Gamma_0 + \sum_{1 \leq \sigma \leq \delta} \Gamma_{1,\sigma} a_{1\sigma}^{\dagger} + \sum_{1 \leq \sigma \leq \delta} \Gamma_{1,\sigma} a_{1\sigma}^{\dagger} a_{2\sigma} + \sum_{1 \leq \sigma \leq \delta} \Gamma_{1,\sigma} a_{1\sigma}^{\dagger} a_{2\sigma}^{\dagger} a_{3\sigma} a_{4\sigma}^{\dagger} + \cdots \} \psi_0,$$

$$\psi_1 = \{ \sum_{1 \leq \sigma \leq \delta} \Gamma_{1,\sigma} d_{\sigma}^{\dagger} a_{1\sigma} + \sum_{1 \leq \sigma \leq \delta} \Gamma_{1,\sigma} d_{\sigma}^{\dagger} a_{2\sigma}^{\dagger} a_{3\sigma} a_{4\sigma}^{\dagger} a_{5\sigma} + \cdots \} \psi_0,$$

$$\psi_2 = \{ \sum_{1 \leq \sigma \leq \delta} \Gamma_{1,\sigma} d_{\sigma}^{\dagger} a_{1\sigma}^{\dagger} a_{2\sigma} + \sum_{1 \leq \sigma \leq \delta} \Gamma_{1,\sigma} d_{\sigma}^{\dagger} a_{2\sigma}^{\dagger} a_{3\sigma} a_{4\sigma}^{\dagger} a_{5\sigma} + \cdots \} \psi_0,$$

(2.2)

where 1, 2 and 3 stand for wave numbers $k_1$, $k_2$ and $k_3$ for simplicity. The wave function $\psi_0$ represents the Fermi vacuum, $\psi_0$ the component of the ground state with unoccupied $d$-state, and $\psi_1(\psi_2)$ with $d$-state occupied by an electron with up (down) spin. The state with two $d$-electrons is excluded by infinite $U$.

The coefficient $\Gamma_{1,\sigma}$ denotes the amplitude of the state with excited $n$-electrons and $m$-holes (The suffixes which come before a semicolon denote excited electrons and those after a semicolon excited holes.), and $\Gamma_{1,\sigma,1\sigma,2\sigma}$ that of the $d$-occupied state with excited $(n-1)$ electrons and $m$ holes. This singlet wave
function (2·2) is analog of Yosida's wave function for the s-d exchange model, and its zeroth order approximate wave function in which only $\Gamma_0$ and $\Gamma_{d;1}$ are taken into account was discussed by Varma and Yafeel and recently by Yosida and Sakurai.

Inserting the wave function in the Schrödinger equation

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

we obtain a hierarchy of equations which connects the amplitudes $\Gamma_{d;1}$, $\Gamma_{d;2}$, $\Gamma_{d;1;1}$, $\Gamma_{1;2;1}$, $\Gamma_{1;2;2}$, ... with $\Gamma_0$. The first five equations of the hierarchy are written down below:

$$-E \cdot \Gamma_0 + V \sum_{\sigma} \Gamma_{d;1;\sigma} = 0 ,$$

$$\begin{align*}
(E_d - \varepsilon_1 - E) \Gamma_{d;1;\sigma} + & V \sum_{\sigma} \Gamma_{d;1;\sigma} = 0 , \\
(\varepsilon_1 - \varepsilon_2 - E) \Gamma_{1;2;1;\sigma} + V \sum_{\sigma} \Gamma_{1;2;1;\sigma} = 0 , \\
(E_d + \varepsilon_1 - \varepsilon_2 - E) \Gamma_{d;1;\sigma} + V \sum_{\sigma} \Gamma_{d;1;\sigma} = 0 , \\
(E_d + \varepsilon_1 - \varepsilon_2 - E) \Gamma_{d;1;2;3;\sigma} + V \sum_{\sigma} \Gamma_{d;1;2;3;\sigma} = 0 , \\
(E_d + \varepsilon_1 - \varepsilon_2 - E) \Gamma_{d;1;2;3;\sigma} + V \sum_{\sigma} \Gamma_{d;1;2;3;\sigma} = 0 .
\end{align*}$$

where $\sigma$ indicates the spin opposite to $\sigma$, and the coefficients with $[1, 2]$, etc., denote the antisymmetrized sum; $\Gamma_{d;1;2;3}$ means

$$\Gamma_{d;1;2;3} = \Gamma_{d;1;2;3}^{\text{d}} - \Gamma_{d;1;2;3}^{\text{d} \dagger} .$$

Expressing higher order amplitudes in terms of the lower order amplitudes by iterative procedure, we can finally express $\Gamma_0$, ... $\Gamma_{1;2;1}$ and $\Gamma_{d;1;2;3}$ in a power series in $V$ which includes $\Gamma_0$ alone. The equation determining $\Gamma_{d;1;\sigma}$ exactly up to the seventh order in $V$ is shown below.

$$\Gamma_{d;1}\left\{ E_d - \varepsilon_1 - E \right. \begin{array}{c}
- V^2 \sum_{\sigma} \frac{1}{\varepsilon_2 - \varepsilon_1 - E - 2V^2 \sum_{\sigma} 1} \\
\times \frac{1}{E_d + \varepsilon_1 - \varepsilon_2 - E - V^2 \sum_{\sigma} 1} \\
+ \frac{1}{E_d + \varepsilon_2 - \varepsilon_1 - E - V^2 \sum_{\sigma} 1} \\
\times \frac{1}{E_d + \varepsilon_4 - \varepsilon_1 - E} \\
\times \frac{1}{E_d + \varepsilon_3 - \varepsilon_1 - E} \end{array} \right\}$$
The iterative solution of this equation gives $T_d;_i$ in terms of $T_0$. Substituting this expression for $T_d;_i$ in Eq. (2.4a), we can obtain the secular equation for the ground state energy. In a power series in $V$ it is written down as follows:

$$-E = V^2 \sum_{i<j} \frac{1}{E_{dd} - \varepsilon_i - E} + V^4 \sum_{i<j} \frac{1}{(E_{dd} - \varepsilon_i - E)^2} \sum_{k} \frac{1}{\varepsilon_k - \varepsilon_i - E}$$

$$+ V^6 \sum_{i<j} \frac{1}{(E_{dd} - \varepsilon_i - E)^3} \left( \sum_{k} \frac{1}{\varepsilon_k - \varepsilon_i - E} \right)^2$$

$$+ V^6 \sum_{i<j} \frac{1}{(E_{dd} - \varepsilon_i - E)^2} \sum_{k} \frac{1}{\varepsilon_k - \varepsilon_i - E} \sum_{l} \frac{1}{E_{dd} + \varepsilon_k - \varepsilon_i - E}$$

$$- V^6 \sum_{i<j} \frac{1}{E_{dd} - \varepsilon_i - E} \sum_{k} \frac{1}{\varepsilon_k - \varepsilon_i - E} \sum_{l} \frac{1}{E_{dd} + \varepsilon_k - \varepsilon_i - E}$$

$$\times \frac{1}{E_{dd} - \varepsilon_i - E} + \cdots. \quad (2.7)$$

Here the spin suffix $\sigma$ is added to $E_d$ in order to indicate the origin of the factor 2 appearing in such an expression as Eq. (2.6), and we write down terms only up to the sixth order in $V$ for saving space.

Each term in Eq. (2.7) can be represented by a diagram which is depicted in Fig. 1. The $V^2$ term in Eq. (2.7) corresponds to (a), the $V^4$ term to (b), and the three $V^6$ terms to (c) ~ (e) in Fig. 1. Here the time direction is fixed, and the
dashed line represents the $d$-electron line. The solid lines represent a conduction electron line to the right and a hole line to the left, and dots represent the mixing integral $V$. The Pauli principle and the fact that $U$ is infinite prevent two dotted lines from running at the same time.

Replacing summations over $1(k_i)$ in Eq. (2.7) by integrations with the band energy $\varepsilon$ on the assumption of the constant density of states $\rho$ for $-D \leq \varepsilon \leq D$ ($\varepsilon$ is measured from the Fermi level), we can evaluate the contribution of each diagram to the ground state energy. The calculated results are given as follows:

\begin{align}
\text{(a)} &= 2 \frac{d}{\pi} \log \frac{D}{|E|}, \\
\text{(b)} &= 2 \cdot \left( \frac{d}{\pi} \right)^2 \frac{1}{|E|} \left( \log \frac{D}{|E|} - 1 \right), \\
\text{(c)} &= 2 \cdot \left( \frac{d}{\pi} \right)^3 \frac{1}{2E^2} \left( \log^2 \frac{D}{|E|} - \log \frac{D}{|E|} + \frac{1}{2} \right), \\
\text{(d)} &= 4 \cdot \left( \frac{d}{\pi} \right)^3 \frac{1}{2E^2} \left( \log \frac{D}{|E|} - \frac{3}{2} \right), \\
\text{(e)} &= -2 \cdot \left( \frac{d}{\pi} \right)^3 \frac{1}{E^2} \left( 3\zeta(3) - 2\zeta(2) \right),
\end{align}

where $\zeta(n)$ is Riemann's Zeta function, $d$ the energy width of the localized $d$-level given by $d=\pi\rho V^2$, and we have set $E_d=0$ to discuss the typical case of the asymmetric Anderson model. Each term consists of terms of the order of $|E| \cdot (d/\pi|E|)^n \cdot \log^{n-1} D/|E|$.

By the perturbation calculations up to the eighth order in $V$, we found that the most dominant contributions ($m=0$) appear only in the $V^2$ term ($n=1$) (We assume $d/\pi|E| \cdot \log D/|E|$ is of order unity for $d/D \ll 1$). The next dominant contribution ($m=1$) comes from the type of the diagrams shown in Fig. 2(a), whose examples are found in Fig. 1(b) and (c). The third dominant contribution ($m=2$) comes from the ones shown in Fig. 2(b) and (c). The diagrams with
any crossings of electron lines and/or of hole lines, the simplest example of which is the diagram 1(c), are less dominant ($m \geq 3$). On the other hand, the contributions from all the diagrams with no crossings can be collected in the infinite continued fraction of the form

$$-E = V_t \sum_{i,j} \frac{1}{\Delta_{ij} - \varepsilon_i - E - \varepsilon_j - \varepsilon_k} + \frac{1}{\Delta_{ij} - \varepsilon_i - E - \varepsilon_j - \varepsilon_k - \varepsilon_m} + \ldots$$

(2.9)

This is easily proved diagrammatically by comparison of terms appearing when this expression is expanded with respect to $V$ with terms in the perturbation series (2.7). This expression for $E$ is equivalent to neglect of all vertex corrections and self-energies in Eq. (2.6) for $t_{ij}$ except for the one appearing first.

All we do in the remaining part of this paper is to discuss Eq. (2.9) since it includes the perturbation terms exactly at least up to the third dominant order. It will be shown that the ground state energy derived by using this equation satisfies our assumption that $\Delta_i/\pi|E| \log D/|E|$ be of order unity ($\sim 1/2$).

The approach so far developed is valid also for $U = 0$. For this case up- and down-spin electrons are independent of each other, and we have only to consider electrons with the same spin. Then, the above-mentioned formulation works if we remove the sum with respect to the spin suffix: The ground state energy is given by Eq. (2.9) without the spin sum. It can be shown that the energy derived by following the approach developed in § 3 reproduces correctly the leading terms of the exact ground state energy for this case.

$\ast$ The variable $s$ appearing there is now defined by $g/f$. 

Fig. 2. (a) Next dominant diagram ($m = 1$) and (b), (c) third dominant diagrams ($m = 2$). Aside from simple electron-hole excitations appearing in (a), diagrams (b) and (c) have a single electron-hole excitation accompanied with any number of d-electron-hole excitations.
§ 3. The ground state energy

In this section we derive the ground state energy satisfying our basic equation (2.9). In the next section we will calculate the physical quantities of the ground state, such as the number of the d-electrons, the spin- and charge-susceptibilities. For this purpose we here include the magnetic field $H$ through the $\sigma$ dependence of $E_{ds}$:

$$E_{ds} = E_{ds} - \sigma \cdot H, \quad \sigma = \pm 1.$$  \hspace{1cm} (3.1)

We take the unit $\tilde{g} \mu_B/2 = 1$ where $\tilde{g}$ is the $g$-factor. The resulting ground state energy is given as a function of $D$, $J$, $E_d$ and $H$.

(1) The coupled integral equations

If we introduce the self-energies of d-occupied and d-unoccupied states, $\Sigma_1(\varepsilon)$ and $\Sigma_0(\varepsilon)$, defined by

$$\Sigma_1(\varepsilon) = -V^2 \sum_1 \frac{1}{\varepsilon_1 + \varepsilon + \Sigma_0(\varepsilon_1 + \varepsilon)},$$  \hspace{1cm} (3.2)

$$\Sigma_0(\varepsilon) = -V^2 \sum_\sigma \frac{1}{E_{ds} + \varepsilon - \varepsilon_1 + \Sigma_1(\varepsilon - \varepsilon_1)},$$  \hspace{1cm} (3.3)

Eq. (2.9) can be compactly written as

$$-E = -\Sigma_0(-E).$$  \hspace{1cm} (3.4)

The coupled integral equations, (3.2) and (3.3), can be transformed into the coupled differential equations. Replacing the summation over 1 in Eq. (3.2) by the integration with the band energy $\varepsilon_0$, we have

$$\Sigma_1(\varepsilon) = -\frac{d}{d\varepsilon} \int_0^\infty \frac{d\varepsilon_1}{\varepsilon_1 + \varepsilon + \Sigma_0(\varepsilon_1 + \varepsilon)} = -\frac{d}{d\varepsilon} \int_0^\infty \frac{d\varepsilon_1}{\varepsilon_1 + \Sigma_0(\varepsilon_1)}.$$  \hspace{1cm} (3.5)

Here we have replaced the upper bound of the integral, $D + \varepsilon$, by $D$ since such a replacement in the band edge gives no significant influence on the ground state energy. In the same way we have

$$\Sigma_0(\varepsilon) = -\frac{d}{d\varepsilon} \sum_{\varepsilon_0} \int_{E_{ds}}^\infty \frac{d\varepsilon_1}{E_{ds} + \varepsilon - \varepsilon_1 + \Sigma_1(\varepsilon - \varepsilon_1)} = -\frac{d}{d\varepsilon} \sum_{\varepsilon_0} \int_{E_{ds}}^\infty \frac{d\varepsilon_1}{E_{ds} + \varepsilon + \Sigma_1(\varepsilon_1)},$$  \hspace{1cm} (3.6)

where we have changed the sign of $\varepsilon$. Differentiation of $\Sigma_1$ and $\Sigma_0$ by $\varepsilon$ gives

$$\frac{d\Sigma_1(\varepsilon)}{d\varepsilon} = \partial \cdot \frac{1}{\varepsilon + \Sigma_0(\varepsilon)},$$  \hspace{1cm} (3.7)

$$\frac{d\Sigma_0}{d\varepsilon} = \partial \cdot \left\{ \frac{1}{E_d - H + \varepsilon + \Sigma_1(\varepsilon)} + \frac{1}{E_d + H + \varepsilon + \Sigma_1(\varepsilon)} \right\},$$  \hspace{1cm} (3.8)
where $\delta = D/\pi D$ and we have normalized all the energy variables by $D(\Sigma_0/D \rightarrow \Sigma_0, \Sigma_1/D \rightarrow \Sigma_1, \varepsilon/D \rightarrow \varepsilon, E_d/D \rightarrow E_d$ and $H/D \rightarrow H)$. Our task then is to solve these coupled differential equations with the boundary condition that

$$\Sigma_0 = \Sigma_1 = 0 \quad \text{at} \quad \varepsilon = 1. \quad (3.9)$$

(2) Solution of the equations

When we introduce two functions defined by

$$f(\varepsilon) = \varepsilon + \Sigma_0(\varepsilon), \quad (3.10)$$

$$g(\varepsilon) = \varepsilon + \Sigma_1(\varepsilon) + E_d, \quad (3.11)$$

Eqs. (3.7) and (3.8) are reduced to the coupled differential equations for $f$ and $g$:

$$\frac{df}{d\varepsilon} = 1 + \delta \left( \frac{1}{g - H} + \frac{1}{g + H} \right), \quad (3.12)$$

$$\frac{dg}{d\varepsilon} = 1 + \delta \cdot \frac{1}{f}. \quad (3.13)$$

Their boundary conditions (3.9) are written as

$$f(1) = 1, \quad g(1) = 1 + E_d, \quad (3.14)$$

and Eq. (3.4) becomes $f(-E) = 0$. From Eq. (3.12) and the boundary condition (3.14), we have

$$\varepsilon - 1 = \int^f_0 \frac{df}{1 + \delta \left( \frac{1}{g - H} + \frac{1}{g + H} \right)}. \quad (3.15)$$

Thus the ground state energy is given by

$$E = -2\delta \int^1_0 \frac{g}{g^2 - H^2 + 2\delta \cdot g} \, df. \quad (3.16)$$

The first integral of the coupled differential equations, (3.12) and (3.13), is obtained by eliminating $\varepsilon$ from them as

$$\frac{df}{dg} = \frac{1 + \delta \left( \frac{1}{g - H} + \frac{1}{g + H} \right)}{1 + \delta \cdot \frac{1}{f}.} \quad (3.17)$$

Integration of it yields
where the constant of the integration has been determined so as to satisfy the condition (3.14).

If we introduce an auxiliary variable defined by

\[ s = \sqrt{\frac{g^2 - H^2}{f}} , \]  

(3.19)

the two functions, \( f \) and \( g \), can be expressed by the variable \( s \): Eliminating \( g \) in Eq. (3.18) by (3.19), we have

\[ f = f_+ \quad 0 < f < f_1 \]

\[ = f_- \quad f_1 < f < 1 \]

\[ f_+ = \frac{1}{2} s^2 + \delta \cdot \log \left[ \frac{s^2}{(1 + E_d)^2 - H^2} \cdot e^{-E_d/\beta} \right] \]

\[ \pm \sqrt{\frac{1}{4} s^4 + \delta \cdot s^2 \cdot \log \left[ \frac{s^2}{(1 + E_d)^2 - H^2} \cdot e^{-E_d/\beta} \right] + H^2} , \]  

(3.20)

where \( f_1 \) is defined by

\[ f_1 = \frac{1}{2} s_1^2 + \delta \cdot \log \left[ \frac{s_1^2}{(1 + E_d)^2 - H^2} \cdot e^{-E_d/\beta} \right] \]  

(3.21)

with \( s_1 \), the minimum value of \( s \), determined by the equation

\[ \frac{1}{4} s_1^4 + \delta \cdot s_1^2 \cdot \log \left[ \frac{s_1^2}{(1 + E_d)^2 - H^2} \cdot e^{-E_d/\beta} \right] + H^2 = 0 . \]  

(3.22)

The function \( f = f(s) \) is schematically shown in Fig. 3, where the boundary values \( s_\pm \) of \( s \) are given by

\[ s_+ = \sqrt{(1 + E_d)^2 - H^2} , \]

\[ s_- = \sqrt{(1 + E_d)^2 - H^2} \cdot e^{\beta H \cdot |H|} . \]  

(3.23)

These values have been derived so as to satisfy the condition (3.14) and the condition that \( g = |H| \) for \( f = 0 \).

Fig. 3. A schematic figure of the function \( f = f(s) \).
Expressing all the variables in terms of \( s \) (\( g \) is given by \( \sqrt{H^2 + f \cdot s^2} \)), we can rewrite after some manipulations the expression (3.16) for the ground state energy by the integrals in the two intervals of \( s \) (\( s_1 < s < s_0, \mu = \pm \)). By changing the variable from \( s \) to \( y \) where \( s = s_1 \cdot (1 + y) \), the expression is finally given by

\[
E = E_d - |H| - 2\delta \sum_{\mu = \pm} \int_{s_1}^{s_{1,\mu}} dy \frac{1}{\sqrt{y^2 + 2y + \frac{8\delta}{s_1^2} \cdot \log(1 + y)} + \frac{4H^2}{s_1^4} \cdot \left( \frac{1}{(1 + y)^2} - 1 \right)},
\]

(3.24)

where use has been made of Eqs. (3.22) and (3.23).

This expression gives the ground state energy as an explicit function of \( E_d, H \) and \( \delta \). In the remaining part of this section we calculate the ground state energy for \( E_d = H = 0 \).

(3) The ground state energy

In the limit \( \delta \to 0 \) calculations are carried out analytically. When \( E_d = H = 0 \), \( s_1 \) defined by Eq. (3.22) is reduced to \( s_0 \) which satisfies the equation

\[
s_0^2 + 4\delta \cdot \log s_0^2 = 0.
\]

(3.25)

In the limit \( \delta \to 0 \) \( s_0^2 \) is given by

\[
s_0^2 = 4\delta \cdot \left( \log \frac{1}{\delta} - \log \log \frac{1}{\delta} - \log 4 + O \left( \frac{\log \log (1/\delta)}{\log (1/\delta)} \right) \right).
\]

(3.26)

The integral in Eq. (3.24) is evaluated as follows. We use the inequality that

\[
\int_{0}^{1/\delta} dy \frac{1}{\sqrt{y^2 + 2y + \alpha y}} < \int_{0}^{1/\delta} dy \frac{1}{\sqrt{y^2 + 2y + \alpha \log(1 + y)}} < \int_{0}^{1/\delta} dy \frac{1}{\sqrt{y^2 + 2y}}.
\]

(3.27)

where \( \alpha = 8\delta/s_0^2 \). The integrals appearing in both sides are calculated as

\[
\int_{0}^{1/\delta} dy \frac{1}{\sqrt{y^2 + 2y + \alpha y}} = \log \left( \frac{1}{s_0} + \frac{\alpha}{2} + \sqrt{\left( \frac{1}{s_0} + \frac{\alpha}{2} \right)^2 - (1 + \frac{\alpha}{2})^2} - \log \left( 1 + \frac{\alpha}{2} \right) \right)
\]

\[
= \log \left( \frac{2}{s_0} + O \left( \frac{1}{\log (1/\delta)} \right) \right),
\]

(3.28)

because \( 1/s_0 \) is much larger than 1 for \( \delta \to 0 \), and \( \alpha \sim 2/\log (1/\delta) \) is much smaller than 1. Since the leading term in Eq. (3.28) is independent of \( \alpha \), the integral in Eq. (3.24) is also given by Eq. (3.28). Hence the ground state energy is obtained as
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\[ E_{\text{g.s}} = -4\delta \log \frac{2}{\delta} + O\left(\frac{\delta}{\log(1/\delta)}\right) \]

\[ = -2\delta \left( \log \frac{1}{\delta} - \log \log \frac{1}{\delta} \right) + O\left(\frac{\delta \cdot \log(1/\delta)}{\log(1/\delta)}\right). \quad (3.29) \]

For moderately small values of \( \delta \) numerical calculations have been carried out by using Eq. (3.24) with \( E_d = H = 0 \). The solid line in Fig. 4 indicates the calculated value of the ground state energy divided by \( \delta \), and the dashed line the limiting expression \( E_{\text{g.s.}}/\delta \). The bars shown in the latter line for not too small values of \( \delta \) come from the last term of Eq. (3.29) whose coefficient is taken unity.

Fig. 4. The ground state energy divided by \( \delta(=10^{-x}) \). The abscissa is \( x = \log_{10}(1/\delta) \).

§ 4. The properties of the ground state

In this section we calculate the number of \( d \)-electrons, and the spin- and charge-susceptibilities for \( E_d = H = 0 \). The coefficient linear in temperature of the specific heat is also obtained. We discuss first the limit of \( \delta \to 0 \) where analytical calculations are possible. Numerical calculations are shown later.

1. The number of \( d \)-electrons in the limit \( \delta \to 0 \)

The number of \( d \)-electrons is given by the derivative of the ground state energy with respect to \( E_d \):

\[ \langle n_{d\delta} \rangle = \frac{1}{2} \cdot \frac{dE}{dE_d}, \quad (4.1) \]

since \( E_d \) is regarded as a variable conjugate to \( n_{d\delta} \). For the ground state energy we use Eq. (3.24). It can be shown that this corresponds to taking account of the perturbation series for \( n_{d\delta} \) up to the next dominant order exactly (The order is \( (A/\pi|E|)^n \cdot \log^{n-m}(D/|E|) \) with \( m = 1 \)).

The result of the differentiation with respect to \( E_d \) yields
\[ \langle n_{de} \rangle = \frac{1}{2} - \delta \sum_{\pi} \left\{ \frac{d}{dE_d} \log \frac{s_{\pi}}{s_1} \right\}_{E_d = H = 0}, \tag{4.2} \]

where we have used Eq. (3.25). The integral in Eq. (4.2) can be estimated as

\[ \int_0^{1/s_0} \frac{\log (1 + y)}{(y^2 + 2y + \alpha \log (1 + y))^{5/2}} dy, \tag{4.3} \]

for \( 1/s_0 \gg 1 \). The derivative \( d/dE_d (8\delta/s_0^5) \) is calculated as

\[ \frac{d}{dE_d} \left( \frac{8\delta}{s_0^5} \right)_{E_d = H = 0} = - \frac{32\delta}{s_0^2} + \frac{1}{2s_0^2} \frac{1}{s_0^4} + 4\delta \log \left( \frac{1}{\delta} \right) + O \left( \frac{1}{\log (1/\delta)} \right). \tag{4.4} \]

Thus the contribution from the last term in Eq. (4.2) to \( \langle n_{de} \rangle \) is of order \( 1/\log^2 (1/\delta) \).

By using Eqs. (3.22) and (3.23) the second term in Eq. (4.2) is calculated as

\[ \frac{d}{dE_d} \left( \log \frac{s_+}{s_1} \right)_{E_d = H = 0} = - \frac{2}{s_0^2} + \frac{8\delta}{s_0^5} + \ldots, \tag{4.5a} \]

\[ \frac{d}{dE_d} \left( \log \frac{s_-}{s_1} \right)_{E_d = H = 0} = \frac{1}{2s_0} + \frac{d}{dE_d} \left( \log \frac{s_+}{s_1} \right)_{E_d = H = 0}. \tag{4.5b} \]

The term \( 1/2s_0 \) appearing in the right-hand side of (4.5b) just cancels \( 1/2 \) appearing in Eq. (4.2), and \( \langle n_{de} \rangle \) is finally given by

\[ \langle n_{de} \rangle = \frac{4\delta}{s_0^2} + O \left( \frac{1}{\log^2 (1/\delta)} \right) = \frac{1}{\log (1/\delta)} + \log \log (1/\delta) + O \left( \frac{1}{\log^2 (1/\delta)} \right). \tag{4.6} \]

(2) The charge susceptibility

The charge susceptibility \( \chi_c \) is given by the second derivative of the energy (3.24) with respect to \( E_d, (-1) \cdot d^2 E/dE_d^2 \). It can be calculated in a way similar to that for \( \langle n_{de} \rangle \). Omitting the details, we show only the result.

\[ \chi_c = 4\delta \cdot \frac{d^2}{dE_d^2} \log \frac{s_+}{s_1} + O \left( \frac{1}{\delta \log^2 (1/\delta)} \right) \]

\[ = \frac{32\delta}{s_0^2} + O \left( \frac{1}{\delta \log^2 (1/\delta)} \right) \]

\[ = \frac{2}{\delta \log^2 (1/\delta)} \cdot \left( 1 + 2 \log \log (1/\delta) \right) + O \left( \frac{1}{\delta \log^2 (1/\delta)} \right). \tag{4.7} \]
(3) The spin susceptibility

The spin susceptibility $\gamma_s$ is given by the second derivative with respect to $H$. Up to the second order in $H$ the integral in Eq. (3.24) is written as

$$\int_0^{s} \frac{dy}{\sqrt{y^2+2y+(s+1)/(s-1)} \log(1+y)}$$

Both terms of Eq. (4.8) contribute to the spin susceptibility. The first term can be calculated in a way parallel to that for $\langle n_d \rangle$. We obtain

$$\frac{d^2}{dH^2} \int_0^{s} \frac{dy}{\sqrt{y^2+2y+(s+1)/(s-1)} \log(1+y)} = \frac{d^2}{dH^2} \log \frac{s+1}{s-1} + O\left(\frac{1}{s^2 \log^3(1/\delta)}\right) = \frac{4}{s^4} + O\left(\frac{1}{s^2 \log^3(1/\delta)}\right),$$

where we have used the facts that $s_+$ and $s_1$ are even functions of $H$, and that

$$\log \frac{s_+}{s_1} = \log \frac{s_+}{s_1} + \frac{1}{2\delta} (-|H|).$$

The integral appearing in the second term of Eq. (4.8) can be estimated as

$$\int_0^{1/s} \frac{dy}{\sqrt{y^2+2y+\alpha \log(1+y)}} = -1 + O(\alpha),$$

since

$$\int_0^{1/s} \frac{dy}{\sqrt{y^2+2y+\alpha \log(1+y)}} = -1 + \left(4 - \frac{3\alpha}{4}\right)\alpha + \cdots.$$

Thus, summing up contributions from Eqs. (4.9) and (4.11), we finally obtain $\gamma_s$ as

$$\gamma_s = \frac{32\delta}{s^4} + O\left(\frac{1}{s^2 \log^3(1/\delta)}\right),$$

which coincides with $\gamma_c$, Eq. (4.7). It is reasonable because the spin fluctuations equal to the charge fluctuations for vanishingly small number of $d$-electrons.

(4) The specific heat

There is a general relation proved in perturbation theory with respect to the electron interaction $U_{\parallel}=\beta$ that the $T$-linear coefficient $\gamma$ of the specific heat of the impurity is related to the spin susceptibility due to parallel spin correlations as
where we employ the usual definition for $\chi_{\eta \eta}$, and $k_B$ is the Boltzmann constant. Then, with the use of the general relation that\(^{10-13}\)

\[
\begin{align*}
\left( \frac{\bar{g}_B^2}{2} \right)^2 \cdot \chi_s / D &= \chi_{\eta \eta} - \chi_s, \\
\left( \frac{\bar{g}_B^2}{2} \right)^2 \cdot \chi_s / D &= \chi_{\eta \eta} + \chi_s,
\end{align*}
\]

(4·15)

$\gamma$ in our system is given by

\[
\gamma = \frac{2\pi k_B^2}{3} \cdot \frac{1}{4D} \cdot (\chi_s + \chi_c).
\]

(4·16)

(5) The case where $\delta$ is moderately small

Figures 5 and 6 show the quantities $n_{de}$, $\chi_s$ and $\chi_c$ calculated numerically for moderately small values of $\delta$. For the calculations we have used the following equations:

\[
\langle n_{de} \rangle = \delta \cdot \int_0^1 \frac{df}{(g+2\delta)(f+\delta)^2} + O(\delta),
\]

(4·17)

\[
\chi_s = 2\delta \cdot \int_0^1 \frac{gdf}{(g+2\delta)^2(f+\delta)^2} \cdot (1+2\delta)^2 + O(\delta^2),
\]

(4·18)

\[
\chi_c = 4\delta \cdot \int_0^1 \frac{df}{g} \cdot \frac{1}{(g+2\delta)^2} - \delta \cdot \frac{1-g^2}{g(g+2\delta)^2}.
\]

(4·19)

Expression (4·17) is obtained as follows. Using the relation (4·1) and Eq. (3·16), we have $(H=0)$

\[
\langle n_{de} \rangle = \delta \cdot \int_0^1 \frac{df}{(g+2\delta)^2} \cdot \frac{dg}{dE_d}.
\]

(4·20)

From Eq. (3·18) we have

\[
\frac{dg}{dE_d} \bigg|_{E_d=0} = \frac{g}{g+2\delta} \cdot (1-2\delta).
\]

(4·21)

Inserting Eq. (4·21) into Eq. (4·20) and using Eq. (3·17), we obtain

\[
\langle n_{de} \rangle = \delta \cdot (1+2\delta) \cdot \int_0^1 \frac{f}{(g+2\delta)^2(f+\delta)} df.
\]

(4·22)

By the partial integration it can be written down as

\[
\langle n_{de} \rangle = \delta \cdot (1+2\delta) \left\{ \frac{1}{g+2\delta} \cdot \frac{1}{f+\delta} \bigg|_{g=0}^{f=1} + \int_0^1 \frac{1}{g+2\delta} \cdot \frac{\delta}{(f+\delta)^2} df \right\},
\]

(4·23)
which gives the expression (4·17). Other expressions, (4·18) and (4·19), can be obtained similarly.

The quantities \( n_{d\tau}, \chi_s \) and \( \chi_c \) are calculated after expressing \( f \) and \( g \) in Eqs. (4·17) \( \sim \) (4·19) in terms of the variable \( s \), Eq. (3·19). In Figs. 5 and 6 the solid lines indicate these quantities, and the dashed lines indicate their limiting expressions, (4·6) and (4·7). The arrow in Fig. 5 indicates \( \langle n_{d\tau} \rangle = 1/4 \), whose value is taken for the case \( D = 0 \). The number \( \langle n_{d\tau} \rangle \) is always smaller than this value as was remarked by Yosida and Sakurai.\(^6\) (The wave function \( \psi \) consistent with our approximation leading to Eq. (2·9) satisfies Anderson’s compensation theorem on which the arguments of Ref. 6) are based. This will be reported elsewhere.\(^6\))

Table I shows the values of \( n_{d\tau}, \chi_s \) and \( \chi_c \) for very small values of \( \delta \). For these values of \( \delta \), we may expand \( \chi_s \) and \( \chi_c \) in terms of the small quantities \( n_{d\tau} \) as

\[
\chi_s = \frac{2}{\delta} \cdot (n_{d\tau}^2 + \alpha \cdot n_{d\tau}^3 + \cdots),
\]

\[
\chi_c = \frac{2}{\delta} \cdot (n_{d\tau}^2 + \beta \cdot n_{d\tau}^3 + \cdots),
\]

\((4·24)\)

\(^6\) The theorem states that there are no localized charge of conduction electrons for the constant density of states. We can calculate the charge and show that its magnitude is of order \( \delta \). As \( \delta \) is negligible compared with \( \log (1/\delta)^{-1} \), the theorem holds in our wave function.
where the coefficients, $\alpha$ and $\beta$, are shown in Table I. From this we guess that $\alpha=3$ and $\beta=-1$. For the zeroth order solution in which only $I_0$ and $I_{e1}$ are retained in Eq. (2.4), we have $\alpha=-\beta=2$. Quite recently Fukuyama and Sakurai investigated the ground state of the asymmetric Anderson model with $D=\infty$ but finite $U$ within the $T$-matrix (ladder) approximation. Their results for large $U$ region are very similar to ours if one interchanges their $U$ by our $D$. However, the expansion coefficients are different. They obtained $\alpha=-\beta=3$. At present we do not know which of these coefficients is correct.

§ 5. Conclusion and discussion

In this paper we have performed the perturbation expansion for the ground state energy in a power series of $V$ up to the eighth order in the case of infinite $U$. On the basis of the perturbation calculations, coupled integral equations have been derived which include for $E_d=0$ all the perturbation terms up to the third dominant order exactly and some of less dominant terms. By solving the equations which are generalized for arbitrary values of $E_d$ and $H$, we have given the expression for the ground state energy as an explicit function of $\delta$, $D$, $E_d$ and $H$.

The number of $d$-electrons, the spin- and charge-susceptibilities are evaluated explicitly in the case $E_d=0$. We have shown analytically that $n_{de}$ is given by $4\delta/s_0^2$ with $s_0^2$, Eq. (3.26), and tends to zero as $(\log 1/\delta)^{-1}$ in the limit $\delta=D/\pi D\to 0$. The two susceptibilities are equal, and tend to zero as $(\bar{g}\mu_b)^2/2.\pi/4.\gamma.\delta$. (Here we use the usual definition for the susceptibility. It is given by $(\bar{g}\mu_b/2)^2\chi/D$ with $\chi$ appearing up to § 4.) The ground state energy (3.29) is determined also by $\delta$ and $s_0^2$ only. If we identify $s_0^2/4=\delta(\log 1/\delta-\log 1/\delta + \cdots)$ as the energy of the effective $d$-level $E_d$ with the width $\delta\ll E_d$, these results are reproduced by the second order perturbation theory in $V$. That is, the $d$-level is effectively shifted upwards, leaving small $n_{de}\sim(\log 1/\delta)^{-1}$, and the valence mixing weakens. This $E_d$ seems to correspond to $T^*$ in Haldane's scaling argument. His $\alpha$ is given by our theory as $\alpha=4$. 

Table I. The values of $n_{de}$, $\bar{z}_i=(\delta/2)\chi_i$ and $\bar{z}_e=(\delta/2)\chi_e$ for small values of $\delta$.

<table>
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<tr>
<th>$\delta$</th>
<th>$10^{-10}$</th>
<th>$10^{-8}$</th>
<th>$10^{-5}$</th>
<th>$10^{-2}$</th>
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</thead>
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<tr>
<td>$n_{de}$</td>
<td>4.717$\times10^{-2}$</td>
<td>2.305$\times10^{-2}$</td>
<td>1.516$\times10^{-2}$</td>
<td>1.257$\times10^{-2}$</td>
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<tr>
<td>$\bar{z}_i$</td>
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<td>5.713$\times10^{-4}$</td>
<td>2.409$\times10^{-4}$</td>
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<tr>
<td>$\bar{z}_e$</td>
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<td>5.180$\times10^{-4}$</td>
<td>2.262$\times10^{-4}$</td>
<td>1.559$\times10^{-4}$</td>
</tr>
<tr>
<td>$\alpha$</td>
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<td>3.27</td>
<td>3.2</td>
<td>3.1</td>
</tr>
<tr>
<td>$\beta$</td>
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<td>-1.09</td>
<td>-1.0</td>
<td>-1.1</td>
</tr>
</tbody>
</table>
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References