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Anisotropic s-d Exchange Interaction

Normal State I

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Summary

In this paper we have dealt with an anisotropic s-d exchange interaction and calculated physical quantities such as specific heat and resistivity using the Hamann's approximation.

Since partial breakdown of the rotational symmetry arises in this system, we have introduced a special type of T-operation for matrices and utilized it to construct equations of the t's matrices which appear in the one-particle Green's function.

1. Introduction

The phenomena of the resistance minimum in some metals and alloys has been a puzzling problem in the theory of metals for a long time.

The first theoretical explanation has been given by kondo,¹⁾ who has considered the spin flip scattering of conduction electrons using s-d exchange model²⁾ as the origin of the resistance minimum. He has calculated the life time of conduction electrons due to this anomalous scattering in the second Born approximation, and has shown that there appears the "singular" term proportional to $\ln T$. Combining this singular term with the usual term due to the scattering by phonons, he has succeeded to explain the occurrence of the resistance minimum at a certain temperature. It is to be noted that this occurs only when the exchange coupling between the "localized spin" of the paramagnetic impurity and the spin density of conduction electrons is antiferromagnetic. While we have believed for a long time that the ordinary perturbational theory could have accounted for all effects of interest, but the appearance of such a singular term has meant that the perturbational treatment of this anomalous scattering problem becomes very doubtful at sufficiently low temperatures.

There have been a number of attempts to treat the s-d exchange model by nonperturbative methods.

Suhl³⁾ has used the Chew-Low method⁴⁾ in calculating the scattering t-matrix of conduction electrons by the paramagnetic impurity. His result is similar to that of Abrikosov⁵⁾ and Doniach⁶⁾, who have calculated the self-energy of conduction electrons by using the technique of the Feynman diagram⁴⁾ and summed up the most "divergent terms",⁵⁾⁶⁾ so Suhl's result shows the instability; that is, the breakdown of the analytical property of the t-matrix at low temperatures.

Later, Suhl and Wong⁷⁾ have succeeded to remove this instability and to obtain the t-matrix which is analytic even at low temperatures.

Nagaoka⁸⁾ has developed a special decoupling scheme for double time Green's functions.⁹⁾ As a result of the decoupling procedure, he has obtained the complex closed sets of equations and proceeded by further approximations to solve these

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equations. His result has been shown to be similar to that of Suhl, Abrikosov, and Doniach at high temperatures but to give the finite value for the life time of conduction electrons at low temperatures, especially at. 0°K. An improvement of the calculations have been achieved by Hamann.¹⁰⁾

He has shown that all the informations contained in Nagaoka's equations can be exactly obtained from the solution of a nonlinear integral equation for the t-matrix which appear in the one-particle Green's function, derived a simpler integral equation than the original one by retaining only those parts of the integral operators which give rise to Fermi surface anomalies of the Kondo type, and solved it approximately to obtain physical quantities. This simplified equation has been studied exactly by Bloomfield and Hamann¹⁰⁾ using special mathematical techniques in the theory of "singular integral equations."¹¹⁾ Zittartz and Muller-Hartmann¹²⁾ have, recently, solved exactly the original non-linear integral equation derived by Hamann, which is equivalent to solving the Nagaoka equation, and given physical quantities.

This Green's function method has been shown to be equivalent to the Suhl's method, mentioned above, by Schotte,¹³⁾ and Zittartz,¹⁴⁾ respectively.

Giving "reasonable" physical quantities, if we utilize the exact solutions in calculations, nonperturbative theories for the s-d exchange system seem to be successful.

Now we must refer to the ground state of this system.

Yoshida¹⁵⁾ and his coworkers¹⁶⁾ have investigated the ground state of the system by the variational method and obtained a possibility forming a singlet ground state for $s = \frac{1}{2}$, as Cooper pairs¹⁷⁾ in superconductors. Kondo¹⁸⁾ has used the different method and got the similar result. This singlet ground state had been conjectured by Anderson.¹⁹⁾

If this is true, the susceptibility χ multiplied by absolute temperature T should vanish at $T=0$.

Recently, Zittartz²⁰⁾ have examined, using nonperturbative exact solution, the susceptibility and obtained the unfavorable result that χ , which should certainly be either positive or zero, is negative at $T=0$ for $S = \frac{1}{2}$.

This fault seems to result from either the Nagaoka's decoupling scheme, or the model with a single impurity spin.

This question ought to be answered, but it is extremely difficult.

Having interests of this problems, the authors would like to propose an anisotropic model: i. e.,

$$\sigma \hat{J} S = \lambda \sigma_z S_z + \mu (\sigma_+ S_- + \sigma_- S_+),$$

instead of the usual isotropic interaction: i. e.,

$$J \sigma S = J \{ \sigma_z S_z + \frac{1}{2} (\sigma_+ S_- + \sigma_- S_+) \},$$

where

$$\hat{J} = \begin{pmatrix} \lambda & 0 & 0 \\ 0 & 2\mu & 0 \\ 0 & 0 & 2\mu \end{pmatrix},$$

and λ and μ are assumed to be real and independent from each other.

The reason for proposition of the anisotropic interaction model is that, for $\mu=0$, we can obtain a solution without an approximation, and for $\mu \neq 0$, we will be able to hope to discuss the Nagaoka's decoupling scheme.

In this paper, first we will discuss the anisotropic exchange model in Hamann's treatment, and then give observable quantities except susceptibility.

Since in our system the rotational symmetry breaks down partly, we will employ a matrix form of Green's functions rather than the usual form³⁾ used for the normal states.

2. Formulation

The starting point for the following calculations is the anisotropic s-d exchange Hamiltonian

$$H = \sum_{l, \sigma} \xi_l C_{l\sigma}^+ C_l - \sum_{l, l'} \{ (C_{l'}^+ C_{l+1} - C_l^+ C_{l'-1}) \lambda S_z + C_{l'}^+ C_{l'-1} \mu S_- + C_l^+ C_{l+1} \mu S_+ \}, \quad (2-1)$$

where ξ_k is the free electron energy measured relative to the chemical potential, and $C_{k\sigma}^+$ and $C_{k\sigma}$ creates and annihilates conduction electrons with momentum k and spin σ , respectively.

λ and μ are the coupling constants, per an electron, of the anisotropic exchange interaction between conduction electrons and an impurity spin S ($S = \frac{1}{2}$).

We introduce the Green's functions in matrix forms

$$\hat{G}_{kk'}(Z) = \begin{pmatrix} \langle\langle C_{k+1} | C_{k'+1}^+ \rangle\rangle_Z & 0 \\ 0 & \langle\langle C_{-k+1}^+ | C_{-k'+1} \rangle\rangle_Z \end{pmatrix}, \quad (2-2)$$

$$\hat{F}_{kk'}(Z) = \begin{pmatrix} \langle\langle C_{k+1} S_z | C_{k'+1}^+ \rangle\rangle_Z & 0 \\ 0 & \langle\langle C_{-k+1}^+ S_z | C_{-k'+1} \rangle\rangle_Z \end{pmatrix}, \quad (2-3)$$

and

$$\hat{A}_{kk'}(Z) = \begin{pmatrix} \langle\langle C_{-k+1} S_- | C_{k'+1}^+ \rangle\rangle_Z & 0 \\ 0 & -\langle\langle C_{k+1}^+ S_- | C_{-k'+1} \rangle\rangle_Z \end{pmatrix}, \quad (2-4)$$

where $\langle\langle A | B \rangle\rangle_{i\omega_n}$ denotes the n -th Fourier coefficient of the temperature dependent Green's function³⁾ of two operators A and B , i. e.,

$$-\langle T A(\tau) B(\tau') \rangle \quad (2-5)$$

with $0 \leq \tau, \tau' \leq \beta$ and

$$\omega_n = \frac{2n+1}{\beta} \pi \quad (2-6)$$

The bracket $\langle BA \rangle$ is the usual statistical average of operators BA and T is the time ordering operator.⁴⁾ The thermal averages are related to the Green's functions. This relation is given by the general expression

$$\langle BA \rangle = \frac{1}{\beta} \sum_n e^{i\omega_n \delta} \langle\langle A | B \rangle\rangle_{i\omega_n} = \mathfrak{F}_n \{ \langle\langle A | B \rangle\rangle_{i\omega_n} \}, \quad (2-7)$$

where δ is positive and infinitesimal.

We will follow Nagaoka's treatments⁸⁾ for the constructions of equations of the Green's functions as closely as possible, especially for the decoupling scheme of the Green's functions higher in order than the three Green's functions introduced above.

The closed equations of these Green's functions are

$$\hat{\Omega}_k(Z) \hat{G}_{kh'}(Z) + \lambda \Sigma_l \hat{F}_{lh'}(Z) + \mu \Sigma_l \hat{\Lambda}_{lh'}(Z) = \delta_{kh'}, \quad (2-8)$$

$$\hat{\Omega}_k(Z) \hat{F}_{kh'}(Z) + \hat{N}_k \Sigma_l \hat{\Lambda}_{lh'}(Z) + \hat{M}_k \Sigma_l \hat{G}_{lh'}(Z) = 0, \quad (2-9)$$

$$\hat{\Omega}_k(Z) \hat{\Lambda}_{kh'}(Z) + \hat{O}_k \Sigma_l \hat{F}_{lh'}(Z) + \hat{P}_k \Sigma_l \hat{\Lambda}_{lh'}(Z) + \hat{L}_k \Sigma_l \hat{G}_{lh'}(Z) = 0, \quad (2-10)$$

where Z is a complex energy, and

$$\hat{\Omega}_k(Z) = \begin{pmatrix} Z - \xi_k & 0 \\ 0 & Z + \xi_k \end{pmatrix} \quad (2-11)$$

$$\hat{N}_k = \frac{\mu}{2} - \mu \Sigma_l \left(\langle C_{k\uparrow} C_{l\uparrow}^\dagger \rangle \quad \langle C_{k\uparrow}^0 C_{l\uparrow}^0 \rangle \right), \quad (2-12)$$

$$\hat{M}_k = \frac{\lambda}{4} + \mu \Sigma_l \left(\langle C_{k\uparrow} C_{l\uparrow}^\dagger S_z \rangle \quad -\langle C_{k\uparrow}^0 C_{l\uparrow}^0 S_z \rangle \right), \quad (2-13)$$

$$\hat{O}_k = \mu - 2\mu \Sigma_l \left(\langle C_{k\uparrow} C_{l\uparrow}^\dagger \rangle \quad \langle C_{k\uparrow}^0 C_{l\uparrow}^0 \rangle \right), \quad (2-14)$$

$$\hat{P}_k = \frac{\lambda}{2} - \lambda \Sigma_l \left(\langle C_{k\uparrow} C_{l\uparrow}^\dagger \rangle \quad \langle C_{k\uparrow}^0 C_{l\uparrow}^0 \rangle \right), \quad (2-15)$$

and

$$\begin{aligned} \hat{L}_k = \lambda \Sigma_l \left(\langle C_{l\uparrow} C_{l\uparrow}^\dagger S_z \rangle \quad -\langle C_{k\uparrow}^0 C_{l\uparrow}^0 S_z \rangle \right) \\ - 2\mu \Sigma_l \left(\langle C_{k\uparrow} C_{l\uparrow}^\dagger S_z \rangle \quad \langle C_{k\uparrow}^0 C_{l\uparrow}^0 S_z \rangle \right) + \frac{\mu}{2} \end{aligned} \quad (2-16)$$

To obtain the formal solutions of these closed set of the equations, it is convenient to define t-matrices without spin flip,¹⁰⁾ i. e.,

$$\hat{F}_k(Z) \equiv \Sigma_l \hat{F}_{lk}(Z) \equiv -\hat{t}_1(Z) \hat{\Omega}_k^{-1}(Z), \quad (2-17)$$

$$\hat{\Lambda}_k(Z) \equiv \Sigma_l \hat{\Lambda}_{lk}(Z) \equiv -\hat{t}_2(Z) \hat{\Omega}_k^{-1}(Z), \quad (2-18)$$

Consequently, we have the following:

$$\begin{aligned} \hat{G}_k(Z) \equiv \Sigma_l \hat{G}_{kl}(Z) = \Sigma_l \hat{G}_{lk}(Z) \\ = \hat{\Omega}_k^{-1}(Z) + \hat{F}(Z) [\lambda \hat{t}_1(Z) + \mu \hat{t}_2(Z)] \hat{\Omega}_k^{-1}(Z), \end{aligned} \quad (2-19)$$

where

$$\hat{F}(Z) \equiv \Sigma_l \hat{\Omega}_l^{-1}(Z) \quad (2-20)$$

Now we must write down the equations satisfied with t-matrices. They are given by

$$[1 - \lambda \hat{M}(Z) \hat{F}(Z)] \hat{t}_1(Z) + [\hat{N}(Z) - \mu \hat{M}(Z) \hat{F}(Z)] \hat{t}_2(Z) = \hat{M}(Z), \quad (2-21)$$

$$[\hat{O}(Z) - \lambda \hat{L}(Z) \hat{F}(Z)] \hat{t}_1(Z) + [1 + \hat{P}(Z) - \mu \hat{L}(Z) \hat{F}(Z)] \hat{t}_2(Z) = \hat{L}(Z), \quad (2-22)$$

where

$$\hat{N}(Z) = \sum_t \hat{\Omega}_t^{-1}(Z) \hat{N}_t, \quad (2-23)$$

$$\hat{M}(Z) = \sum_t \hat{\Omega}_t^{-1}(Z) \hat{M}_t, \quad (2-24)$$

$$\hat{O}(Z) = \sum_t \hat{\Omega}_t^{-1}(Z) \hat{O}_t, \quad (2-25)$$

$$\hat{P}(Z) = \sum_t \hat{\Omega}_t^{-1}(Z) \hat{P}_t, \quad (2-26)$$

and

$$\hat{L}(Z) = \sum_t \hat{\Omega}_t^{-1}(Z) \hat{L}_t. \quad (2-27)$$

Next step is to express the eqs. (2-23)~(2-27) in terms of \hat{t}_1 and \hat{t}_2 , using the eq. (2-7).

It is easy to express \hat{N} by the matrices \hat{t} 's. Using eqs. (2-2), (2-7), (2-12), (2-19) and (2-23), we can write

$$\begin{aligned} \hat{N}(Z) &= \sum_t \hat{\Omega}_t^{-1}(Z) \left\{ \mu \mathfrak{F}_n \{ \hat{G}(i\omega_n) \} - \frac{\mu}{2} \right\} \\ &= \mu \hat{g}(Z) \\ &\quad + \lambda \mu \mathfrak{F}_n \left\{ \frac{\hat{F}(i\omega_n) - \hat{F}(Z)}{Z - i\omega_n} \hat{t}_1(i\omega_n) \hat{F}(i\omega_n) \right\} \\ &\quad + \mu^2 \mathfrak{F}_n \left\{ \frac{\hat{F}(i\omega_n) - \hat{F}(Z)}{Z - i\omega_n} \hat{t}_2(i\omega_n) \hat{F}(i\omega_n) \right\} \end{aligned} \quad (2-28)$$

where the function $\hat{g}(Z)$ is given by

$$\begin{aligned} \hat{g}(Z) &= \mathfrak{F}_n \left\{ \frac{\hat{F}(i\omega_n) - \hat{F}(Z)}{Z - i\omega_n} \right\} - \frac{1}{2} \hat{F}(Z) \\ &= \frac{1}{4\pi i} \int_{-\infty}^{\infty} d\omega \frac{\text{th} \frac{\beta\omega}{2}}{Z - i\omega} \left[\hat{F}^R(\omega) - \hat{F}^*(\omega) \right] \end{aligned} \quad (2-29)$$

To obtain similar expressions for the rest of functions \hat{M} etc, it is necessary to have a little manipulations where we take complex conjugate of the matrices and use T_1 -operation defined by

$$\begin{pmatrix} a & 0 \\ 0 & b \end{pmatrix} T_1 = - \begin{pmatrix} b & 0 \\ 0 & a \end{pmatrix} \quad (2-30)$$

As the result, we have explicit forms for the rest of functions \hat{M} etc., as the follows:

$$\hat{M}(Z) = \frac{\lambda}{4} \hat{F}(Z) - \mu \mathfrak{F}_n \left\{ \frac{\hat{F}(i\omega_n) - \hat{F}(Z)}{Z - i\omega_n} \hat{t}_2(i\omega_n) \right\}, \quad (2-31)$$

$$\hat{O}(Z) = \mu \hat{F}(Z) - 2\mu \mathfrak{F}_n \left\{ \frac{\hat{F}^{T_1}(i\omega_n) - \hat{F}(Z)}{Z + i\omega_n} \right\}$$

$$\begin{aligned}
& -2\lambda\mu\mathfrak{F}_n\left\{\frac{\hat{F}^{T_1}(i\omega_n)-\hat{F}(Z)}{Z+i\omega_n}\hat{t}_1^{T_1}(i\omega_n)\hat{F}^{T_1}(i\omega_n)\right\} \\
& -2\mu^2\mathfrak{F}_n\left\{\frac{\hat{F}^{T_1}(i\omega_n)-\hat{F}(Z)}{Z+i\omega_n}\hat{t}_2^{T_1}(i\omega_n)\hat{F}^{T_1}(i\omega_n)\right\} \\
& = -2\mu\hat{g}(Z) \\
& -2\lambda\mu\mathfrak{F}_n\left\{\frac{\hat{F}(i\omega_n)-\hat{F}(Z)}{Z-i\omega_n}\hat{t}_1^{T_1}(-i\omega_n)\hat{F}(i\omega_n)\right\} \\
& -2\mu^2\mathfrak{F}_n\left\{\frac{\hat{F}(i\omega_n)-\hat{F}(Z)}{Z-i\omega_n}\hat{t}_2^{T_1}(-i\omega_n)\hat{F}(i\omega_n)\right\}, \tag{2-32}
\end{aligned}$$

$$\hat{P}(Z) = -\lambda\hat{g}(Z)$$

$$\begin{aligned}
& -\lambda^2\mathfrak{F}_n\left\{\frac{\hat{F}(i\omega_n)-\hat{F}(Z)}{Z-i\omega_n}\hat{t}_1^{T_1}(-i\omega_n)\hat{F}(i\omega_n)\right\} \\
& -\lambda\mu\mathfrak{F}_n\left\{\frac{\hat{F}(i\omega_n)-\hat{F}(Z)}{Z-i\omega_n}\hat{t}_2^{T_1}(-i\omega_n)\hat{F}(i\omega_n)\right\}, \tag{2-33}
\end{aligned}$$

and

$$\begin{aligned}
\hat{L}(Z) &= -\frac{\mu}{2}\hat{F}(Z) \\
& -2\mu\mathfrak{F}_n\left\{\frac{\hat{F}(i\omega_n)-\hat{F}(Z)}{Z-i\omega_n}\hat{t}_1^{T_1}(-i\omega_n)\right\} \\
& -\lambda\mathfrak{F}_n\left\{\frac{\hat{F}(i\omega_n)-\hat{F}(Z)}{Z-i\omega_n}\hat{t}_2^{T_1}(-i\omega_n)\right\}, \tag{2-33'}
\end{aligned}$$

where we have used the relation;

$$\hat{F}^{T_1}(-Z) = \hat{F}(Z), \tag{2-34}$$

which is easily checked using eqs. (2-11) and (2-20). Here, we have assumed that the state density ρ is an even function of a free electron energy: $\rho(\xi_k) = \rho(-\xi_k)$, analytic in a neighbourhood of the real axis, and falls off rapidly enough at infinity.

As pointed out by Takano and Matayoshi,²¹⁾ we have also

$$\hat{t}_1(Z) = t_1(Z) \tag{2-35}$$

and

$$\hat{t}_2(Z) = t_2(Z) \tag{2-36}$$

for

$$\hat{F}(Z) = F(Z) = \sum_t \frac{1}{Z - \xi_t} = \int_{-\infty}^{\infty} d\omega \frac{\rho(\omega)}{Z - \omega} \tag{2-37}$$

and

$$\hat{g}(Z) = g(Z) = -\frac{1}{2} \int_{-\infty}^{\infty} d\omega \operatorname{th} \frac{\beta\omega}{2} \frac{\rho(\omega)}{Z - \omega}. \tag{2-38}$$

From eqs. (2-21), (2-22), (2-28), and from (2-31) through (2-38) except (2-34), we can obtain the explicit closed sets in terms of t_1 and t_2 , dropping out

the symbol " \wedge " and T_1 operator (since $t_{T_1} = -t_j$, for $j=1, 2$).

To derive the closed sets in terms of t_1 and t_2 , we have used the T_1 -operator, but not the rotational symmetry relations such as $\langle C_{k_1}^+ C_{k_1} \rangle = \langle C_{k_1}^+ C_{k_1'} \rangle$, etc., which had been used in many works.¹⁰⁾ Therefore, it ought to be stressed that our approaches are of great significance especially in treating a system without the rotational symmetry; for example, systems with a finite external field.

Attentions are paid to the relations in the system without fields;

$$\hat{t}_j(-Z) = -t_j(Z) \quad \text{for } j=1 \text{ and } 2, \quad (2-39)$$

which are easily checked in the closed sets in terms of t_1 and t_2 , and were pointed out by Zittartz and Muller-Hartmann.²²⁾

Now, we write down the desired forms of the closed sets in terms of t_1 and t_2 ;

$$A(Z)t_1(Z) + B(Z)t_2(Z) = C(Z) \quad (2-40)$$

and

$$\tilde{B}(Z)t_1(Z) + \tilde{A}(Z)t_2(Z) = \tilde{C}(Z), \quad (2-41)$$

where

$$A(Z) = 1 - \frac{\lambda^2}{4} F^2(Z) - \lambda \mu F(Z) \mathfrak{F}_n \left\{ \frac{F(i\omega_n) - F(Z)}{Z - i\omega_n} t_2(i\omega_n) \right\}, \quad (2-42)$$

$$B(Z) = -\frac{\mu^2}{4} F^2(Z) + \mu g(Z) + \lambda \mu \mathfrak{F}_n \left\{ \frac{F(i\omega_n) - F(Z)}{Z - i\omega_n} F(i\omega_n) t_1(i\omega_n) \right\} \\ + \mu^2 \mathfrak{F}_n \left\{ \frac{[F(i\omega_n) - F(Z)]^2}{Z - i\omega_n} t_2(i\omega_n) \right\}, \quad (2-43)$$

$$\tilde{A}(Z) = 1 - \frac{\mu^2}{2} F^2(Z) + \lambda g(Z) \\ + \lambda^2 \mathfrak{F}_n \left\{ \frac{F(i\omega_n) - F(Z)}{Z - i\omega_n} F(i\omega_n) t_1(i\omega_n) \right\} \\ - 2\mu^2 F(Z) \mathfrak{F}_n \left\{ \frac{F(i\omega_n) - F(Z)}{Z - i\omega_n} t_1(i\omega_n) \right\} \\ + \lambda \mu \mathfrak{F}_n \left\{ \frac{[F(i\omega_n) - F(Z)]^2}{Z - i\omega_n} t_2(i\omega_n) \right\}, \quad (2-44)$$

$$\tilde{B}(Z) = -\frac{\lambda \mu}{2} F^2(Z) + 2\mu g(Z) \\ + 2\lambda \mu \mathfrak{F}_n \left\{ \frac{[F(i\omega_n) - F(Z)]^2}{Z - i\omega_n} t_1(i\omega_n) \right\} \\ + 2\mu^2 \mathfrak{F}_n \left\{ \frac{F(i\omega_n) - F(Z)}{Z - i\omega_n} F(i\omega_n) t_2(i\omega_n) \right\} \\ - \lambda^2 F(Z) \mathfrak{F}_n \left\{ \frac{F(i\omega_n) - F(Z)}{Z - i\omega_n} t_2(i\omega_n) \right\}, \quad (2-45)$$

$$C(Z) = \frac{\lambda}{4} F(Z) + \mu \mathfrak{F}_n \left\{ \frac{F(i\omega_n) - F(Z)}{Z - i\omega_n} t_2(i\omega_n) \right\}, \quad (2-46)$$

and

$$\begin{aligned} \tilde{C}(Z) = & -\frac{\mu}{2} F(Z) + \lambda \mathfrak{F}_n \left\{ \frac{F(i\omega_n) - F(Z)}{Z - i\omega_n} t_2(i\omega_n) \right\} \\ & + 2\mu \mathfrak{F}_n \left\{ \frac{F(i\omega_n) - F(Z)}{Z - i\omega_n} t_1(i\omega_n) \right\}, \end{aligned} \quad (2-47)$$

Our closed sets are clearly equivalent to the eq.(20) in the ref.(12) for $\lambda = \mu = J/2N$

The summation in the function A, etc., can be expressed in the usual way as a contour integral bent over to the real axis. This gives

$$\begin{aligned} A(Z) = & 1 - \frac{\lambda^2}{4} F^2(Z) \\ & - \frac{\lambda \mu}{4\pi i} F(Z) \int_{-\infty}^{\infty} d\omega \frac{\text{th} \frac{\beta \omega}{2}}{Z - \omega} \left\{ [F^R(\omega) - F(Z)] t_2^R(\omega) \right. \\ & \left. - [F^a(\omega) - F(Z)] t_2^a(\omega) \right\}, \end{aligned} \quad (2-48)$$

$$\begin{aligned} B(Z) = & -\frac{\mu^2}{4} F^2(Z) + \mu g(Z) \\ & + \frac{\lambda \mu}{4\pi i} \int_{-\infty}^{\infty} d\omega \frac{\text{th} \frac{\beta \omega}{2}}{Z - \omega} \left\{ [F^R(\omega) - F(Z)] F^R(\omega) t_1^R(\omega) \right. \\ & \left. - [F^a(\omega) - F(Z)] F^a(\omega) t_1^a(\omega) \right\} \\ & + \frac{\mu^2}{4\pi i} \int_{-\infty}^{\infty} d\omega \frac{\text{th} \frac{\beta \omega}{2}}{Z - \omega} \left\{ [F^R(\omega) - F(Z)]^2 t_2^R(\omega) \right. \\ & \left. - [F^a(\omega) - F(Z)]^2 t_2^a(\omega) \right\}, \end{aligned} \quad (2-49)$$

$$\begin{aligned} \tilde{A}(Z) = & 1 - \frac{\mu^2}{2} F^2(Z) + \lambda g(Z) \\ & + \frac{\lambda^2}{4\pi i} \int_{-\infty}^{\infty} d\omega \frac{\text{th} \frac{\beta \omega}{2}}{Z - \omega} \left\{ [F^R(\omega) - F(Z)] F^R(\omega) t_1^R(\omega) \right. \\ & \left. - [F^a(\omega) - F(Z)] F^a(\omega) t_1^a(\omega) \right\} \\ & - \frac{2\mu^2}{4\pi i} F(Z) \int_{-\infty}^{\infty} d\omega \frac{\text{th} \frac{\beta \omega}{2}}{Z - \omega} \left\{ [F^R(\omega) - F(Z)] t_1^R(\omega) - [F^a(\omega) - F(Z)] t_1^a(\omega) \right\} \\ & + \frac{\lambda \mu}{4\pi i} \int_{-\infty}^{\infty} d\omega \frac{\text{th} \frac{\beta \omega}{2}}{Z - \omega} \left\{ [F^R(\omega) - F(Z)]^2 t_2^R(\omega) - [F^a(\omega) - F(Z)]^2 t_2^a(\omega) \right\}, \end{aligned} \quad (2-50)$$

$$\begin{aligned}
\tilde{B}(Z) = & -\frac{\lambda \mu}{2} F^2(Z) + 2 \mu g(Z) \\
& + \frac{2 \lambda \mu}{4 \pi i} \int_{-\infty}^{\infty} d \omega \frac{\operatorname{th} \frac{\beta \omega}{2}}{Z - \omega} \left\{ [F^R(\omega) - F(Z)]^2 t_1^R(\omega) \right. \\
& \quad \left. - [F^A(\omega) - F(Z)]^2 t_1^A(\omega) \right\} \\
& + \frac{2 \mu^2}{4 \pi i} \int_{-\infty}^{\infty} d \omega \frac{\operatorname{th} \frac{\beta \omega}{2}}{Z - \omega} \left\{ [F^R(\omega) - F(Z)] F^R(\omega) t_2^R(\omega) \right. \\
& \quad \left. - [F^A(\omega) - F(Z)] F^A(\omega) t_2^A(\omega) \right\} \\
& - \frac{\lambda^2}{4 \pi i} F(Z) \int_{-\infty}^{\infty} d \omega \frac{\operatorname{th} \frac{\beta \omega}{2}}{Z - \omega} \left\{ [F^R(\omega) - F(Z)] t_2^R(\omega) \right. \\
& \quad \left. - [F^A(\omega) - F(Z)] t_2^A(\omega) \right\}, \tag{2-51}
\end{aligned}$$

$$\begin{aligned}
C(Z) = & \frac{\lambda}{4} F(Z) + \frac{\mu}{4 \pi i} \int_{-\infty}^{\infty} d \omega \frac{\operatorname{th} \frac{\beta \omega}{2}}{Z - \omega} \left\{ [F^R(\omega) - F(Z)] t_2^R(\omega) \right. \\
& \quad \left. - [F^A(\omega) - F(Z)] t_2^A(\omega) \right\}, \tag{2-52}
\end{aligned}$$

and

$$\begin{aligned}
\tilde{C}(Z) = & -\frac{\mu}{2} F(Z) + \frac{\lambda}{4 \pi i} \int_{-\infty}^{\infty} d \omega \frac{\operatorname{th} \frac{\beta \omega}{2}}{Z - \omega} \left\{ [F^R(\omega) - F(Z)] t_2^R(\omega) \right. \\
& \quad \left. - [F^A(\omega) - F(Z)] t_2^A(\omega) \right\} \\
& + \frac{2 \mu}{4 \pi i} \int_{-\infty}^{\infty} d \omega \frac{\operatorname{th} \frac{\beta \omega}{2}}{Z - \omega} \left\{ [F^R(\omega) - F(Z)] t_1^R(\omega) \right. \\
& \quad \left. - [F^A(\omega) - F(Z)] t_1^A(\omega) \right\}. \tag{2-53}
\end{aligned}$$

3. Hamann's Approximation

According to Hamann's discussions,¹⁰⁾ we can obtain the functions A, etc., in the simpler form and define them on the real axis ω as follows:

$$\begin{aligned}
A^R(\omega + i \delta) & \equiv A(\omega) \\
& = 1 + \frac{\pi^2}{4} \lambda^2 - \frac{i \pi \lambda \mu}{2} \int_{-D}^D d \eta \frac{\operatorname{th} \frac{\beta \eta}{2}}{\omega - \eta + i \delta} t_2^A(\eta), \tag{3-1}
\end{aligned}$$

$$\begin{aligned}
 B(\omega) &= \frac{\pi^2}{4} \mu^2 + \mu g^R(\omega) - \frac{i\pi\lambda\mu}{2} \int d\eta \frac{\text{th} \frac{\beta\eta}{2}}{\omega - \eta + i\delta} t_1^a(\eta) \\
 &\quad - \frac{2i\pi\mu^2}{2} \int d\eta \frac{\text{th} \frac{\beta\eta}{2}}{\omega - \eta + i\delta} t_2^a(\eta), \quad (3-2)
 \end{aligned}$$

$$\begin{aligned}
 \tilde{A}(\omega) &= 1 + \frac{\pi^2}{2} \mu^2 + \lambda g^R(\omega) - \frac{i\pi\lambda^2}{2} \int d\eta \frac{\text{th} \frac{\beta\eta}{2}}{\omega - \eta + i\delta} t_1^a(\eta) \\
 &\quad - \frac{2\pi i\mu^2}{2} \int d\eta \frac{\text{th} \frac{\beta\eta}{2}}{\omega - \eta + i\delta} t_1^a(\eta) \\
 &\quad - \frac{2\pi i\lambda\mu}{2} \int d\eta \frac{\text{th} \frac{\beta\eta}{2}}{\omega - \eta + i\delta} t_2^a(\eta), \quad (3-3)
 \end{aligned}$$

$$\begin{aligned}
 \tilde{B}(\omega) &= \frac{\pi^2}{2} \lambda\mu + 2\mu g^R(\omega) - \frac{4\pi i\lambda\mu}{2} \int d\eta \frac{\text{th} \frac{\beta\eta}{2}}{\omega - \eta + i\delta} t_1^a(\eta) \\
 &\quad - \frac{2\pi i\mu^2}{2} \int d\eta \frac{\text{th} \frac{\beta\eta}{2}}{\omega - \eta + i\delta} t_2^a(\eta) - \frac{\pi i\lambda^2}{2} \int d\eta \frac{\text{th} \frac{\beta\eta}{2}}{\omega - \eta + i\delta} t_2^a(\eta), \quad (3-4)
 \end{aligned}$$

$$C(\omega) = -\frac{i\pi}{4} \lambda - \frac{\mu}{2} \int d\eta \frac{\text{th} \frac{\beta\eta}{2}}{\omega - \eta + i\delta} t_2^a(\eta) \quad (3-5)$$

and

$$\begin{aligned}
 \tilde{C}(\omega) &= -\frac{i\pi}{2} \mu - \frac{2\mu}{2} \int d\eta \frac{\text{th} \frac{\beta\eta}{2}}{\omega - \eta + i\delta} t_1^a(\eta) \\
 &\quad - \frac{\lambda}{2} \int d\eta \frac{\text{th} \frac{\beta\eta}{2}}{\omega - \eta + i\delta} t_2^a(\eta), \quad (3-6)
 \end{aligned}$$

where we put λ and μ instead of $\lambda\rho$ and $\mu\rho$, respectively, ρ denoting the state density at the Fermi energy $\omega = 0$.

The essential approximation in the Hamann's treatments¹⁰⁾ is

$$-\frac{1}{2} \int_{-D}^D d\eta \frac{\text{th} \frac{\beta\omega}{2}}{\omega - \eta \pm i\delta} t^{a,R}(\eta) \simeq \int_0^{\beta\omega} d\eta t^{R,a}(\eta), \quad (3-7)$$

which includes exactly the most divergent terms pointed out by Abrikosov⁵⁾ at least and has an error of only a few percents.¹⁰⁾

Consequently, we can establish the simultaneous non-linear differential equations from eqs. (2-40), (2-41), and from (3-1) through (3-6); namely

$$\begin{aligned} & \left[1 + \frac{\pi^2}{4} \lambda^2 + \pi^2 \lambda \mu \psi_2 \right] \psi_1' + \left[\frac{\pi^2}{4} \mu^2 + \mu x + \pi^2 \lambda \mu \psi_1 + 2\pi^2 \mu^2 \psi_2 \right] \psi_2' \\ & = -\frac{\lambda}{4} - \mu \psi_2, \end{aligned} \quad (3-8)$$

$$\begin{aligned} & \left[\frac{\pi^2}{2} \lambda \mu + 2 \mu x + 4\pi^2 \lambda \mu \psi_1 + \pi^2 (\lambda^2 + 2\mu^2) \psi_2 \right] \psi_1' \\ & + \left[1 + \frac{\pi^2}{2} \mu^2 + \lambda x + \pi^2 (\lambda^2 + 2\mu^2) \psi_1 + 2\pi^2 \lambda \mu \psi_2 \right] \psi_2' \\ & = -\frac{\mu}{2} - 2\mu \psi_1 - \lambda \psi_2, \end{aligned} \quad (3-9)$$

and

$$\psi_j(0) = 0 \quad \text{for } j=1,2, \quad (3-10)$$

where, for convenience, we put as follows;

$$x = g^R(\omega), \quad (3-11)$$

$$\psi_j = \frac{1}{2\pi i} \int d\eta \frac{\text{th} \frac{\beta \eta}{2}}{\omega - \eta + i\delta} t_j^a(\eta) \quad \text{for } j=1,2, \quad (3-12)$$

and

$$\psi_j' = \frac{\partial \psi_j}{\partial x} \quad \text{for } j=1,2. \quad (3-13)$$

The eqs (3-8), (3-9), and (3-10) can be solved easily to give the formal solutions;

$$\begin{aligned} & \left[1 + \frac{\pi^2}{4} \lambda^2 \right] \psi_1 + \left[\frac{\pi^2}{4} \mu^2 + \mu x \right] \psi_2 + \pi^2 \lambda \mu \psi_1 \psi_2 \\ & + \pi^2 \mu^2 \psi_2^2 = -\frac{\lambda}{4} x, \end{aligned} \quad (3-14)$$

and

$$\begin{aligned} & \left[\frac{\pi^2}{2} \lambda \mu + 2\mu x \right] \psi_1 + \left[1 + \frac{\pi^2}{2} \mu^2 + \lambda x \right] \psi_2 + 2\pi^2 \lambda \mu \psi_1^2 \\ & + \pi^2 (\lambda^2 + 2\mu^2) \psi_1 \psi_2 + \pi^2 \lambda \mu \psi_2^2 = -\frac{\mu}{2} x \end{aligned} \quad (3-15)$$

or, eliminating ψ_1 , from eqs (3-14) and (3-15), we have

$$a_0 \psi_2^3 + a_1 \psi_2^2 + a_2 \psi_2 + a_3 = 0, \quad (3-16)$$

and

$$\psi_1 = \frac{-\frac{\lambda}{4} x - \left[\frac{\pi^2}{4} \mu^2 + \mu x \right] \psi_2 - \pi^2 \mu^2 \psi_2^2}{1 + \frac{\pi^2}{4} \lambda^2 + \pi^2 \lambda \mu \psi_2} \quad (3-16')$$

where

$$a_0 = 2\pi^4 (\lambda^2 - \mu^2) \mu^2 + \frac{\pi^6}{4} [\lambda^3 \mu^2 (\lambda - \mu) - 2\lambda \mu^4 (\lambda - \mu)], \quad (3-17)$$

$$a_1 = 3\pi^2 \lambda \mu + \frac{\pi^4}{4} [4\lambda^3 \mu - \lambda^2 \mu^2 + 2\mu^3 (\lambda - \mu)] \\ + \frac{\pi^6}{16} [\lambda^4 \mu (\lambda - \mu) + 2\lambda \mu^3 (\lambda - \mu)^2] + \pi^2 [\lambda^2 \mu - 4\mu^3] x \\ - \frac{\pi^4}{2} \lambda \mu^3 [\lambda - \mu] x, \quad (3-18)$$

$$a_2 = 1 + \frac{\lambda^2 + \mu^2}{2} \pi^2 + \frac{\lambda^4 + 4\lambda^2 \mu^2 - 2\lambda \mu^3}{16} \pi^4 + \lambda^3 \mu^2 \frac{\lambda - \mu}{32} \pi^6 \\ + \lambda x + \frac{\lambda^3 - 2\mu^3}{4} \pi^2 x - \lambda^2 \mu^2 \frac{\lambda - \mu}{8} \pi^4 x - 2\mu^2 x^2, \quad (3-19)$$

and

$$a_3 = \frac{\mu}{2} x + \frac{\lambda^2 \mu}{8} \pi^2 x - \frac{1}{2} \lambda \mu x^2. \quad (3-20)$$

Now, we must check our solutions in several limiting cases.

Case A $\lambda = \gamma$ and $\mu = 0$.

We have the trivial solutions as follows;

$$\psi_2 = 0 \quad (3-21)$$

and

$$\psi_1 = -\frac{\gamma}{4} \frac{x}{1 + \frac{\pi^2}{4} \gamma^2} \quad (3-22)$$

from eqs. (3-16) and (3-14).

Case B. $\lambda = \mu = \gamma$.

In the same way as in Case A, we obtain

$$\psi_2 = -\frac{[1 + \frac{3\pi^2}{4} \gamma^2 + 2\gamma x] \pm \sqrt{[1 - \frac{3\pi^2}{4} \gamma^2 + 2\gamma x]^2 + 3\pi^2 \gamma^2}}{6\pi^2 \gamma^2} \quad (3-23)$$

and

$$\psi_1 = \frac{1}{2} \psi_2, \quad (3-24)$$

which are equivalent to the Hamann's solutions.

Case C. Approximation taking only the most divergent terms which mean the terms for the smallest ℓ_1 and ℓ_2 in

$$\lambda^{m+\ell_1} \mu^{n+\ell_2} x^{m+n}.$$

This gives

$$\psi_2 = -\frac{a_3}{a_2} \simeq -\frac{1}{2} \frac{\mu x - \lambda \mu x^2}{1 + \lambda x - 2\mu^2 x^2} \quad (3-25)$$

and

$$\psi_1 = -\frac{1}{4} \frac{\lambda x + (\lambda^2 - 2\mu^2) x^2}{1 + \lambda x - 2\mu^2 x^2}, \quad (3-26)$$

or,

$$t_2 = \psi_2' = -\frac{\mu}{2} \frac{1 - 2\lambda x - (\lambda^2 - 2\mu^2) x^2}{(1 + \lambda x - 2\mu^2 x^2)^2} \quad (3-27)$$

and

$$t_1 = \psi_1' = -\frac{\lambda}{4} \frac{1 + 2\lambda x + \lambda^2 x^2}{(1 + \lambda x - 2\mu^2 x^2)^2}, \quad (3-28)$$

which correspond to the perturbational results given by Yamaguchi, Fukuhara, and Matayoshi.²³⁾

As has been checked above, our solutions include various limiting cases reasonably, and therefore informations on physical quantities in general cases could be obtained from the solutions for ψ_1 and ψ_2 .

4. Physical Quantities

A. Resistivity

The life time $\tau(\omega)$ in this system is given by

$$\frac{1}{2\tau(\omega)} = c \text{Im}[\lambda t_1^R(\omega) + \mu t_2^R(\omega)],$$

and we find for the resistivity

$$\frac{\Delta R}{R_0} = -\left[\lambda \frac{\partial \psi_1(x_0)}{\partial x_0} + \mu \frac{\partial \psi_2(x_0)}{\partial x_0} \right], \quad (4-1)$$

where c is impurity concentration,

$$R_0 = \frac{3\pi c}{\rho e^2 v_F^2}$$

and

$$x_0 = g(0)$$

The graphs of the eq. (4-1) are shown in Fig. 1 through Fig. 5.

B. Ground state energy and specific heat.

As in the usual way, we have energy of the system; namely,

$$\begin{aligned} \Delta E &= E - E_0 \\ &= \frac{c\rho}{D} \text{Im} \int d\eta \cdot \eta \text{th} \frac{\beta\eta}{2} \left[\lambda t_1^R(\eta) + \eta \psi_2^R(\eta) \right], \end{aligned} \quad (4-2)$$

which is simply calculated in the following.

Expanding eqs (3-14) and (3-15) as power series of ω for $|\omega| \gg D$, we can obtain

$$\begin{aligned} \left[1 + \frac{\pi^2}{4} \lambda^2 \right] \int d\eta \eta \text{th} \frac{\beta\eta}{2} t_1^R(\eta) + \frac{\pi^2}{4} \mu^2 \int d\eta \eta \text{th} \frac{\beta\eta}{2} t_2^R(\eta) \\ = \frac{i\pi\lambda}{2} \int d\eta \cdot \eta \text{th} \frac{\beta\eta}{2}, \end{aligned} \quad (4-3)$$

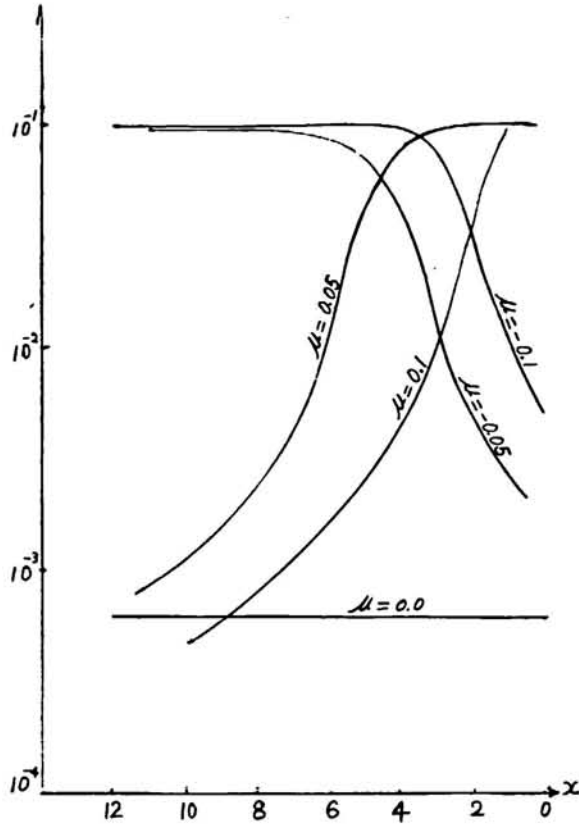


Fig. 2. R vs. x for $\lambda = -0.05$,
where R is resistivity and $x = \log(D/T)$

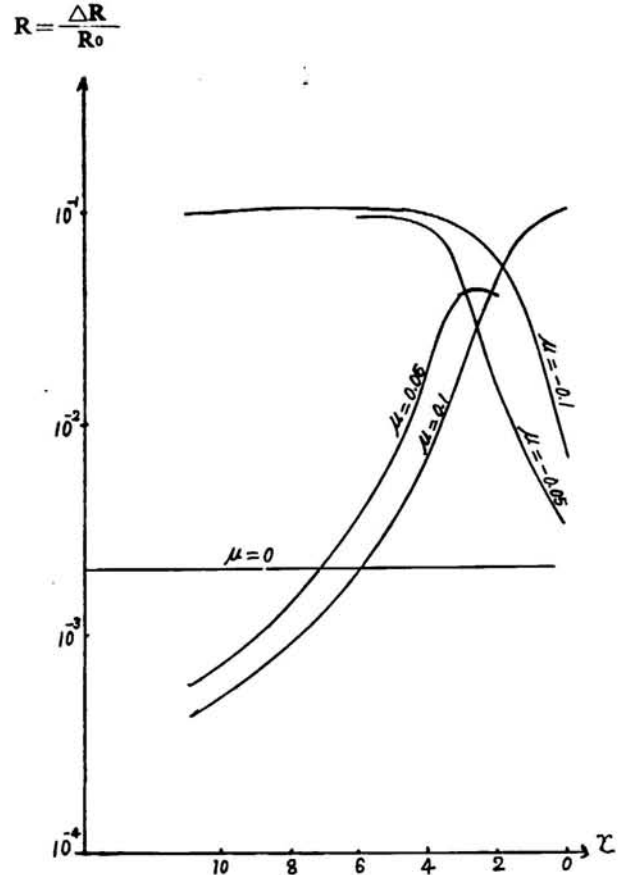


Fig. 1. R vs. x for $\lambda = -0.1$,
where R is resistivity and $x = \log(D/T)$

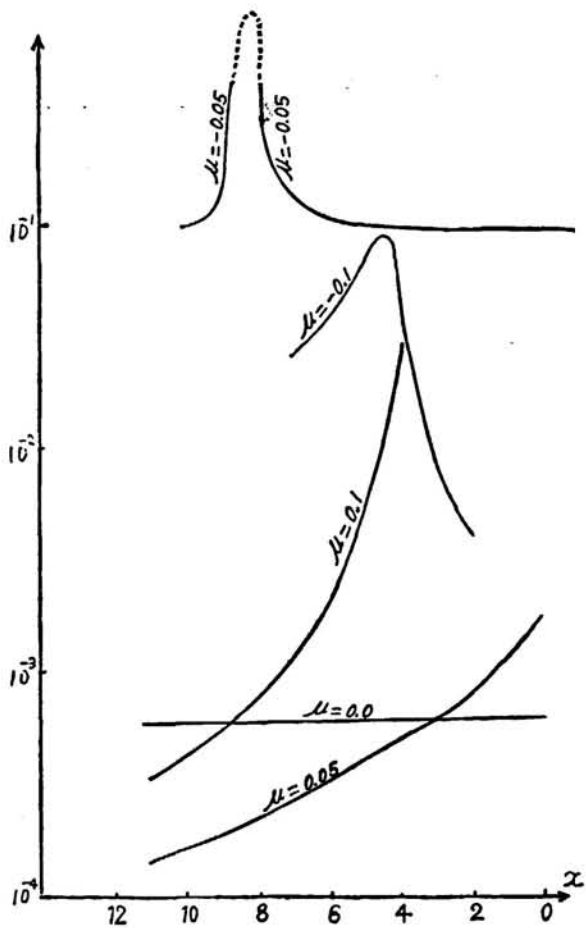


Fig. 4. R vs. x for $\lambda = 0.05$, where R is resistivity and $x = \log(D/T)$

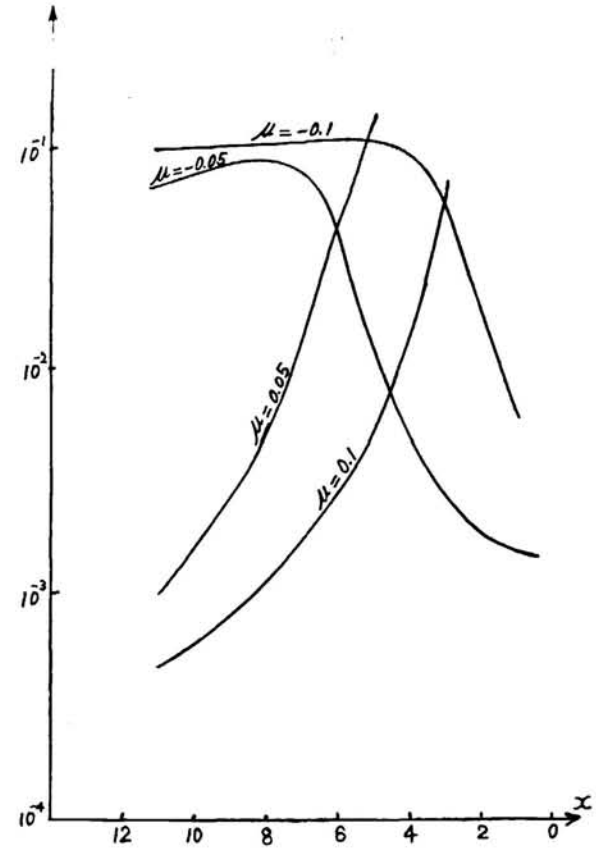


Fig. 3. R vs. x for $\lambda = 0.00$, where R is resistivity and $X = \log(D/T)$

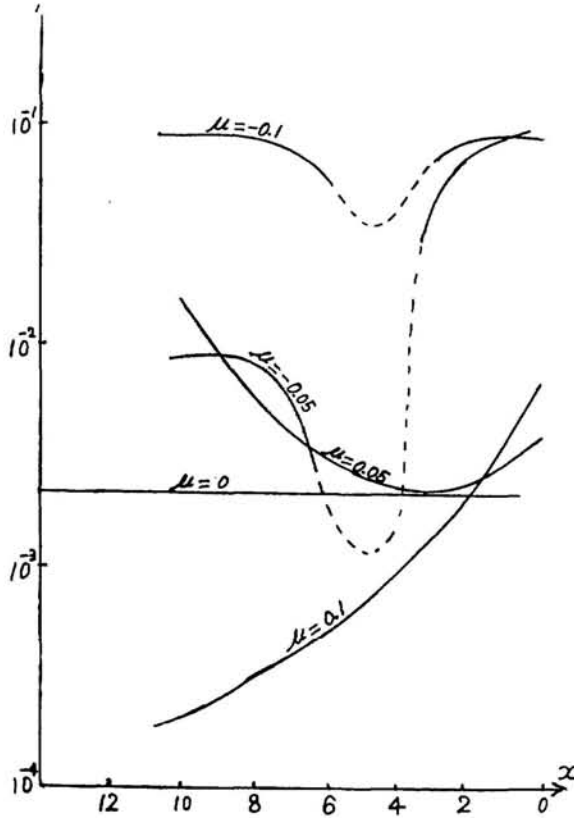


Fig. 5. R vs. x for $\lambda=0.1$, where R is resistivity and $x=\log(D/T)$

and

$$\begin{aligned} \frac{\pi^2}{2} \lambda \mu \int d\eta \cdot \eta \operatorname{th} \frac{\beta \eta}{2} t_1^R(\eta) + \left[1 + \frac{\pi^2}{2} \mu^2 \right] \int d\eta \cdot \eta \operatorname{th} t_2^R(\eta) \\ = i \pi \mu \int d\eta \cdot \eta \operatorname{th} \frac{\beta \eta}{2}, \end{aligned} \quad (4-4)$$

and as a final result we have as follows:

$$\Delta E \approx -\frac{c \rho \pi}{D} \frac{\mu \left[2 + \frac{\pi^2}{2} \mu^2 \right] - \frac{\pi^2}{8} \lambda \mu^2}{\left(1 + \frac{\pi^2}{4} \lambda^2 \right) \left(1 + \frac{\pi^2}{2} \mu^2 \right) - \frac{\pi^4}{8} \lambda \mu^3} \cdot \frac{D^2}{2}. \quad (4-5)$$

using eqs. (4-2), (4-3), and (4-4).

Non-analytic part for λ and μ is not contained, in eq. (4-5), and naturally not in the ground state energy either. In addition we get very easily

$$\Delta C = \frac{\partial \Delta E}{\partial T} = 0, \quad (4-6)$$

as specific heat.

5. Results and Discussions

Since the paper published by Kondo, many works have been done experimentally and theoretically concerning the thermodynamics and transport properties of metals and alloys with small amount of paramagnetic impurities. There have been many works, such as the theories by Abrikosov, Doniach, Suhl, Nagaoka and so on, as stated in the section I. Their works seem to have succeeded to account for the physical quantities, such as the specific heats, etc., in the s-d system. Having known the fault of the susceptibility by Zittartz's calculations, however, we must study to remove the fault in the s-d system. As it is very difficult to treat the usual s-d model in the investigations for the removal of the fault, no one has succeeded in the construction of theory, yet.

To attack this problem from another point of view, we have proposed the model, i. e.,

$$\sigma \hat{J} S$$

instead of the usual isotropic model; i. e.,

$$J \sigma S$$

The reason for the proposition of the new anisotropic model have been stated in the section I.

Since in our system the rotational symmetry breaks down partly any more even in the normal states, the following statistical relations, for example, do not hold,

$$\langle C_{l\uparrow}^{\dagger} C_{l'\uparrow} S_{-} \rangle = 2 \langle C_{l\uparrow}^{\dagger} C_{l'\uparrow} S_z \rangle, \text{ etc.,}$$

which has been utilized by many authors. This makes it difficult to construct a closed set of equations of t' s- matrices.

By introducing matrix type of Green's functions and special type of T_1 operation for matrices, however, we have beautifully got over with this difficulty.

Further merit of our treatment is that it is very suggestive even for the case when the rotational symmetry breaks down completely. We will apply this treatment to the superconducting state in next work.

The results of the ground state energy and specific heat in our calculation do not contain anomalous parts which appear in the Works of Nagaoka, and Bloomfield-Hamann. The anomalous parts for the specific heat have been observed experimentally. This failure, which also appears in Hamann's work, seems to result from the Hamann's approximation. The exact t -solutions, in the B-H treatment,¹⁰⁾ for the simpler integral equations by Hamann have the temperature-dependent phase factor which lacks in the Hamann's approximation. This phase factor does give effect to physical quantities through differentiation with respect to temperature. Therefore, our failure for the specific heat is naturally anticipated.

As for the resistivity, since it does not contain the differentiation in calculation, our result, like Hamann's one, could be considered to be fairly reasonable.

Our results for the reduced resistivity, computed by using the HITAC 10 mini-

computer, are presented in Fig. 1 through Fig. 5. The graphs are drawn for various values of the coupling constants λ and μ . For the cases of $\lambda = \mu$, we have reasonable results corresponding to those of Hamann's. For $\lambda \neq \mu$, excluding a few cases the results have roughly the similar tendencies with those of the cases $\lambda = \mu$.

Because of the limit in practicing of computation, some of the results, especially for $\lambda > 0$, $\mu < 0$, may not be reliable enough. These results, however, do not change monotonously with temperature, but seem to have either minimum or maximum. In realistic system impurity spins ordering through cloud of electron spins may arise and this might be leading to produce some sort of "effective field". At low temperatures this "effective field" might be competitive with temperature in giving effect to electron conduction, producing maximum or minimum in resistivity.

Taking these into consideration, our simple model might have some sort of relation with realistic models, containing many impurity spins. This discussion might be questionable, but seems to of interest enough to be investigated further.

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