

Perturbation Expansion for the Anderson Hamiltonian. III

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Thermodynamical quantities are expanded in perturbation series with respect to the Coulomb repulsion U for the Anderson Hamiltonian with electron-hole symmetry and their general terms of perturbation are investigated. By these processes the mutual relations among these quantities are discussed. It is confirmed that the thermodynamical quantities such as the specific heat and the scattering t -matrix are expressed in terms of two quantities; the even and odd parts of the susceptibility as far as low-lying excitations are concerned. These results are entirely consistent with the Nozières phenomenological Fermi liquid theory based on the s - d exchange model.

§ 1. Introduction

In the first paper^{1),*)} of this series, we presented a perturbation theoretical approach to the Anderson Hamiltonian²⁾ with electron-hole symmetry and showed that each term of the perturbation expansion for the thermodynamical quantities, in particular for the free energy, can be expressed by an imaginary time integral of the product of two antisymmetric determinants constructed by unperturbed local d -electron temperature Green's functions.

In the second paper by Yamada,³⁾ each term in the perturbation expansions for the specific heat, the susceptibility, the resistivity and the density-of-states for the localized d -state has been calculated up to fourth order. In the course of calculation it has been found that some general relations hold between thermodynamical quantities, in particular, the T -linear specific heat is proportional to the even part of the susceptibility. This finding immediately leads us to the result that the ratio of the susceptibility to the coefficient of the T -linear specific heat becomes twice as large in the s - d limit as the value in the case of no correlation.

This paper deals with further development along this line: Here, discussion is mainly concentrated on the general properties of the perturbation series for thermodynamical quantities in the Anderson model.

The basic Hamiltonian in this paper is the Anderson Hamiltonian with electron-hole symmetry ($E_d = -\frac{1}{2}U$), which is divided into two parts, the unperturbed part H_0 and the perturbation H' as follows:

*) This paper is referred to as I.

$$H = H_0 + H', \tag{1.1}$$

$$H_0 = \sum_k \epsilon_{k\sigma} a_{k\sigma}^\dagger a_{k\sigma} + V \sum_{k\sigma} (a_{k\sigma}^\dagger a_{d\sigma} + a_{d\sigma}^\dagger a_{k\sigma}) - \frac{1}{4}U, \tag{1.2}$$

$$H' = U(n_{d\uparrow} - \frac{1}{2})(n_{d\downarrow} - \frac{1}{2}), \tag{1.3}$$

where $a_{k\sigma}$ and $a_{d\sigma}$ are respectively the annihilation fermion operators for the conduction electron with wave vector k and spin σ and for the localized d -electron with spin σ . ϵ_k represents the kinetic energy of the conduction electrons, V the transfer energy between the conducting and local d -states and U the Coulomb repulsion between two d -electrons.

For this Hamiltonian, as shown in I, the free energy F can be expanded in the power series of U , except for the 1st U -linear term, as

$$F = - \sum_{n=2}^{\infty} (-1)^n \frac{U^n}{n!} \frac{1}{\beta} \int_0^\beta \dots \int_0^\beta d\tau_1 d\tau_2 \dots d\tau_n [D^n(1, 2, \dots, n)]_{\text{conn}}^2, \tag{1.4}$$

$$\beta = \frac{1}{kT}.$$

$D^n(1, \dots, n)$ is the n -row, n -column antisymmetric determinant,

$$D^n(1, \dots, n) = \begin{vmatrix} 0 & G_{12} & G_{13} & \dots & G_{1n} \\ G_{21} & & & & \vdots \\ \vdots & & & & \vdots \\ G_{n1} & G_{n2} & \dots & \dots & 0 \end{vmatrix} \tag{1.5}$$

and the element G_{ij} is the unperturbed d -electron temperature Green's function

$$G_{ij} = G(\tau_i - \tau_j) = - \langle T_\tau a_{d\sigma}(\tau_i) a_{d\sigma}^\dagger(\tau_j) \rangle_{\text{unperturbed}} = \frac{1}{\beta} \sum_n G(\omega_n) e^{-i\omega_n(\tau_i - \tau_j)}, \tag{1.6}$$

$$G(\omega_n) = \frac{1}{i(\omega_n + \Delta \operatorname{sgn} \omega_n)}, \quad \omega_n = \frac{\pi}{\beta} (2n + 1), \tag{1.7}$$

where Δ is the width of the virtual d -level and given by

$$\Delta = \pi\rho |V|^2, \tag{1.8}$$

ρ being the state density for the conduction electrons. Since the antisymmetric determinant identically vanishes for odd n , we can easily see from Eq. (1.4) that the free energy is expressed by an even power series of U , exclusive of the U -linear term included in the unperturbed part H_0 .

For our purpose of discussing the general properties of the thermodynamical quantities, the determinantal expressions of their perturbation series as (1.4) for the free energy are particularly convenient and such expressions are fully used in this paper.

§ 2. Dynamical susceptibility

The perturbation expansion for the static local susceptibility is given in our scheme as^{3), 4)}

$$\chi = \chi_{\text{even}} + \chi_{\text{odd}}, \quad (2.1)$$

$$\chi_{\text{even}} = \frac{(g\mu_B)^2}{2} \sum_{n=0}^{\infty} \frac{U^{2n}}{(2n)!} \frac{1}{\beta} \int_0^\beta \cdots \int_0^\beta d\tau_1 d\tau_2 \cdots d\tau_{2n+2} \\ \times [D^{2n+2}(1, 2, \dots, 2n+2) D^{2n}(1, 2, \dots, 2n)]_{\text{conn}}, \quad (2.2)$$

$$\chi_{\text{odd}} = \frac{(g\mu_B)^2}{2} \sum_{n=0}^{\infty} \frac{U^{2n+1}}{(2n+1)!} \frac{1}{\beta} \int_0^\beta \cdots \int_0^\beta d\tau_1 d\tau_2 \cdots d\tau_{2n+3} \\ \times [D^{2n+2}(1, 2, \dots, 2n+2) D^{2n+2}(2, 3, \dots, 2n+3)]_{\text{conn}}. \quad (2.3)$$

In this section, these expressions for the static susceptibilities are extended to the dynamical susceptibilities.

We consider a case in which a time-dependent local magnetic field with circular frequency ω is applied in the z -direction. The magnetic moment induced by this applied field is calculated by the time-dependent perturbation theory. The perturbation in this case is the Zeeman energy:

$$H_z = -\frac{g\mu_B}{2} (n_{d\uparrow} - n_{d\downarrow}) (H_\omega e^{i\omega t + \eta t} + H_\omega^* e^{-i\omega t + \eta t}) \quad (2.4)$$

and the induced moment M is given by

$$M = \chi_\omega H_\omega^* e^{-i\omega t + \eta t} + \chi_\omega^* H_\omega e^{i\omega t + \eta t}. \quad (2.5)$$

The dynamical susceptibility is calculated as

$$\chi_\omega = \left(\frac{g\mu_B}{2}\right)^2 Z^{-1} \sum_{n,n} e^{-\beta E_n} |A_{nm}|^2 \left\{ \frac{1}{\omega + \omega_{nm} + i\eta} + \frac{1}{-\omega + \omega_{nm} - i\eta} \right\}, \\ Z = \sum_m e^{-\beta E_m}, \quad \omega_{nm} = E_n - E_m, \\ A_{nm} = \langle n | n_{d\uparrow} - n_{d\downarrow} | m \rangle. \quad (2.6)$$

Here, if we put $\omega + i\eta \rightarrow i\omega_n$, we obtain the temperature expression for the dynamical susceptibility as

$$\chi(\omega_n) = \left(\frac{g\mu_B}{2}\right)^2 Z^{-1} \sum_m e^{-\beta E_m} (1 - e^{-\beta \omega_{nm}}) \frac{|A_{mn}|^2}{\omega_{nm} - i\omega_n}, \\ \omega_n = 2n \frac{\pi}{\beta}. \quad (2.7)$$

(2.7) can be rewritten in the following form:

$$\chi(\omega_n) = \left(\frac{g\mu_B}{2}\right)^2 \frac{1}{\beta} \int_0^\beta \int_0^\beta d\tau d\tau' e^{i\omega_n(\tau - \tau')} \langle T_\tau (n_{d\uparrow}(\tau) - n_{d\downarrow}(\tau)) (n_{d\uparrow}(\tau') - n_{d\downarrow}(\tau')) \rangle, \quad (2.8)$$

where $\langle\langle A \rangle\rangle$ denotes the thermal average of A

$$\langle\langle A \rangle\rangle = \frac{\sum_n e^{-\beta E_n} \langle m | A | m \rangle}{\sum_n e^{-\beta E_n}}$$

and

$$A(\tau) = e^{H\tau} A e^{-H\tau}.$$

(2.8) can be again rewritten as

$$\chi(\omega_n) = \frac{(g\mu_B)^2}{2} \frac{1}{\beta} \int_0^\beta \int_0^\beta d\tau d\tau' e^{i\omega_n(\tau-\tau')} [\langle\langle T_\tau n_{d\uparrow}(\tau) n_{d\uparrow}(\tau') \rangle\rangle - \langle\langle T_\tau n_{d\uparrow}(\tau) n_{d\downarrow}(\tau') \rangle\rangle]. \tag{2.9}$$

The integrand of (2.9) gives the time(imaginary)-dependent susceptibility $\chi(\tau-\tau')$, namely

$$\chi(\tau-\tau') = \chi_{\text{even}}(\tau-\tau') + \chi_{\text{odd}}(\tau-\tau'), \tag{2.10}$$

$$\chi_{\text{even}}(\tau-\tau') / \frac{(g\mu_B)^2}{2} = \chi'_{\text{even}}(\tau-\tau') = \langle\langle T_\tau n_{d\uparrow}(\tau) n_{d\uparrow}(\tau') \rangle\rangle, \tag{2.11}$$

$$\chi_{\text{odd}}(\tau-\tau') / \frac{(g\mu_B)^2}{2} = \chi'_{\text{odd}}(\tau-\tau') = -\langle\langle T_\tau n_{d\uparrow}(\tau) n_{d\downarrow}(\tau') \rangle\rangle. \tag{2.12}$$

The perturbation expansion of $\chi(\tau-\tau')$ is easily obtained in a way similar to the case for the free energy as

$$\chi'_{\text{even}}(\tau-\tau') = \sum_{n=0}^{\infty} \frac{U^{2n}}{(2n)!} \int_0^\beta \cdots \int_0^\beta d\tau_1 \cdots d\tau_{2n} [D^{2n+2}(\tau, 1, 2, \dots, 2n, \tau') \times D^{2n}(1, 2, \dots, 2n)]_{\text{conn}}, \tag{2.13}$$

$$\chi'_{\text{odd}}(\tau-\tau') = \sum_{n=0}^{\infty} \frac{U^{2n+1}}{(2n+1)!} \int_0^\beta \cdots \int_0^\beta d\tau_1 \cdots d\tau_{2n+1} [D^{2n+2}(\tau, 1, 2, \dots, 2n+1) \times D^{2n+2}(1, 2, \dots, 2n+1, \tau')]_{\text{conn}}. \tag{2.14}$$

Now, we expand the determinant D^{2n+2} by their cofactors as follows:

$$\begin{aligned} D^{2n+2}(\tau, 1, 2, \dots, 2n, \tau') &= \sum_{\substack{j'i, j'i' \\ \text{incl. } j=i, j'=i'}} G_{\tau i} G_{j\tau} G_{\tau' i'} G_{j'\tau'} \\ &\times D_{\tau i, j\tau, \tau' i', j'\tau'}^{2n+2} + \sum_{ji} \{G_{\tau\tau'} G_{j\tau} G_{\tau' i} D_{\tau\tau', j\tau, \tau' i}^{2n+2} \\ &+ G_{\tau i} G_{\tau' \tau} G_{j\tau'} D_{\tau i, i'\tau, j\tau'}^{2n+2}\} + G_{\tau\tau'} G_{\tau' \tau} D_{\tau\tau', \tau' \tau}^{2n+2} \\ &= \sum_{\substack{j'i, j'i' \\ \text{incl. } j=i, j'=i'}} G_{\tau i} G_{j\tau} G_{\tau' i'} G_{j'\tau'} D_{ji, j'i'}^{2n} \\ &+ 2 \sum_{ji} G_{\tau\tau'} G_{j\tau} G_{\tau' i} D_{ji}^{2n} - G_{\tau\tau'} G_{\tau' \tau} D^{2n}. \end{aligned} \tag{2.15}$$

On the right-hand side of the second equation, $D_{ji, j'i'}^{2n}$, etc., are the cofactors of the $2n$ -th order determinant constructed by G_{ij} , where $i, j=1, \dots, 2n$. By

using (2.15) in (2.13), its Fourier component can be written as

$$\begin{aligned} \chi'_{\text{even}}(\omega_n) = & -\frac{1}{\beta} \sum_{\omega_1} G(\omega_1) G(\omega_1 - \omega_n) \\ & + \sum_{n=1}^{\infty} \frac{U^{2n}}{(2n)!} \frac{1}{\beta} \int_0^\beta \cdots \int_0^\beta d\tau_1 \cdots d\tau_{2n} \left[\sum_{\substack{j_t, j'_t \\ \text{incl. } j=j', j'=j'}} \frac{1}{\beta} \sum_{\omega_1} G(\omega_1) \right. \\ & \times G(\omega_1 - \omega_n) e^{-i\omega_1(\tau_j - \tau_t) + i\omega_n \tau_j} \frac{1}{\beta} \sum_{\omega_2} G(\omega_2) G(\omega_2 + \omega_n) \\ & \times e^{-i\omega_2(\tau_{j'} - \tau_{t'}) - i\omega_n \tau_{j'}} D_{j_t j'_t}^{2n} D_{j'_t j_t}^{2n} \\ & \left. + 2 \sum_{j_t} \frac{1}{\beta} \sum_{\omega_1} G(\omega_1 + \omega_n) G^2(\omega_1) e^{-i\omega_1(\tau_j - \tau_t)} D_{j_t}^{2n} D_{j_t}^{2n} \right]_{\text{conn}}. \end{aligned} \quad (2.16)$$

Similarly, by the use of the relation

$$D^{2n+2}(\tau, 1, \dots, 2n+1) = - \sum_{\substack{j_t \\ \text{incl. } j=t}} G_{\tau t} G_{j\tau} D_{j_t}^{2n+1},$$

the Fourier component of (2.14) is obtained as

$$\begin{aligned} \chi'_{\text{odd}}(\omega_n) = & \sum_{n=0}^{\infty} \frac{U^{2n+1}}{(2n+1)!} \frac{1}{\beta} \int_0^\beta \cdots \int_0^\beta d\tau_1 \cdots d\tau_{2n+1} \\ & \times \left[\sum_{\substack{j_t \\ \text{incl. } j=t}} \frac{1}{\beta} \sum_{\omega_1} G(\omega_1) G(\omega_1 - \omega_n) e^{-i\omega_1(\tau_j - \tau_t)} \right. \\ & \times \sum_{\substack{j'_t \\ \text{incl. } j'=t'}} \frac{1}{\beta} \sum_{\omega_2} G(\omega_2) G(\omega_2 + \omega_n) e^{-i\omega_2(\tau_{j'} - \tau_{t'})} \\ & \left. \times e^{i\omega_n(\tau_j - \tau_{j'})} D_{j_t}^{2n+1} D_{j'_t}^{2n+1} \right]_{\text{conn}}. \end{aligned} \quad (2.17)$$

§ 3. Relation between the free energy and the dynamical susceptibility

The $2n$ -th order term of the free energy is, from (1.4), written as

$$F^{2n} = - \frac{U^{2n}}{(2n)!} \frac{1}{\beta} \int_0^\beta \cdots \int_0^\beta d\tau_1 \cdots d\tau_{2n} [D^{2n}(1, \dots, 2n)]_{\text{conn}}^2. \quad (3.1)$$

Here, we expand D^{2n} with respect to the elements of $2n$ -th row and $2n$ -th column as

$$D^{2n} = - \sum_{\substack{j_t \\ \text{incl. } t=j}} G_{2nt} G_{j2n} D_{j_t}^{2n-1} \quad (3.2)$$

and carry out the integration with respect to τ_{2n} . Then, (3.1) is written as

$$F^{2n} = - \frac{U^{2n}}{(2n)!} \frac{1}{\beta} \int_0^\beta \cdots \int_0^\beta d\tau_1 \cdots d\tau_{2n-1} \sum_{\substack{j_t j'_t \\ \text{incl. } j=t, j'=t'}} \dots$$

$$\begin{aligned} & \times \left[\frac{1}{\beta} \sum_{\omega_n} e^{i\omega_n(\tau_j - \tau_{j'})} \frac{1}{\beta} \sum_{\omega_1} G(\omega_1) G(\omega_1 - \omega_n) e^{-i\omega_1(\tau_j - \tau_i)} \right. \\ & \left. \times \frac{1}{\beta} \sum_{\omega_2} G(\omega_2) G(\omega_2 + \omega_n) e^{-i\omega_2(\tau_{j'} - \tau_{i'})} D_{j'i}^{2n-1} D_{j'j}^{2n-1} \right]_{\text{conn}}. \end{aligned} \quad (3.3)$$

Comparing this result with (2.17), we obtain the relation

$$F^{2n} = - \int_0^U dU \frac{1}{\beta} \sum_{\omega_n} \chi'_{\text{odd}}{}^{2n-1}(\omega_n) \quad (3.4)$$

or

$$F = - \int_0^U dU \frac{1}{\beta} \sum_{\omega_n} \chi'_{\text{odd}}(\omega_n). \quad (3.5)$$

This result can be derived indirectly by putting

$$\frac{1}{\beta} \sum_{\omega_n} \chi'_{\text{even}}{}^{2n}(\omega_n) = 0 \quad \text{for } n \neq 0 \quad (3.6)$$

in the well-known relation which generally holds between the free energy and the dynamical susceptibility. (3.6) can easily be proved in the expression for $\chi'_{\text{even}}(\omega_n)$ given by (2.16).

The ground state energy E_g is given in terms of $\chi_{\text{odd}}(\omega_n)$ at the absolute zero by

$$E_g = E_0 - \frac{U}{4} - \frac{1}{\pi} \int_0^U dU \int_0^\infty \chi'_{\text{odd}}(\omega) d\omega. \quad (3.7)$$

§ 4. Static susceptibility at $T=0$

The expressions for the static susceptibility, $\chi'_{\text{even}}(0)$ and $\chi'_{\text{odd}}(0)$, can be rewritten in a more compact form for $T=0$.

First we consider $\chi'_{\text{even}}{}^{2n}(\omega_n=0)$ and take out its integrand:

$$\begin{aligned} & \sum_{\text{incl. } j=i, j'=i'} \frac{1}{\beta} \sum_{\omega_1} G(\omega_1)^2 e^{-i\omega_1(\tau_j - \tau_i)} \frac{1}{\beta} \sum_{\omega_2} G(\omega_2)^2 \\ & \times e^{-i\omega_2(\tau_{j'} - \tau_{i'})} D_{j'i}^{2n} D_{j'j}^{2n} + 2 \sum_{j'i} \frac{1}{\beta} \sum_{\omega_1} G(\omega_1)^3 \\ & \times e^{-i\omega_1(\tau_j - \tau_i)} D_{j'i}^{2n} D^{2n}. \end{aligned} \quad (4.1)$$

At $T=0$, the sum over ω_n can be replaced by integration as

$$\frac{1}{\beta} \sum_{\omega_1} G(\omega_1) \rightarrow \frac{1}{2\pi} \int_{-\infty}^\infty G(\omega) d\omega.$$

By partial integration, we have

$$2\frac{1}{2\pi} \int G(\omega_1)^2 e^{-i\omega_1(\tau_j - \tau_i)} d\omega_1 = -\frac{1}{2\pi} \int G(\omega_1)^2 e^{-i\omega_1(\tau_j - \tau_i)} d\omega_1 (\tau_j - \tau_i). \quad (a)$$

By the cofactor expansion, we rewrite $(\tau_j - \tau_i) D_{ji}^{2n}$ as follows:

$$\begin{aligned} (\tau_j - \tau_i) D_{ji}^{2n} &= - \left[\sum_{j' \neq j} \tau_{j'} \sum_{i'} G_{j'i'} D_{ji'j'}^{2n} - \sum_{i' \neq i} \tau_{i'} \sum_{j'} G_{j'i'} D_{ji'j'}^{2n} \right] \\ &= - \sum_{\substack{j' \neq j \\ i' \neq i, j' \neq i'}} (\tau_{j'} - \tau_{i'}) G_{j'i'} D_{ji'j'}^{2n}. \end{aligned} \quad (b)$$

One more partial integration yields

$$\begin{aligned} (\tau_{j'} - \tau_{i'}) \frac{1}{2\pi} \int G(\omega) e^{-i\omega(\tau_{j'} - \tau_{i'})} d\omega \\ = -\frac{1}{\pi A} - \frac{1}{2\pi} \int G(\omega)^2 e^{-i\omega(\tau_{j'} - \tau_{i'})} d\omega. \end{aligned} \quad (c)$$

After the above three manipulations, the second term in (4.1) is rewritten as

$$\begin{aligned} &-\frac{1}{\pi A} \sum_{\substack{j \neq i, j' \neq i' \\ j \neq i, j' \neq i'}} \frac{1}{\beta} \sum_{\omega_1} G(\omega_1)^2 e^{-i\omega_1(\tau_j - \tau_i)} D_{ji'j'}^{2n} D^{2n} \\ &- \sum_{\substack{j \neq i, j' \neq i' \\ j \neq i, j' \neq i'}} \frac{1}{\beta} \sum_{\omega_1} G(\omega_1)^2 e^{-i\omega_1(\tau_j - \tau_i)} \\ &\quad \times \frac{1}{\beta} \sum_{\omega_2} G(\omega_2)^2 e^{-i\omega_2(\tau_{j'} - \tau_{i'})} D_{ji'j'}^{2n} D^{2n}. \end{aligned}$$

The second term is cancelled out with the $j \neq i$ and $j' \neq i'$ terms of the first term of (4.1). Thus, the following terms survive in (4.1):

$$\begin{aligned} &\left(\frac{1}{\pi A}\right)^2 \sum_{jj'} D_{jjj'j'}^{2n} D^{2n} \\ &- 2\frac{1}{\pi A} \sum_{\substack{j \neq i, j' \neq i' \\ j \neq i, j' \neq i'}} \frac{1}{\beta} \sum_{\omega} G(\omega)^2 e^{-i\omega(\tau_{j'} - \tau_{i'})} D_{jjj'j'}^{2n} D^{2n} \\ &- \frac{1}{\pi A} \sum_{\substack{j \neq i, j' \neq i' \\ j \neq i, j' \neq i'}} \frac{1}{\beta} \sum_{\omega} G(\omega)^2 e^{-i\omega(\tau_j - \tau_i)} D_{jjj'j'}^{2n} D^{2n}. \end{aligned} \quad (4.2)$$

By the reversed processes of (c) and (b),

$$\frac{1}{2\pi} \int G(\omega)^2 e^{-i\omega(\tau_{j'} - \tau_{i'})} d\omega = -\frac{1}{\pi A} - (\tau_{j'} - \tau_{i'}) G_{j'i'}, \quad (c')$$

$$\sum_{i'} (\tau_{j'} - \tau_{i'}) G_{j'i'} D_{ji'j'}^{2n} = -(\tau_j - \tau_i) D_{ji}^{2n}, \quad (b')$$

(4.2) becomes

$$\left(\frac{1}{\pi A}\right)^2 \left[\sum_{jj'} D_{jjj'j'}^{2n} + 2 \sum_{\substack{j \neq i \\ j' \neq i'}} D_{jjj'j'}^{2n} + \sum_{\substack{j \neq i, j' \neq i'}} D_{ji'j'}^{2n} \right] D^{2n}$$

$$-\frac{1}{\pi A} \sum_{ji} (\tau_j - \tau_i) D_{ji}^{2n} D^{2n}. \tag{4.3}$$

If we notice the relations

$$\begin{aligned} D_{jii}^n &= -D_{jjj}^n, & D_{jij'j}^n &= -D_{jjj'i}^n, \\ D_{jij'i}^n &= -D_{j'j'i}^n, \end{aligned} \tag{4.4}$$

we see that the quantities in the square brackets are cancelled out and we finally obtain

$$\begin{aligned} \chi'_{\text{even}} &= \chi'_{\text{even}}{}^0 - \frac{1}{\pi A} \lim_{\beta \rightarrow \infty} \sum_{n=1}^{\infty} \frac{U^{2n}}{(2n)!} \frac{1}{\beta} \int_0^\beta \dots \int_0^\beta d\tau_1 d\tau_2 \dots d\tau_{2n} \\ &\times \sum_{ji} [(\tau_j - \tau_i) D_{ji}^{2n} D^{2n}]_{\text{conn}}. \end{aligned} \tag{4.5}$$

By similar but simpler manipulations, the odd part of the static susceptibility χ'_{odd} at $T=0$ can be written in the following compact form:

$$\begin{aligned} \chi'_{\text{odd}} &= \frac{1}{(\pi A)^2} \lim_{\beta \rightarrow \infty} \sum_{n=0}^{\infty} \frac{U^{2n+1}}{(2n+1)!} \frac{1}{\beta} \int_0^\beta \int_0^\beta d\tau_1 \dots d\tau_{2n+1} \\ &\times \left[\sum_{\substack{ji \\ \text{incl. } j=i}} D_{ji}^{2n+1} \right]_{\text{conn}}. \end{aligned} \tag{4.6}$$

§ 5. T^2 -part of the free energy

The free energy of $2n$ -th order is given by

$$F^{2n} = -\frac{U^{2n}}{(2n)!} \frac{1}{\beta} \int_0^\beta \int_0^\beta d\tau_1 \dots d\tau_{2n} [D^{2n}]_{\text{conn}},$$

where temperature dependence arises from the d -electron Green's function,

$$\begin{aligned} G_{ji} &= \frac{1}{\beta} \sum_n G(\omega_n) e^{-i\omega_n(\tau_j - \tau_i)}, \\ \omega_n &= (2n+1) \frac{\pi}{\beta}. \end{aligned}$$

Now, we consider a function $F(\omega)$ which has a singularity at $\omega=0$, just as $G(\omega)$. Then, a discrete sum of $F(\omega_n)$ with respect to n can be expanded in a series of T^{2n} as

$$\begin{aligned} \frac{2\pi}{\beta} \sum_{\omega_n} F(\omega_n) &= \int_{-\infty}^{\infty} F(\omega) d\omega - \frac{1}{6} \left(\frac{\pi}{\beta}\right)^2 [F'(0-) - F'(0+)] \\ &+ \frac{7}{360} \left(\frac{\pi}{\beta}\right)^4 [F'''(0-) - F'''(0+)] - \dots. \end{aligned} \tag{5.1}$$

Using this relation, we have

$$G_{ji} = \frac{1}{2\pi} \int G(\omega) e^{-i\omega(\tau_j - \tau_i)} d\omega - \frac{1}{6} \left(\frac{\pi}{\beta}\right)^2 \frac{1}{\pi\Delta} (\tau_j - \tau_i) + \frac{7}{360} \left(\frac{\pi}{\beta}\right)^4 \frac{1}{\pi\Delta} \left(\frac{6}{\Delta^2} (\tau_j - \tau_i) - (\tau_j - \tau_i)^3\right) + \dots \quad (5.2)$$

If we use the relation (5.2), it is an easy task to take out the T^2 -part from F^{2n} . The result is obtained as

$$\Delta^{(2)} F^{2n} = \frac{1}{3} \left(\frac{\pi}{\beta}\right)^2 \frac{1}{\pi\Delta} \frac{U^{2n}}{(2n)!} \lim_{\beta \rightarrow \infty} \frac{1}{\beta} \int_0^\beta \dots \int_0^\beta d\tau_1 \dots d\tau_{2n} \times \sum_{ji} [(\tau_j - \tau_i) D_{ji}^{2n} D^{2n}]_{\text{conn}}. \quad (5.3)$$

From this result, we obtain the coefficient of the T -linear specific heat γ as

$$\gamma^{2n} = -\frac{2}{3} (\pi k)^2 \frac{1}{\pi\Delta} \frac{U^{2n}}{(2n)!} \lim_{\beta \rightarrow \infty} \frac{1}{\beta} \int_0^\beta \dots \int_0^\beta d\tau_1 \dots d\tau_{2n} \times \sum_{ji} [(\tau_j - \tau_i) D_{ji}^{2n} D^{2n}]_{\text{conn}}. \quad (5.4)$$

Comparing (5.4) with (4.5), we are led immediately to

$$\chi'_{\text{even}} = \left[\frac{2}{3} (\pi k)^2 \right]^{-1} \gamma^{2n}. \quad (5.5)$$

By noting that

$$\chi^{0'} = \frac{1}{\pi\Delta}, \quad \gamma^0 = \frac{2}{3} (\pi k)^2 \frac{1}{\pi\Delta}, \quad (5.6)$$

an important relation for the Anderson Hamiltonian is derived:

$$\chi'_{\text{even}} = \gamma / \frac{2}{3} (\pi k)^2. \quad (5.7)$$

It is more convenient to define dimensionless quantities, $\tilde{\chi}$ and $\tilde{\gamma}$, for later use by

$$\chi' = \frac{1}{\pi\Delta} \tilde{\chi}, \quad \gamma = \frac{2}{3} (\pi k)^2 \frac{1}{\pi\Delta} \tilde{\gamma}. \quad (5.8)$$

Another proof by the diagram method of this relation was presented in II, where it was shown that this relation immediately leads to the result that the ratio

$$\frac{\tilde{\chi}}{\tilde{\gamma}} = 1 + \frac{\tilde{\chi}_{\text{odd}}}{\tilde{\chi}_{\text{even}}} \quad (5.9)$$

tends to 2 in the limit of large U , namely in the s - d limit. Thus, we can see that $\tilde{\chi}_{\text{odd}}$ represents the many-body effect for the Anderson Hamiltonian.

The procedures used in this and the preceding sections enable us also to obtain the T^4 -part of the free energy and the T^2 -part of the static susceptibility.

Here, we write down only the obtained results.

$$\begin{aligned}
 \Delta^{(4)} F^{2n} &= -\frac{1}{18} (\pi k)^4 \frac{1}{(\pi \Delta)^2} \frac{U^{2n}}{(2n)!} \lim_{\beta \rightarrow \infty} \frac{1}{\beta} \int_0^\beta \cdots \int_0^\beta d\tau_1 \cdots d\tau_{2n} \\
 &\quad \times \left[\sum_{j_i j'_i} (\tau_j - \tau_i) (\tau_{j'} - \tau_{i'}) D_{j_i j'_i}^{2n} D^{2n} \right. \\
 &\quad + \frac{7}{10} \pi \Delta \sum_{j_i} \left\{ \frac{6}{\Delta^2} (\tau_j - \tau_i) - (\tau_j - \tau_i)^3 \right\} D_{j_i}^{2n} D^{2n} \\
 &\quad \left. + \frac{1}{2} \sum_{j_i} (\tau_j - \tau_i) D_{j_i}^{2n} \sum_{j'_i} (\tau_{j'} - \tau_{i'}) D_{j'_i}^{2n} \right]_{\text{conn}}, \\
 \Delta^{(4)} F^{\circ} &= +\frac{7}{90} (\pi k)^4 \frac{1}{\pi \Delta} \frac{1}{\Delta^2}, \tag{5.10}
 \end{aligned}$$

$$\begin{aligned}
 \Delta^{(2)} \chi'_{\text{even}}{}^{2n} &= \frac{1}{6} (\pi k)^2 \left(\frac{1}{\pi \Delta} \right)^2 \frac{U^{2n}}{(2n)!} \lim_{\beta \rightarrow \infty} \frac{1}{\beta} \int_0^\beta \cdots \int_0^\beta d\tau_1 \cdots d\tau_{2n} \\
 &\quad \times \left[\sum_{j_i j'_i} (\tau_j - \tau_i) (\tau_{j'} - \tau_{i'}) D_{j_i j'_i}^{2n} D^{2n} \right. \\
 &\quad + \pi \Delta \sum_{j_i} \left\{ \frac{6}{\Delta^2} (\tau_j - \tau_i) - (\tau_j - \tau_i)^3 \right\} D_{j_i}^{2n} D^{2n} \\
 &\quad + 2 \sum_{\substack{j_i j'_i \\ \text{incl. } j'=i'}} (\tau_j - \tau_i)^2 D_{j_i j'_i}^{2n} D^{2n} \\
 &\quad \left. + \sum_{j_i} (\tau_j - \tau_i) D_{j_i}^{2n} \sum_{j'_i} (\tau_{j'} - \tau_{i'}) D_{j'_i}^{2n} \right]_{\text{conn}}, \\
 \Delta^{(2)} \chi'_{\text{even}}{}^{\circ} &= \frac{1}{6} (\pi k)^2 \frac{1}{(\pi \Delta)^2} \frac{\pi}{\Delta}, \tag{5.11}
 \end{aligned}$$

$$\begin{aligned}
 \Delta^{(2)} \chi'_{\text{odd}}{}^{2n+1} &= -\frac{2}{3} (\pi k)^2 \left(\frac{1}{\pi \Delta} \right)^2 \frac{U^{2n+1}}{(2n+1)!} \lim_{\beta \rightarrow \infty} \frac{1}{\beta} \int_0^\beta \cdots \int_0^\beta d\tau_1 \cdots d\tau_{2n+1} \\
 &\quad \times \left[\frac{1}{\Delta^2} \sum_{\substack{j_i \\ \text{incl. } j=i}} D_{j_i}^{2n+1} \sum_{\substack{j'_i \\ \text{incl. } j'=i'}} D_{j'_i}^{2n+1} \right. \\
 &\quad + \frac{1}{2} \frac{1}{(\pi \Delta)} \sum_{\substack{j_i j'_i \\ \text{incl. } j=i}} (\tau_{j'} - \tau_{i'}) D_{j_i j'_i}^{2n+1} \\
 &\quad \left. \times \sum_{\substack{j'_i \\ \text{incl. } j'=i'}} D_{j'_i}^{2n+1} \right]_{\text{conn}}. \tag{5.12}
 \end{aligned}$$

§ 6. Scattering *t*-matrix

The electrical conductivity σ of the system described by the Anderson Hamiltonian is calculated by the following expression:

$$\sigma = -\frac{2e^2}{3} \int \tau_k(\omega) v_k^2 \frac{df}{d\varepsilon_k} \rho d\varepsilon_k \tag{6.1}$$

and

$$\frac{1}{\tau_k(\omega)} = -2c \operatorname{Im} t_{kk}(\omega). \quad (6.2)$$

t -matrix is obtained from the retarded Green's function as

$$t_{kk}(\omega) = V_{kd} G_{d\sigma}^R(\omega) V_{dk} = \frac{1}{\pi\rho} \frac{A}{(\omega - R) + i(\Delta - I)}, \quad (6.3)$$

where $R(\omega)$ and $I(\omega)$ are, respectively, the real and imaginary parts of the self-energy

$$\Sigma^R(\omega) = R(\omega) + iI(\omega). \quad (6.4)$$

Therefore, the following relation holds between t -matrix and the retarded self-energy of the local d -electron:

$$1 - 2\pi i \rho t_{kk} = \frac{\omega - R - i(\Delta + I)}{\omega - R + i(\Delta - I)} = \left[\frac{\Delta^2 + \{(\omega - R)^2 + 2\Delta I + I^2\}}{\Delta^2 + \{(\omega - R)^2 - 2\Delta I + I^2\}} \right]^{1/2} e^{-2i\delta}. \quad (6.5)$$

Since, as will be seen later, $\Sigma^R(0) = 0$ and $R \propto \omega$, $I \propto \omega^2$, T^2 , (6.5) is written down for low frequency and low temperatures as

$$1 - 2\pi i \rho t_{kk}(\omega) = \left[1 + \frac{4I}{\Delta} \right]^{1/2} e^{-2i\delta},$$

$$\delta(\omega) = \frac{\pi}{2} - \frac{\omega - R}{\Delta}. \quad (6.6)$$

The imaginary part of the phase shift $\delta' = I/\Delta$ represents contributions from inelastic channels. In the low-energy and low-temperature regions, the inelastic channel is dominated by two-particle scattering. The transition rate for this type of inelastic scattering is calculated by Nozières.⁵⁾ If we here use his result in our case, we have

$$\frac{4I}{\Delta} = -2\pi^2 \rho^4 (\pi^2 T^2 + \omega^2) \left[|A_{\uparrow\downarrow}|^2 + \frac{1}{2} |A_{\uparrow\uparrow}|^2 \right], \quad (6.7)$$

where $A_{\uparrow\downarrow}$ and $A_{\uparrow\uparrow}$ are the notations employed by Nozières⁵⁾ and represent the transition amplitudes with which two electrons in the states of $k_{1\uparrow}$ and $k_{2\downarrow}$, or $k_{1\uparrow}$ and $k_{2\uparrow}$ on the Fermi surface are, respectively, scattered to the states of $k_{3\downarrow}$ and $k_{4\uparrow}$, or $k_{3\uparrow}$ and $k_{4\uparrow}$ on the Fermi surface.

On the other hand, the self-energy $\Sigma(\omega)$ can be directly calculated from the improper self-energy $\Sigma'(\omega)$ which is in the following relation to the proper one $\Sigma(\omega)$:

$$\Sigma'(\omega) = \frac{\Sigma(\omega)}{1 - \Sigma(\omega)G(\omega)} = R'(\omega) + iI'(\omega), \quad (6.8)$$

namely, $R'(\omega) = R(\omega) + \dots$, $I'(\omega) = I(\omega) - (1/\Delta)R^2(\omega) + \dots$.

The perturbed Green's function $G^p(\tau - \tau')$

$$G^p(\tau - \tau') = -\langle\langle T_{\tau} a_{d\sigma}(\tau) a_{d\sigma}^\dagger(\tau') \rangle\rangle$$

is expanded in a power series of U as

$$G^p(\tau - \tau') = G_{\tau\tau'} + \sum_{n=1}^{\infty} \frac{U^{2n}}{(2n)!} \int_0^\beta \dots \int_0^\beta d\tau_1 \dots d\tau_{2n} \times [D^{2n+1}(\tau, \tau'; 1, 2, \dots, 2n) D^{2n}(1, \dots, 2n)]_{\text{conn}}. \quad (6.9)$$

Therefore, its Fourier component is given by

$$G^p(\omega_n) = G(\omega_n) - \sum_{n=1}^{\infty} \frac{U^{2n}}{(2n)!} \frac{1}{\beta} \int_0^\beta \dots \int_0^\beta e^{i\omega_n(\tau - \tau')} \times d\tau d\tau' d\tau_1 \dots d\tau_{2n} [\sum_{ji} G_{\tau i} G_{j\tau} D_{ji}^{2n}(1, \dots, 2n) D^{2n}]_{\text{conn}}. \quad (6.10)$$

Noting the relation

$$G^p(\omega_n) = G(\omega_n) + G(\omega_n) \Sigma'(\omega_n) G(\omega_n), \quad (6.11)$$

we obtain the improper self-energy as

$$\Sigma'(\omega_n) = -\sum_{n=1}^{\infty} \frac{U^{2n}}{(2n)!} \frac{1}{\beta} \int_0^\beta \dots \int_0^\beta d\tau_1 \dots d\tau_{2n} \times [\sum_{ji} e^{-i\omega_n(\tau_j - \tau_i)} D_{ji}^{2n} D^{2n}]_{\text{conn}}. \quad (6.12)$$

From (6.12), we can see $\Sigma'(\omega \rightarrow 0) = 0$ because $D_{ji}^{2n} = -D_{ij}^{2n}$. The first-order term with respect to ω_n is given by

$$A^{(1)} \Sigma'(\omega_n) = i\omega_n \sum_{n=1}^{\infty} \frac{U^{2n}}{(2n)!} \frac{1}{\beta} \int_0^\beta \dots \int_0^\beta d\tau_1 \dots d\tau_{2n} \times \sum_{ji} [(\tau_j - \tau_i) D_{ji}^{2n} D^{2n}]_{\text{conn}}. \quad (6.13)$$

Comparing this with χ'_{even} given by (4.5), we obtain

$$A^{(1)} \Sigma'(\omega_n) = -i\omega_n (\tilde{\chi}_{\text{even}} - 1) \quad (6.14)$$

and replacing ω_n by $-i\omega$, we obtain

$$R'(\omega) = R(\omega) = -\omega (\tilde{\chi}_{\text{even}} - 1) \quad (6.15)$$

or

$$\omega - R(\omega) = \omega \tilde{\chi}_{\text{even}}. \quad (6.16)$$

As for $I(\omega)$, we pursue an indirect way without obtaining it directly from $\Sigma'(\omega_n)$. We first calculate inelastic scattering amplitudes $A_{\uparrow\downarrow}$ and $A_{\uparrow\uparrow}$. In order to get them, we have to calculate the two-particle Green's functions

$$G^{\text{II}}(k_1\sigma\nu_1, k_2\sigma'\nu_2; k_3\sigma'\nu_3, k_4\sigma\nu_4)$$

$$\begin{aligned}
 &= \int_0^\beta \cdots \int_0^\beta ds_1 ds_2 ds_3 ds_4 e^{i\nu_1 s_1 + i\nu_2 s_2 - i\nu_3 s_3 - i\nu_4 s_4} \\
 &\quad \times \langle\langle T_\tau a_{k_1\sigma}(s_1) a_{k_2\sigma'}(s_2) a_{k_3\sigma'}^\dagger(s_3) a_{k_4\sigma}^\dagger(s_4) \rangle\rangle. \tag{6.17}
 \end{aligned}$$

First we calculate the Green's function for $\sigma = \uparrow$ and $\sigma' = \downarrow$. This can be done in the following way:

$$\begin{aligned}
 &G^{\text{II}}(k_1\nu_1\uparrow, k_2\nu_2\downarrow; k_3\nu_3\downarrow, k_4\nu_4\uparrow) \\
 &= \int_0^\beta \cdots \int_0^\beta ds_1 ds_2 ds_3 ds_4 e^{i\nu_1 s_1 + i\nu_2 s_2 - i\nu_3 s_3 - i\nu_4 s_4} \\
 &\quad \times \sum_{n=0}^\infty (-1)^n \frac{U^n}{n!} \int_0^\beta \cdots \int_0^\beta d\tau_1 \cdots d\tau_n [D^{n+1}(s_1 s_4; 1, 2, \dots, n) \\
 &\quad \times D^{n+1}(s_2 s_3; 1, 2, \dots, n)]_{\text{conn}}, \tag{6.18}
 \end{aligned}$$

where

$$\begin{aligned}
 &D^{n+1}(s_1 s_4; 1, 2, \dots, n) \\
 &= \begin{vmatrix} G_{k_1 k_4}(s_1 - s_4) & G_{k_1 a}(s_1 - \tau_1) & G_{k_1 a}(s_1 - \tau_2) & \cdots & G_{k_1 a}(s_1 - \tau_n) \\ G_{a k_4}(\tau_1 - s_4) & 0 & G_{12} \cdots \cdots \cdots & \cdots & G_{1n} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ G_{a k_4}(\tau_n - s_4) & G_{n1} \cdots \cdots \cdots & \cdots & \cdots & 0 \end{vmatrix}.
 \end{aligned}$$

Expanding $D^{n+1}(s_1 s_4; 1, 2, \dots, n)$ with respect to the first row and column and carrying out the integration over s_i , we obtain

$$\begin{aligned}
 &G^{\text{II}}(k_1\nu_1\uparrow, k_2\nu_2\downarrow; k_3\nu_3\downarrow, k_4\nu_4\uparrow) \\
 &= \beta [\beta G_{k_1 k_4}(\nu_1) G_{k_2 k_3}(\nu_2) \delta_{\nu_1 \nu_4} \delta_{\nu_2 \nu_3} \\
 &\quad + \sum_{n=1}^\infty (-1)^n \frac{U^n}{n!} \frac{1}{\beta} \int_0^\beta \cdots \int_0^\beta d\tau_1 \cdots d\tau_n \{ \sum_{j_i} G_{k_1 a}(\nu_1) G_{a k_4}(\nu_4) \\
 &\quad \times e^{-i\nu_4 \tau_j + i\nu_1 \tau_i} D_{j_i}^n \sum_{j'_i} G_{k_2 a}(\nu_2) G_{a k_3}(\nu_3) \\
 &\quad \times e^{-i\nu_3 \tau_{j'} + i\nu_2 \tau'_i} D_{j'_i}^n \}_{\text{conn}}]. \tag{6.19}
 \end{aligned}$$

By the use of the relations

$$\begin{aligned}
 &G_{k k'}(\nu) = V^2 G(\nu) G_k^\circ(\nu) G_{k'}^\circ(\nu), \\
 &G_{a k}(\nu) = V G(\nu) G_k^\circ(\nu), \tag{6.20}
 \end{aligned}$$

where $G_k^\circ(\nu)$ is the free electron Green's function in the absence of the s - d mixing, (6.19) can be calculated as

$$\begin{aligned}
 (6.19) &= \beta G_{k_1}^\circ(\nu_1) G_{k_2}^\circ(\nu_2) G_{k_3}^\circ(\nu_3) G_{k_4}^\circ(\nu_4) \{ \beta V^4 G(\nu_1) G(\nu_2) \delta_{\nu_1 \nu_4} \delta_{\nu_2 \nu_3} \\
 &\quad + V^4 G(\nu_1) G(\nu_2) G(\nu_3) G(\nu_4) \\
 &\quad \times \sum_{n=1}^\infty \frac{(-1)^n}{n!} U^n \frac{1}{\beta} \int_0^\beta \cdots \int_0^\beta d\tau_1 \cdots d\tau_n [\sum_{\text{incl. } j=i}^{j'_i} e^{-i\nu_4 \tau_j + i\nu_1 \tau_i}
 \end{aligned}$$

$$\times D_{jt}^n \sum_{\substack{j'j'' \\ \text{incl. } j'=t'}} e^{-i\nu_1\tau_{j'}+i\nu_2\tau_{j''}} D_{j'j''}^n]_{\text{conn}}\}.$$
 (6.21)

If we put $\nu_i=0$, only the terms with odd n remain, because $\sum_{jt} D_{jt}^n=0$ as n is even. Then, the sum in (6.21), the vertex part, is proportional to $\tilde{\chi}_{\text{odd}}$. Compared with χ_{odd} given by (4.6), this vertex part, which should be put as $A_{\uparrow\downarrow}$, is expressed as

$$\begin{aligned} A_{\uparrow\downarrow} &= -\frac{V^4}{\Delta^4} \pi \Delta \tilde{\chi}_{\text{odd}} \\ &= -\frac{1}{\pi \rho^2 \Delta} \tilde{\chi}_{\text{odd}}. \end{aligned}$$
 (6.22)

The two-particle Green's function for $\sigma=\uparrow$ and $\sigma'=\uparrow$ is also calculated in a similar way and the result is

$$\begin{aligned} G^{\text{II}}(k_1\uparrow\nu_1, k_2\uparrow\nu_2; k_3\uparrow\nu_3, k_4\uparrow\nu_4) &= \beta V^4 G_{k_1}^{\circ}(\nu_1) G_{k_2}^{\circ}(\nu_2) G_{k_3}^{\circ}(\nu_3) G_{k_4}^{\circ}(\nu_4) [G(\nu_1) G(\nu_2) \beta (\delta_{\nu_1\nu_2} \delta_{\nu_3\nu_4} - \delta_{\nu_1\nu_3} \delta_{\nu_2\nu_4}) \\ &+ G(\nu_1) G(\nu_2) G(\nu_3) G(\nu_4) \sum_{n=1}^{\infty} \frac{U^{2n}}{(2n)!} \frac{1}{\beta} \int_0^{\beta} \dots \int_0^{\beta} d\tau_1 d\tau_2 \dots d\tau_{2n} \\ &\times \sum_{\substack{j_i j'_i j''_i \\ \text{incl. } j=i, j'=i'}} e^{i\nu_1\tau_i - i\nu_2\tau_j + i\nu_3\tau_{j''} - i\nu_4\tau_{j'}} D_{j_i j'_i j''_i}^{2n}]_{\text{conn}}. \end{aligned}$$

Here we put $\nu_i=0$. Then, the second vertex part identically vanishes since

$$\sum_{\substack{j_i j'_i j''_i \\ \text{incl. } j=i, j'=i'}} D_{j_i j'_i j''_i}^{2n} = 0,$$

which results from (4.4). Thus, we have

$$A_{\uparrow\uparrow} = 0.$$
 (6.23)

Inserting (6.22) and (6.23) into (6.7), we obtain

$$I = -\frac{1}{2} \Delta \tilde{\chi}_{\text{odd}}^2 \left(\frac{\pi^2 T^2}{\Delta^2} + \frac{\omega^2}{\Delta^2} \right).$$
 (6.24)

With the results of (6.16) and (6.24), the imaginary part of the t -matrix becomes

$$-\text{Im } t_{kk} = \pi \rho |t|^2 + \pi \rho |\tau_{\text{in}}|^2,$$
 (6.25)

$$\begin{aligned} \pi \rho |t|^2 &= \frac{1}{\pi \rho} \frac{\Delta^2}{(\omega - R)^2 + (I - I)^2} \sim \frac{1}{\pi \rho} \left\{ 1 - \frac{(\omega - R)^2}{\Delta^2} + \frac{2I}{\Delta} \right\} \\ &\sim \frac{1}{\pi \rho} \left\{ 1 - \tilde{\chi}_{\text{even}}^2 \frac{\omega^2}{\Delta^2} - \tilde{\chi}_{\text{odd}}^2 \left(\frac{\pi^2 T^2}{\Delta^2} + \frac{\omega^2}{\Delta^2} \right) \right\}, \end{aligned}$$
 (6.26)

$$\pi \rho |\tau_{\text{in}}|^2 = -\frac{1}{\pi \rho} \frac{I \Delta}{(\omega - R)^2 + (I - \Delta)^2} \sim -\frac{1}{\pi \rho} \frac{I}{\Delta}$$

$$\simeq \frac{1}{\pi\rho} \frac{1}{2} \tilde{\chi}_{\text{odd}}^2 \left(\frac{\pi^2 T^2}{D^2} + \frac{\omega^2}{D^2} \right). \quad (6 \cdot 27)$$

The second term of (6.25) expresses contributions from inelastic channels and plays a role of spin-flip scattering in the Suhl-Nagaoka theory⁸⁾ based on the s - d model. However, here in our case it arises from two-particle scattering whose mechanism is different from the so-called 'spin-flip' mechanism.

§ 7. Discussion and conclusion

It has been well established that the ground state of the system described by the s - d model is in a locally singlet state, or non-magnetic state.^{7),8)} However, up to date not so much about the low-lying excitations from the ground state has yet been clarified although the low-temperature behavior is known to be completely normal. Wilson's recent theory⁹⁾ was successful in obtaining the low-temperature specific heat and susceptibility with the aid of numerical calculations. At the same time, however, it seems to show how difficult it is to develop the theory analytically. On the other hand, the Anderson Hamiltonian from which the s - d model is derived in the limit of a large value of U always gives a non-magnetic ground state. The small system described by the Anderson Hamiltonian should have no singularity in its behavior in the whole range of U from zero to infinity. Thus, it is expected that the low-energy and low-temperature behavior of the system described by the Anderson Hamiltonian for not so large a value of U is essentially the same as the one described by the s - d model. Therefore, it might be of great help in clarifying the low-temperature behavior of the s - d model to investigate the Anderson Hamiltonian without using any approximate methods such as Hartree-Fock, RPA, etc. This is the main reason for our present work on the perturbation theoretical approach.

In the Anderson Hamiltonian, inelastic channels always exist besides the elastic channel for scattering of conduction electrons and the former scattering represents the many-body character of this system, as has been pointed out by Nozières.⁵⁾ This inelastic scattering is different from 'spin-flip' scattering in the Suhl-Nagaoka theory on the s - d model and it arises from two or more electron scattering.

In this paper, perturbation terms of general order for thermodynamical quantities—the specific heat, the susceptibility, and the scattering t -matrix—are investigated and mutual relations between them are examined. The main results obtained in this paper are that the low-temperature or low-energy behavior of these quantities is described in terms of the even part $\tilde{\chi}_{\text{even}}$ and the odd part $\tilde{\chi}_{\text{odd}}$ of the local susceptibility at the absolute zero temperature. The Coulomb repulsion U is included in these two quantities. Therefore, as far as the low-lying excitations are concerned, the thermodynamical behavior of this system is scaled by these two quantities. This is also true in the s - d limit where the two quantities

become identical and equal to $\pi\Delta/4T_K$. These facts are entirely consistent with the phenomenological Fermi liquid theory presented recently for the s - d model by Nozières and confirm it from the microscopic point of view.

On the other hand, we have developed the theory of the singlet ground state for the s - d exchange Hamiltonian and calculated the zero-temperature susceptibility for the s - d system.⁸⁾ Thus, if one combines this separately calculated susceptibility with the present results, they can be regarded as the expressions describing the low-temperature behavior of the s - d system.

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Note added in proof:

When the condition of electron-hole symmetry, $2E_d = -U$, is removed, $\chi_{\uparrow\uparrow}$ and $\chi_{\uparrow\downarrow}$ defined by (2·11) and (2·12) include both even- and odd-order terms in U , because for the unsymmetric case the determinants constructed by d -electron temperature Green's functions are no longer antisymmetric. However, the relation between the T -linear specific heat and χ_{even} remains to hold for $\chi_{\uparrow\uparrow}$. The proof for this can easily be given in a quite parallel way.