Progress of Theoretical Physics, Vol. 35, No. 3, March 1966

Simple Self-Consistent Treatment of Kondo's Effect in Dilute Alloys

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(Received November 10, 1965)

The self-consistent treatment of Kondo's effect by Nagaoka is revised by using the method of Gor'kov in the theory of superconductivity. Expressing the spin operators in terms of Fermi operators, such as $s_z=(a_\uparrow^+a_\uparrow-a_\downarrow^+a_\downarrow)/2$, the Green's functions of the type $\langle\langle c_{k'\uparrow}S_z|c_{k\uparrow}\rangle\rangle$ are decomposed into the sum of terms like $\langle a_\uparrow^+c_{k'\uparrow}\rangle\langle\langle a_\uparrow|c_{k\uparrow}^+\rangle\rangle$. The existence of these terms implies the existence of the bound state between the localized spin and the spin density of conduction electrons. Essentially the same expression for the Green's function of conduction electrons as in Nagaoka's treatment is obtained, but we also have the bound state in the case of ferromagnetic coupling.

Magnetic susceptibility is calculated in our approximation and is shown to be finite at $T=0$ and increase with the increasing temperature tending to infinity like $(T_c-T)^{-1}$ as $T\to T_c$.

§ 1. Introduction

Kondo[1] has first pointed out that the exchange interaction between conduction electrons and a localized spin in metals has the anomalous effects on various properties. He has shown that the resistivity calculated up to the third order of this interaction has a logarithmically divergent term as the temperature goes to zero.

His treatment is, however, essentially the perturbational one, which cannot be considered to be valid in the case where such a singularity occurs. Many authors have tried to develope other methods in order to see what is the nature of this singularity.[2),3),4),7)] In particular, Nagaoka[2] (henceforth, referred to as N) has developed the method which has the direct analogy with Zubarev's treatment[5] of superconductivity, and has shown that the two-time Green's function of conduction electrons has a pole on the imaginary axis when the temperature is low enough, and that the resistivity increases with decreasing temperature, and has a finite value at $T=0$. The equation determining the position of this pole is analogous to the gap equation in the theory of superconductivity, and has a non-zero solution only below a certain temperature T_c. This means that below T_c the perturbational treatment breaks down and a sort of bound state is formed between the localized spin and the spin density of conduction electrons. This bound state has the direct analogy with the Cooper pair in superconductors.

The existence of such a bound state is also suggested in the calculation by

Abrikosov.[3] He has summed up all of the most divergent terms in the perturbation expansion, and obtained the result similar to N. The summation of infinite number of terms of special type in the perturbation series usually implies the existence of a bound state.

Although the results of N seems to be quite reasonable, his calculation is very complicated. Actually, his equation determining the imaginary pole is an approximate one, and cannot be used when $T \sim T_c$. This complication comes partly from the use of the method of Zubarev in the theory of superconductivity. In this paper, we show that essentially the same results can be obtained very easily by the use of Gor'kov's method[6] in the theory of superconductivity. The self-consistent equation obtained can be solved exactly, and then, the magnetic susceptibility of the system is calculated very easily.

The results obtained here are essentially the same as N with one exception. All these authors have concluded that the singularity occurs only in the case of anti-ferromagnetic coupling, but the similar singularity also occurs in the case of ferromagnetic coupling in our treatment. Because we cannot find the suitable physical interpretation of the difference between ferro- and anti-ferromagnetic coupling, it may be possible that the singularity occurs in both cases.

The magnetic susceptibility of the localized spin is shown to remain finite even at $T=0°$K, and to increase with the temperature tending to infinity as $(T_c-T)^{-1}$ when $T \to T_c$.

Above T_c, the perturbational calculation will be good, but, in our treatment, the system behaves like free and the susceptibility obeys the Curie law. This is the same as the situation in the Gor'kov or BCS theory of superconductivity. In these theories, the short range order is completely neglected, and the system is completely free above the transition temperatures. It is true that the short range order is unimportant in superconductivity, but it might not be true in our case. In the theory of second order phase transition, however, the molecular field or Bragg-Williams approximation which neglects the short range order gives the essential nature of the transition and, in a similar sense, our treatment may be considered to give the essential nature of the system in this case.

In § 2, we construct the basic equations using the retarded Green's function, and in § 3, these equations are solved when there is no external magnetic field. In § 4, we calculate the magnetic susceptibility.

§ 2. Basic equations

The system considered here is the conduction electrons interacting with a localized spin at the origin. For later convenience, we write down the Hamiltonian of the system with a uniform external magnetic field H,*)

*) We take the unit $\hbar=1$ and the Boltzmann constant $k_B=1$.

$$\mathcal{H}=\sum_{k,\sigma}\epsilon_k c_{k\sigma}^+ c_{k\sigma}-\frac{J}{2N}\sum_{k,k'}\{(c_{k\uparrow}^+ c_{k'\uparrow}-c_{k\downarrow}^+ c_{k'\downarrow})S^z+c_{k\uparrow}^+ c_{k'\downarrow}S^-$$

$$+C_{k\downarrow}^+ c_{k'\uparrow}S^+\}-\mu_B H\{g'S^z+\frac{1}{2}g\sum_k(c_{k\uparrow}^+ c_{k\uparrow}-c_{k\downarrow}^+ c_{k\downarrow})\}. \qquad (2\cdot1)$$

The notations used are almost the same as in N; μ_B is the Bohr magneton, and g and g' are the g factors of the conduction electrons and the localized spin, respectively. We consider only the case $S=1/2$ for simplicity.

As in N, we use the retarded Green's function defined by

$$G_{kk'}(t)=-i\langle[c_{k'\uparrow}(t),\ c_{k\uparrow}^+]_+\rangle,\quad t>0,$$
$$=0,\qquad t<0, \qquad (2\cdot2)$$

and its Fourier transform is denoted by $G_{kk'}(\omega)=\langle\langle C_{k'\uparrow}|C_{k\uparrow}^+\rangle\rangle$. When we construct the equation of motion of G, there appear terms which contain the higher order Green's function such as

$$\Gamma_{kk'}^z(\omega)=\langle\langle c_{k'\uparrow}S^z|c_{k\uparrow}^+\rangle\rangle. \qquad (2\cdot3)$$

N has constructed the equation of motion of Γ, and Green's functions of higher order than Γ are decomposed into the product of G or Γ with the statistical averages of some quantities. As mentioned in N and in § 1, this procedure is the direct analogy of Zubarev's procedure in the theory of superconductivity. On the other hand, it is well known that there exists a much simpler procedure by Gor'kov, which gives essentially the same results as Zubarev's. Gor'kov's procedure in this case corresponds to the following approximation. First, we express the spin operators in terms of Fermi operators,

$$S^z=\frac{1}{2}(a_\uparrow^+ a_\uparrow-a_\downarrow^+ a_\downarrow),$$

$$S^+=a_\uparrow^+ a_\downarrow,\quad S^-=a_\downarrow^+ a_\uparrow, \qquad (2\cdot4)$$

where*)

$$[a_\sigma,\ a_{\sigma'}^+]_+=\delta_{\sigma,\sigma'},$$
$$[a_\sigma,\ c_{k\sigma'}]_+=0.$$

Using this expression, we can decompose Γ into the product of G and the thermal average of two Fermi operators. For example,

$$\langle\langle c_{k'\uparrow}S^z|c_{k\uparrow}^+\rangle\rangle=\frac{1}{2}\langle\langle c_{k'\uparrow}(a_\uparrow^+ a_\uparrow-a_\downarrow^+ a_\downarrow)|c_{k\uparrow}^+\rangle\rangle$$

$$\to\frac{1}{2}\{\langle a_\uparrow^+ a_\uparrow-a_\downarrow^+ a_\downarrow\rangle\langle\langle c_{k'\uparrow}|c_{k\uparrow}^+\rangle\rangle$$

$$-\langle a_\uparrow^+ c_{k'\uparrow}\rangle\langle\langle a_\downarrow|c_{k\uparrow}^+\rangle\rangle+\langle a_\downarrow^+ c_{k'\uparrow}\rangle\langle\langle a_\downarrow|c_{k\uparrow}^+\rangle\rangle\}. \qquad (2\cdot5)$$

*) The commutation relation between a and c can be taken as $[a, c]=0$, but the final results must be the same.

It is true that the only state which has a physical meaning is that in which $n_d \equiv a_\uparrow^+ a_\uparrow + a_\downarrow^+ a_\downarrow = 1$, but that the unphysical states in which $n_d = 0$ or 2 plays some roles in our treatment. In fact, the true average $\langle a^+ c \rangle$ must vanish because n_d is a constant of motion. The assumption of the existence of this quantity, however, is considered to be convenient to describe the bound state between the localized spin and the spin density of conduction electrons. This is the direct analogy of Gor'kov's treatment of superconductivity, where the existence of the average $\langle \psi\psi \rangle$ implies the formation of the bound state (Cooper pair). We shall discuss this question further in a later section.

Following the above procedure, we obtain the closed system of equations for $G_{kk'}$, and

$$G'_{kk'} \equiv \langle\langle c_{k'\downarrow} | c^+_{k\uparrow} \rangle\rangle,$$
$$F_k \equiv \langle\langle a_\uparrow | c^+_{k\uparrow} \rangle\rangle, \qquad (2\cdot6)$$
$$F'_k \equiv \langle\langle a_\downarrow | c^+_{k\uparrow} \rangle\rangle.$$

The equations of motion of these quantities are

$$(\omega - \epsilon_{k'} + \frac{1}{2} g\mu_B H) G_{kk'} + \frac{J}{2N} \{ S^z \mathcal{G}_k - \sqrt{N} (\frac{1}{2} \alpha^+ + \alpha^-) F_k + \sqrt{N} \frac{\beta^-}{2} F'_k \} = \frac{1}{2\pi} \delta_{k,k'},$$

$$(\omega - \epsilon_{k'} - \frac{1}{2} g\mu_B H) G'_{kk'} + \frac{J}{2N} \{ - S^z \mathcal{G}'_k - \sqrt{N} (\frac{1}{2} \alpha^- + \alpha^+) F'_k + \sqrt{N} \frac{\beta^+}{2} F_k \} = 0, \qquad (2\cdot7)$$

$$(\omega + \frac{1}{2} g'\mu_B H) F_k + \frac{J}{2N} \{ \sigma_z(0) F_k - \sqrt{N} (\frac{1}{2} \alpha^+ + \alpha^-) \mathcal{G}_k + \sqrt{N} \frac{\beta^+}{2} \mathcal{G}'_k \} = 0,$$

$$(\omega - \frac{1}{2} g'\mu_B H) F'_k + \frac{J}{2N} \{ - \sigma_z(0) F'_k - \sqrt{N} (\frac{1}{2} \alpha^- + \alpha^+) \mathcal{G}'_k + \sqrt{N} \frac{\beta^-}{2} \mathcal{G}_k \} = 0,$$

where we have denoted as

$$S^z = \frac{1}{2} \langle a_\uparrow^+ a_\uparrow - a_\downarrow^+ a_\downarrow \rangle,$$

$$\sigma_z(0) = \frac{1}{2} \sum_{k,k'} \langle c^+_{k\uparrow} c_{k'\uparrow} - c^+_{k\downarrow} c_{k'\downarrow} \rangle,$$

$$\alpha^+ = \frac{1}{\sqrt{N}} \sum_{k'} \langle a_\uparrow^+ c_{k'\uparrow} \rangle, \qquad \alpha^- = \frac{1}{\sqrt{N}} \sum_{k'} \langle a_\downarrow^+ c_{k'\downarrow} \rangle, \qquad (2\cdot8)$$

$$\beta^+ = \frac{1}{\sqrt{N}} \sum_{k'} \langle a_\uparrow^+ c_{k'\downarrow} \rangle, \qquad \beta^- = \frac{1}{\sqrt{N}} \sum_{k'} \langle a_\downarrow^+ c_{k'\uparrow} \rangle,$$

and

$$\mathcal{G}_k = \sum_{k'} G_{kk'}(\omega), \tag{2·9}$$
$$\mathcal{G}'_k = \sum_{k'} G'_{kk'}(\omega),$$

and, we have assumed that $\alpha^{\pm}$ and $\beta^{\pm}$ are real.

Thermal averages α^+ and β^- defined in Eq. (2·8) can be calculated from F, F' by using the well-known relations

$$\alpha^+ = \frac{1}{\sqrt{N}} \int_{-\infty}^{\infty} \sum_k \{-2\,\mathrm{Im}\, F_k(\omega)\} f(\omega)\, d\omega,$$
$$\beta^- = \frac{1}{\sqrt{N}} \int_{-\infty}^{\infty} \sum_k \{-2\,\mathrm{Im}\, F'_k(\omega)\} f(\omega)\, d\omega \tag{2·10}$$

with

$$f(\omega) = 1/(e^{\omega/T}+1). \tag{2·11}$$

In order to calculate other averages, we need other Green's functions, but we do not write them down until they are necessary.

§ 3. Solution when $H=0$

First of all, we consider the case where no external magnetic field exists. In this case, we can expect the following relations to hold,

$$S^z = \sigma_z(0) = 0,$$
$$\alpha^+ = \alpha^- \equiv \alpha, \ \beta^+ = \beta^- \equiv \beta. \tag{3·1}$$

Then, Eq. (2·7) becomes

$$(\omega - \epsilon_{k'}) G_{kk'} + \frac{J}{2\sqrt{N}} \left(-\frac{3}{2} \alpha F_k + \frac{1}{2} \beta F'_k \right) = \frac{1}{2\pi} \delta_{k,k'},$$
$$(\omega - \epsilon_{k'}) G'_{kk'} + \frac{J}{2\sqrt{N}} \left(\frac{1}{2} \beta F_k - \frac{3}{2} \alpha F_k' \right) = 0, \tag{3·2}$$
$$\omega F_k + \frac{J}{2\sqrt{N}} \left(-\frac{3}{2} \alpha \mathcal{G}_k + \frac{1}{2} \beta \mathcal{G}_k' \right) = 0,$$
$$\omega F'_k + \frac{J}{2\sqrt{N}} \left(\frac{1}{2} \beta \mathcal{G}_k - \frac{3}{2} \alpha \mathcal{G}'_k \right) = 0.$$

Solving this equation, we obtain

$$\mathcal{G}_k = \frac{1}{2\pi} \frac{1}{\omega - \epsilon_k} \frac{\omega(\omega + iA)}{(\omega + iA)^2 + B^2},$$

$$\mathcal{G}'_k=\frac{1}{2\pi}\frac{1}{\omega-\epsilon_k}\frac{i\omega B}{(\omega+iA)^2+B^2},$$

$$F_k=\frac{J}{2\sqrt{N}}\frac{(3/2)\alpha(\omega+iA)-i(1/2)\beta B}{2\pi(\omega-\epsilon_k)[(\omega+iA)^2+B^2]},\qquad(3\cdot3)$$

$$F'_k=\frac{J}{2\sqrt{N}}\frac{i(3/2)\alpha B-(1/2)\beta(\omega+iA)}{2\pi(\omega-\epsilon_k)[(\omega+iA)^2+B^2]},$$

where we put

$$A=\frac{\pi\rho J^2}{4N}\left(\frac{9}{4}\alpha^2+\frac{1}{4}\beta^2\right)$$

and

$$B=\frac{\pi\rho J^2}{4N}\cdot\frac{3}{2}\alpha\beta.\qquad(3\cdot4)$$

In this calculation, there appears the function

$$P(\omega)=\sum_k\frac{1}{\omega-\epsilon_k},\qquad(3\cdot5)$$

and as in N we have taken only the imaginary part of this function as

$$P(\omega)=-i\pi\rho(\omega),\qquad(3\cdot6)$$

where $\rho(\omega)$ is the density of states of conduction electrons and is taken as a constant in the interval $-D\leq\omega\leq D$.

α and β are determined by Eq. (2·10), from which we obtain

$$[1-3V-3(A^2+B^2)U]\alpha+2ABU\beta=0,$$
$$-6ABU\alpha+[1+V+(A^2+B^2)U]\beta=0,\qquad(3\cdot7)$$

where U, V are given by

$$U=\frac{J\rho}{4N}\int_{-D}^{D}f(\omega)\frac{\omega}{[\omega^2+(A+B)^2][\omega^2+(A-B)^2]}d\omega,$$
$$V=\frac{J\rho}{4N}\int_{-D}^{D}f(\omega)\frac{\omega^3}{[\omega^2+(A+B)^2][\omega^2+(A-B)^2]}d\omega.\qquad(3\cdot8)$$

Equations (3·4), (3·7) and (3·8) determine the values of α and β. The set of equations seems to be very complicated, but we can solve it exactly as follows. First of all, we obtain from Eq. (3·7) as a condition of the existence of the non-trivial solution except $\alpha=\beta=0$,

$$[1-3V-3(A^2+B^2)U][1+V+(A^2+B^2)U]$$
$$+12A^2B^2U^2=0.\qquad(3\cdot9)$$

Taking the difference of the upper equation of (3·7) multiplied by β and the lower one multiplied by 3α, and using the definition (3·4) of A, B, we obtain

$$B[(A^2-B^2)U-(\frac{1}{3}+V)]=0. \tag{3·10}$$

The solution of Eq. (3·10) is

$$B=0 \tag{3·11a}$$

or

$$(A^2-B^2)U=\frac{1}{3}+V. \tag{3·11b}$$

We investigate these two cases separately.

Case I. $B\neq 0$

We can solve Eqs. (3·9) and (3·11b) with respect to U, V, getting

$$U=\pm\frac{1}{3A\sqrt{A^2-B^2}},$$

$$V=\pm\frac{\sqrt{A^2-B^2}}{3A}-\frac{1}{3}. \tag{3·12}$$

Because the integral in Eq. (3·8) is negative ($f(\omega)$ is finite for $\omega<0$ and is very small for $\omega>0$), U and V are of opposite sign to J, and the double sign in Eq. (3·12) should be taken as consistent with this sign. The integrals in Eq. (3·8) can be simplified as follows,

$$U=\frac{1}{4AB}[W(A-B)-W(A+B)],$$

$$V=\frac{1}{4AB}[(A+B)^2W(A-B)-(A-B)^2W(A+B)], \tag{3·13}$$

where

$$W(x)\equiv\frac{J\rho}{4N}\int_{-D}^{D}f(\omega)\frac{\omega}{\omega^2+x^2}d\omega. \tag{3·14}$$

From Eqs. (3·12) and (3·13), we obtain

$$W(A-B)=\pm\frac{2B}{3A}\sqrt{\frac{A-B}{A+B}}-\frac{1}{3}, \tag{3·15}$$

$$W(A+B)=\mp\frac{2B}{3A}\sqrt{\frac{A+B}{A-B}}-\frac{1}{3}.$$

At $T=0°$K, $W(x)$ becomes

$$W(x)=\frac{J\rho}{4N}\log\frac{x}{D},$$

if we assume A, $B\ll D$. Therefore, we obtain from Eqs. (3·15)

$$\frac{J\rho}{4N}\log\frac{A-B}{A+B}=\pm\frac{4B}{3\sqrt{A^2-B^2}},$$

which can be written as

$$\frac{J\rho}{2N}\log t=\pm\frac{4}{3}\frac{t^2-1}{t}, \qquad (3\cdot16)$$

by putting

$$\sqrt{\frac{A+B}{A-B}}\equiv t.$$

Equation (3·16) always has a solution $t=1$, which corresponds to $B=0$. In order to have a solution $t\neq1$, it is necessary that

$$\frac{|J|\rho}{N}>\frac{16}{3}. \qquad (3\cdot17)$$

In the actual case, the order of magnitude of $|J|\rho/N$ is 0.1 and, therefore the condition (3·17) can hardly be satisfied. We do not consider this case any longer, and proceed to the case $B=0$.

Case II. $B=0$

In this case, the solution of Eq. (3·7) becomes

$$\beta=0,\ A^2U+V=\frac{1}{3} \qquad (3\cdot18a)$$

or

$$\alpha=0,\ A^2U+V=-1. \qquad (3\cdot18b)$$

Using Eq. (3·8), we can see that

$$A^2U+V=\frac{J\rho}{4N}\int_{-D}^{D}f(\omega)\frac{\omega}{\omega^2+A^2}d\omega,$$

and because the integral on the right-hand side is negative, Eq. (3·18a) has a solution when $J<0$, and (3·18b) when $J>0$. Thus, we can summarize the final results as follows;

(1) $J<0$ (antiferromagnetic coupling)

$\beta=0$, and α is determined from the equation

$$\frac{J\rho}{4N}\int_{-D}^{D}f(\omega)\frac{\omega}{\omega^2+A^2}d\omega=\frac{1}{3},$$

$$A=\frac{9\pi\rho J^2}{16N}\alpha^2, \tag{3·19a}$$

(2) $J>0$ (ferromagnetic coupling)
$\alpha=0$, and β is determined from the equation

$$\frac{J\rho}{4N}\int_{-D}^{D} f(\omega)\frac{\omega}{\omega^2+A^2}d\omega=-1,$$

$$A=\frac{\pi\rho J^2}{16N}\beta^2. \tag{3·19b}$$

It is easily seen that A is essentially the same as Δ in N, and that the Green's function of conduction electrons is of the same form as in N. Thus, the conclusion about the physical behavior of the system is also essentially the same as N.

The important difference is that we have the similar results for $J>0$ as $J<0$. Thus, we can expect the anomalous behavior for $J>0$ as well as $J<0$.

The other important difference is that our equation can be used in any temperature region. In N, the gap equation similar to Eq. (3·19a) cannot be used for small A owing to the approximation used to derive the equation. Thus, nothing can be said about what happens just below the critical temperature T_c. In our treatment, the critical temperature T_c is determined by

$$\frac{J\rho}{4N}\int_0^D \frac{1}{\omega}\tanh\frac{\omega}{2T_c}d\omega=-\frac{1}{3}, \text{ for } J<0,$$

$$\text{or } 1, \text{ for } J>0. \tag{3·20}$$

The physical meaning of the conclusion that $\beta=0$ for $J<0$ and $\alpha=0$ for $J>0$ is clear if we calculate the following quantity,

$$p=\langle(a_\uparrow^+ a_\uparrow - a_\downarrow^+ a_\downarrow)\sum_{kk'}(c_{k\uparrow}^+ c_{k'\uparrow} - c_{k\downarrow}^+ c_{k'\downarrow})\rangle,$$

which can be expressed in terms of α and β as

$$p=2N(-\alpha^2+\beta^2).$$

Thus, we can see that for $J<0$, β vanishes and p is negative, and that for $J>0$, α vanishes and p is positive, as expected.

§ 4. Magnetic susceptibility

As an example of applications, we want to show how the magnetic susceptibility of the system is calculated in our approximation. This quantity has been calculated by Yosida and Okiji,[7] and Miwa[8] by using the perturbation expansion, which is considered to be valid above T_c from our point of view. Our calculation is valid below T_c, and can be said to be complementary to these of references 7) and 8).

In the calculation of the susceptibility, we need all quantities up to linear terms to the magnetic field H. For simplicity, let us consider the case $J<0$, and take $\beta=0$ from the beginning. From the symmetry consideration, it is shown that

$$\alpha^+=\alpha+\delta\alpha,$$
$$\alpha^-=\alpha-\delta\alpha, \tag{4·1}$$

where α is given by Eq. (3·19a) and $\delta\alpha$ is linear to H. Equation (2·7) becomes

$$(\omega-\epsilon_{k'}+\frac{1}{2}g\mu_B H)G_{kk'}+\frac{J}{2N}\left\{S^z\mathcal{G}_k-\sqrt{N}\left(\frac{3}{2}\alpha-\frac{1}{2}\delta\alpha\right)F_k\right\}=\frac{1}{2\pi}\delta_{kk'}, \tag{4·2a}$$

$$(\omega+\frac{1}{2}g'\mu_B H)F_k+\frac{J}{2N}\left\{\sigma_z(0)F_k-\sqrt{N}\left(\frac{3}{2}\alpha-\frac{1}{2}\delta\alpha\right)\mathcal{G}_k\right\}=0. \tag{4·2b}$$

Dividing Eq. (4·2a) by $(\omega-\epsilon_{k'}+(1/2)g\mu_B H)$ and taking the summation over $\boldsymbol{k}'$, we obtain

$$\mathcal{G}_k+\frac{J}{2\pi}(-i\pi\rho_+)\left\{S^z\mathcal{G}_k-\sqrt{N}\left(\frac{3}{2}\alpha-\frac{1}{2}\delta\alpha\right)F_k\right\}=\frac{1}{2\pi}\,\frac{1}{\omega-\epsilon_k+(1/2)g\mu_B H}, \tag{4·3}$$

where we put $\rho_+=\rho(\omega+(1/2)g\mu_B H)$. From Eqs. (4·2b) and (4·3), we obtain

$$\sum_k\mathcal{G}_k=-\frac{i}{2}\,\frac{\omega\rho_+}{\omega+iA_+}+\frac{\rho}{2}\,\frac{1}{(\omega+iA)^2}\left\{A\left(\frac{1}{2}g'\mu_B H+\frac{J}{2N}\sigma_z(0)\right)\right.$$
$$\left.+\omega\left(\frac{J}{2N}\pi\rho\omega S^z+\frac{3J^2}{8N}\pi\rho\alpha\delta\alpha\right)\right\}, \tag{4·4}$$

$$\sum_k F_k=-\frac{3J}{8\sqrt{N}}\alpha\frac{\rho_+}{\omega+iA_+}+\frac{J\rho}{8\sqrt{N}(\omega+iA)^2}\left\{(\omega-iA)\delta\alpha\right.$$
$$\left.+3\alpha\left(\frac{1}{2}g'\mu_B H+\frac{J}{2N}\sigma_z(0)-i\frac{3J}{2N}\pi\rho\alpha S^z\right)\right\} \tag{4·5}$$

up to linear terms to H. Here, A is given by Eq. (3·4) and A_+ is given by replacing ρ in A by ρ_+.

$\sigma_z(0)=\frac{1}{2}\langle\sum_{kk'}(c^+_{k\uparrow}c_{k'\uparrow}-c^+_{k\downarrow}c_{k'\downarrow})\rangle$ and $\delta\alpha$ can be calculated from the relations

$$\langle\sum_{kk'}c^+_{k\uparrow}c_{k'\uparrow}\rangle=-2\int_{-\infty}^{\infty}\mathrm{Im}\sum_k\mathcal{G}_k(\omega)f(\omega)\,d\omega \tag{4·6}$$

and

$$\alpha+\delta\alpha=-\frac{2}{\sqrt{N}}\int_{-\infty}^{\infty}\mathrm{Im}\sum_{k}F_k(\omega)f(\omega)\,d\omega. \tag{4·7}$$

In order to calculate S^z, we need another Green's function,

$$L\equiv\langle\langle a_\uparrow|a_\uparrow^+\rangle\rangle. \tag{4·8}$$

In the equation of motion of L constructed in a same way as before, there appears the Green's function

$$M_k\equiv\langle\langle c_{k\uparrow}^+|a_\uparrow^+\rangle\rangle. \tag{4·9}$$

The set of equations of motion for L and M_k can be solved in a similar way, giving

$$L=\frac{1}{2\pi}\frac{1}{\omega+iA_+}-\frac{1}{2\pi}\frac{1}{(\omega+iA)^2}\left\{\left(\frac{1}{2}g'\mu_B H+\frac{J}{2N}\sigma_z(0)\right)\right.$$
$$\left.-\frac{J}{2N}\pi\rho AS^z-i\pi\rho\frac{3J^2}{8N}\alpha\delta\alpha\right\}, \tag{4·10}$$

and the expression for $\sum_k M_k$ is the same as $\sum_k F_k$, Eq. (4·5).

From Eq. (4·10), we obtain

$$\langle a_\uparrow^+ a_\uparrow\rangle=-2\int_{-\infty}^{\infty}\mathrm{Im}\,L(\omega)f(\omega)\,d\omega, \tag{4·11}$$

and, thus, we can get $S^z=(1/2)\langle(a_\uparrow^+a_\uparrow-a_\downarrow^+a_\downarrow)\rangle$. Calculating $\sigma_z(0)$, $\delta\alpha$ and S^z by using Eqs. (4·6), (4·7) and (4·11), we obtain the closed set of equations for these quantities. In the calculation of the integrals of the first terms of Eqs. (4·4), (4·5) and (4·11), there appear integrals of the type

$$\int_{-\infty}^{\infty}\frac{\omega}{\omega^2+A_+^2}\rho_+ f(\omega)\,d\omega,$$

which can be transformed into the form

$$\int_{-\infty}^{\infty}\frac{\omega-(1/2)g\mu_B H}{(\omega-(1/2)g\mu_B H)^2+A^2}\rho(\omega)f\left(\omega-\frac{1}{2}g\mu_B H\right)d\omega,$$

and is calculated up to linear terms to H.

The set of equations for S^z, $\sigma_z(0)$ and $\delta\alpha$ becomes

$$S^z=-\frac{2A}{\pi}v_1\left[\frac{1}{2}g'\mu_B H+\frac{J}{2N}\sigma_z(0)-\frac{J\rho}{2N}\pi AS^z\right]-\frac{3J^2}{4N}\rho\alpha(v_2-A^2v_0)\delta\alpha,$$

$$\sigma_z(0)=2\rho A^2v_1\left[\frac{1}{2}g'\mu_B H+\frac{J}{2N}\sigma_z(0)-\frac{1}{2}g\mu_B H\right]$$
$$+\frac{3J^2}{8N}\pi\rho^2A\alpha v_2\delta\alpha+\frac{J}{N}\pi\rho^2Av_3S^z,$$

$$\delta\alpha = -\frac{3J}{4N}\rho\alpha(v_2 - A^2 v_0)\left[\frac{1}{2}g'\mu_B H + \frac{J}{2N}\sigma_z(0) - \frac{1}{2}g\mu_B H\right]$$
$$-\frac{J\rho}{2N}(v_3 - 3A^2 v_1)\delta\alpha + \frac{3J^2}{4N^2}\pi\rho^2\alpha A v_2 S^z, \quad (4\cdot 12)$$

where v_n's are defined as

$$v_n \equiv \int_{-D}^{D} \frac{\omega^n}{(\omega^2 + A^2)^2} f(\omega)\, d\omega. \quad (4\cdot 13)$$

The integrals v_0, v_1 and v_2 remain finite in the limit $D \to \infty$, $T \to 0°$K, and, therefore we can put

$$v_0 = \frac{\pi}{4A^3}, \quad v_1 = -\frac{1}{2A^2}, \quad v_2 = \frac{\pi}{4A}.$$

A simple transformation of the integral v_3 and use of Eq. (3·19a) gives

$$v_3 = \frac{4N}{3J\rho} + \frac{1}{2}.$$

Thus, Eqs. (4·12) become very simple and the solution is

$$S^z = \frac{\left(\frac{4}{3} + y\right)(g' + yg)\frac{\rho}{2N}\mu_B H}{\frac{9}{4}\pi^2 y^2 \alpha^2\left[\left(1 + \frac{2}{3}y\right)\left(\frac{4}{3} + y\right) - \frac{\pi^2}{4}y\right]}, \quad (4\cdot 14)$$

where we have put

$$y \equiv \frac{J\rho}{2N}, \quad (4\cdot 15)$$

and the definition (3·19a) of A has been used.

The uniform spin polarization of conduction electrons

$$\sigma_z = \frac{1}{2}\sum_k \langle (c_{k\uparrow}^+ c_{k\uparrow} - c_{k\downarrow}^+ c_{k\downarrow}) \rangle$$

can be calculated by using the Green's function $G_{kk'}$, and is shown to be

$$\sigma_z = \frac{1}{2}\rho g \mu_B H + \frac{J\rho}{2N} S^z. \quad (4\cdot 16)$$

The first term of Eq. (4·16) is nothing but the usual magnetization, and the second term is the additional polarization due to the interaction. It has been shown by Yosida and Okiji[7] that the singular part of this additional term is proportional to S^z and the proportional coefficient is $J\rho/2N$. Their calculation

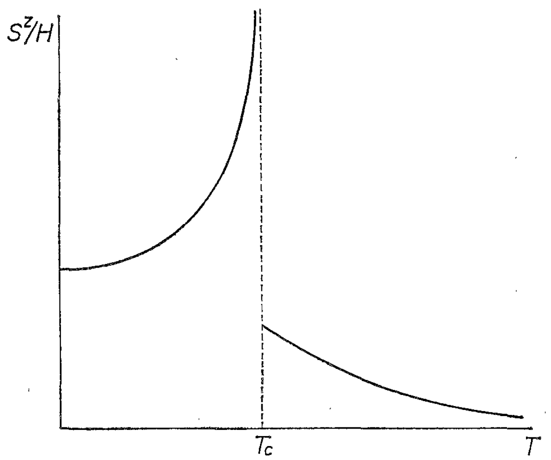

Fig. 1. Schematic behavior of S_z/H as a function of T.

is a perturbational one and seems to be valid above T_c. Our calculation is considered to be valid below T_c, and thus, this character of the polarization may be considered to be a general one.

The temperature dependence of S^z/H comes from α^2 in Eq. (4·14). Since α^2 is proportional to (T_c-T) near $T=T_c$ and increases with decreasing temperature remaining finite at $T=0°$K (see Fig. 1 of reference 2)), S^z/H remains finite at $T=0°$K and increases with increasing temperature, tending to infinity as $(T_c-T)^{-1}$ near $T=T_c$. The schematic behavior of S^z/H is shown in Fig. 1.

As mentioned in § 1, the system is free above T_c in our approximation, so that S^z/H obeys the Curie law.

The calculation for $J>0$ is essentially the same as for $J<0$. Equation (4·16) still holds in this case and S^z is given by

$$S^z=\frac{2}{\pi^2y^2\beta^2}\frac{(g'+yg)\mu_BH}{1+2y-(\pi^2/4)y^2}, \tag{4·17}$$

where y is given by Eq. (4·15) and β is given by Eq. (3·19b). It is easily seen that the qualitative behavior of S^z/H is completely same as in the case of $J<0$.

§ 5. Conclusion and discussions

The self-consistent treatment of N is simplified by using the method similar to Gor'kov's method of superconductivity. Since the expression obtained for the Green's function of conduction electrons is completely the same as in N, the behaviors of the physical quantities such as the resistivity and the specific heat derived in N can be reproduced. The mathematics involved, however, becomes much simpler, and the equations obtained can be solved exactly. It is concluded that some sort of bound state between the localized spin and the spin density of conduction electrons is formed below a certain temperature T_c. While the behaviors of the system near T_c are ambiguous in the treatment of N, our treatment enables one to discuss them clearly.

It is to be noted that our procedure corresponds to that used to obtain a new Hartree-Fock solution, when the normal solution becomes unstable.[9]

Another important conclusion is that the singularity occurs both in ferro- and antiferromagnetic couplings. Although this is in contradiction with those of all other calculations, this conclusion might be true. The reason is that there seems to exist no suitable physical interpretation for the singularity to occur only in the case of $J<0$, as mentioned in § 1.

We have calculated the magnetic susceptibility. The contribution from the localized spin remains finite at $T=0°K$, and increases with the temperature and is proportional to $(T_c-T)^{-1}$ near $T=T_c$. The polarization of conduction electrons has an additional term due to the *s-d* exchange interaction. This additional term has been shown to be of the form $(J\rho/2N)S^z$, irrespective of the sign of J. This fact has also been obtained by Yosida and Okiji,[7] whose calculation is a perturbational one and seems to be valid above T_c. Since our calculation is considered to be valid below T_c, we feel that this fact is a general characteristic of the system.

Finally, one remark must be added on our treatment. As mentioned in § 2, the unphysical states in which $n_d \equiv a_\uparrow^+ a_\uparrow + a_\downarrow^+ a_\downarrow = 0$ or 2 might play some roles in our treatment. The similar situation occurs in Gor'kov's treatment of superconductivity, but there seems to exist one important difference. In the theory of superconductivity, the total number N of electrons is very large, and the fluctuation of this quantity can be neglected completely. On the other hand, n_d in our system is of the order of unity, and the fluctuation of n_d may not be neglected. Therefore, one might argue that our treatment is irrelevant to the singularity of the *s-d* interaction discussed by Kondo.[1] The coincidence of our results to those of N, however, gives the opposite feeling. It might be true that our treatment has nothing to do with the logarithmic singularity of the *s-d* interaction, but it might be also true that our method is closely connected with that of N. A further study is necessary to clarify this situation.

Acknowledgement

The authors wish to express their sincere thanks to Dr. T. Osawa and Mr. K. Takanaka for their valuable discussions. One of authors (T.O.) is indebted to the Iwanami-Fujukai Foundation for financial support.

References

1) J. Kondo, Prog. Theor. Phys. **32** (1964), 37.
2) Y. Nagaoka, Phys. Rev. **138** (1965), 1112 A.
3) A. A. Abrikosov, Soviet Phys.-JETP **21** (1965), 660; Pysics **2** (1965), 5.
4) H. Suhl, Phys. Rev. **138** (1965), 515 A; Physics **2** (1965), 39.
5) D. N. Zubarev, Soviet Phys.-Uspekhi **3** (1960), 320.
6) L. P. Gor'kov, Soviet Phys.-JETP **7** (1958), 505.
7) K. Yosida and A. Okiji, Prog. Theor. Phys. **34** (1965), 505.
8) H. Miwa, Prog. Theor. Phys. **34** (1965), 1040.
9) N. Fukuda, T. Ogawa and T. Soda, Prog. Theor. Phys. Suppl. Extra Number (1965) 492.