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Doctor Thesis

Theory of Itinerant Electron Antiferromagnetism

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## §1. Introduction

§§1.1. Electron Correlation in a Narrow Band

§§1.2. Itinerant Electron Antiferromagnetism

§§1.3. Physical Properties at Finite Temperatures

## §2. The Self-Consistent Renormalization Theory of Spin Fluctuations

§§2.1. Moriya-Kawabata Theory

§§2.2. Hasegawa-Moriya Theory

## §3. Physical Properties Related to the Spin Fluctuations

§§3.1. NMR Relaxation Rate

§§3.2. Specific Heat

§§3.3. Magnetic Excitations

§§3.4. Electrical Resistivity

## §4. Summary and Discussions

Acknowledgments

Appendix

References

Figures

## §1 Introduction

Since the pioneering work of Heisenberg on ferromagnetism,<sup>1)</sup> magnetism of transition metals has been one of the central problems of solid state physics in the past half century and will also continue to be the one in future. Recently, our understanding of itinerant electron magnetism seems to have made a significant progress beyond the conventional Hartree-Fock treatments. The fundamental concept underlying the recent developments is that the thermodynamical properties of itinerant magnets are dominated by the spin fluctuations. This concept manifests that electron correlation or many body effects are essentially important for the excited states.

The main purpose of the present article is to discuss physical properties of itinerant antiferromagnets, with particular emphasis on NMR relaxation rate, electrical resistivity and magnetic excitations. As our treatments of the subjects are in line with the above-mentioned recent developments, their review forms another essential part of the present article. In view of the theoretical nature of the present article we do not intend to survey experimental results systematically but should like to refer to some relevant ones from our theoretical point of view.

The composition of the present article is as follows. In section 1 we review the historical developments of the theory of magnetism and call attention to the importance of the spin fluctuations. The importance becomes evident also by examining experimental results. These discussions play a role of detailed introduction to the later sections. Section 2 is devoted to a review of the self-consistent renormalization theory of spin

fluctuations developed by Moriya and Kawabata<sup>2)</sup> (hereafter abbreviated to MK) for ferromagnetism and Hasegawa and Moriya<sup>3)</sup> (HM) for antiferromagnetism. Section 3 is the main part of the present paper. We discuss several physical quantities which are closely related to the spin fluctuations; NMR relaxation rate, specific heat, spectrum of magnetic excitations and electrical resistivity. Finally in section 4 we briefly summarize the results and comment on important problems still to be solved.

### §§1.1. Electron Correlation in a Narrow Band

From the very early stage of the theory there have been two streams of the theoretical consideration of magnetism of transition metals. One is the localized model initiated by Heisenberg.<sup>1)</sup> His original theory was based on the Heitler and London method, each electron being localized on a particular atom and coupled with each other through ferromagnetic direct exchange. Another is the itinerant model initiated by Bloch<sup>4)</sup> and then developed by Slater<sup>5,6)</sup> and Stoner.<sup>7)</sup>

Bloch studied an electron gas with the Coulomb interaction and discussed possibility of ferromagnetism by using the Hartree-Fock approximation (HFA) and concluded that a low density electron gas was ferromagnetic. In a more rigorous treatment than HFA the electrons keep away from each other owing to the Coulomb repulsion. This effect (correlation) is far more effective for an electron pair of different spins than for a pair of the same spin where Pauli's exclusion principle already prevents the electrons to come across. So the correlation effect acts favoring paramagnetism and Wigner concluded that electron gas could never be ferromagnetic at all metallic densities.<sup>8)</sup>

Taking the d-character of the electrons into consideration, Slater obtained a model hamiltonian and discussed the condition for ferromagnetism within the HFA. A simplified version of the hamiltonian which neglects the d-orbital degeneracy is now generally known as the Hubbard hamiltonian:

$$H = \sum_{i,j,\sigma} t_{ij} a_{i\sigma}^+ a_{j\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow}$$

$$= \sum_{k,\sigma} \epsilon_k a_{k\sigma}^+ a_{k\sigma} + I \sum_{k,k',q} a_{k+q\uparrow}^+ a_{k'-q\downarrow}^+ a_{k'\downarrow} a_{k\uparrow}, \quad (1.1)$$

where  $U=N_0 I$  is the intra atomic Coulomb repulsion and the notations are standard; the first line is in the Wannier representation and the second line in the Bloch representation. Subsequently, Stoner calculated thermodynamical properties of the hamiltonian within the HFA.

The correlation effect in the ground state of hamiltonian (1.1) has been investigated by several authors by various methods; decoupling of two-time Green's function by Hubbard,<sup>9,10)</sup> variational method by Gutzwiller<sup>11)</sup> and Brueckner's t-matrix method by Kanamori.<sup>12)</sup> The essential conclusions about the condition for ferromagnetic instability are the same for all the treatments. The condition of HFA

$$U\rho_a(\epsilon_F) > 1, \quad (1.2)$$

where  $\rho_a(\epsilon_F)$  is the density of states per atom at the Fermi energy is replaced by

$$U_{\text{eff}}\rho_a(\epsilon_F) > 1, \quad (1.3)$$

where  $U_{\text{eff}}$  is the effective interaction whose magnitude is reduced to the order of the band width in the narrow band case. The physical meaning of the reduction to the effective interaction is as follows. When the intra atomic Coulomb repulsion is large the electrons will avoid sharing the same atomic orbital at the expense of the one electron energy of the order of the band width. As  $[\rho_a(\epsilon_F)]^{-1}$  is of the order of the band width, the condition

(1.3) is fulfilled when the Fermi energy lies at the peak of the density of states and this situation is what happens in Ni. As for more detailed discussion on the correlation we refer to Herring's excellent review.<sup>13)</sup>

Before the appearance of the above-mentioned treatments of the correlation Mott presented an important concept.<sup>14)</sup> He stated that the Heisenberg method and the band theoretical treatment were not regarded as compatible approximations to the same electronic state. Alternatively, crystalline solids, which in the ordinary band model have incompletely filled Brillouin zones, fall into two classes according to the strength of the Coulomb repulsion: those for which the Heisenberg treatment is appropriate (insulator) and those for which the other is appropriate (metal). If one varies the band width or the strength of the Coulomb repulsion, a transition between the two states will occur at some critical value of  $t/U$ . The critical value is expected to be of the order of unity. He considered that this metal-insulator transition (Mott transition) is sharp due to the mutual screening effect of the electrons. Actually Hubbard has shown that his decoupling formalism for the two time Green's function can lead to a qualitative description of the transition.<sup>10)</sup> Brinkman and Rice have pointed out that the Gutzwiller's solution also contains the transition.<sup>15)</sup>

Magnetic property of the Mott insulator has been investigated earlier by Anderson,<sup>16)</sup> although the expression of the exchange constant stated below have already been obtained by Slater in connection with spin waves.<sup>6)</sup> He has shown among many other things that the hamiltonian (1.1) in the half-filled case is reduced to

a spin hamiltonian of the Heisenberg type

$$\sum_{i,j} \frac{2|t_{ij}|^2}{U} \vec{s}_i \cdot \vec{s}_j, \quad (1.4)$$

when  $U$  is much greater than the band width. This interaction, which he calls kinetic exchange, is antiferromagnetic. Relative strength of the kinetic exchange and direct exchange which is ferromagnetic determines the magnetic property: antiferro- or ferromagnetism. Insulating magnetic compounds are considered to be the Mott insulators and the major part of them are antiferromagnetic.

## §§1.2. Itinerant Electron Antiferromagnetism

In the preceding subsection we made a sketch of our understanding of magnetism especially referring to the hamiltonian (1.1). We saw there that the insulating limit of hamiltonian (1.1) describes antiferromagnetism of the Heisenberg type. Now we investigate the metallic side of the hamiltonian (1.1). Slater<sup>17)</sup> pointed out that HFA can describe not only para- and ferromagnetism but also antiferromagnetism. Let us assume that the effect of correlation of Kanamori type may be taken account of by replacing the intra atomic Coulomb repulsion by the effective one (hereafter we abbreviate  $U_{\text{eff}}(I_{\text{eff}})$  to  $U(I)$ ), and then we study by the HFA what kind of instability may occur from paramagnetic side. This problem can be treated by using a linear response theory.

The most general transversal dynamical susceptibility (wave vector and frequency dependent susceptibility) is defined by

$$\begin{aligned} \chi^{-+}(q, q'; \omega) \\ = i \int_0^{\infty} dt e^{i\omega t} \langle [s_-(q, t), s_+(q')] \rangle, \end{aligned} \quad (1.5)$$

where

$$\begin{aligned} s_-(q) &= \sum_k a_{k+q\downarrow}^+ a_{k\uparrow}, \\ s_+(q) &= \sum_k a_{k+q\uparrow}^+ a_{k\downarrow}, \\ s_z(q) &= \frac{1}{2} \sum_k (a_{k+q\uparrow}^+ a_{k\uparrow} - a_{k+q\downarrow}^+ a_{k\downarrow}), \end{aligned} \quad (1.6)$$

are the spin density operators and  $\langle A \rangle$  denotes the thermal average of operator A. For diagonal components ( $q' = -q$ ) we abbreviate  $\chi^{-+}(q, -q; \omega)$  to  $\chi^{-+}(q, \omega)$  as usual. Izuyama, Kim and Kubo<sup>18)</sup> investigated  $\chi^{-+}(q, \omega)$  by using random phase approximation (RPA);

$$\chi^{-+}(q, \omega) = \chi_0^{-+}(q, \omega) [1 - I \chi_0^{-+}(q, \omega)]^{-1}, \quad (1.7)$$

with

$$\chi_0^{-+}(q, \omega) = \sum_k \frac{f(\epsilon_k) - f(\epsilon_{k+q})}{\epsilon_{k+q} - \epsilon_k - \omega}, \quad (1.8)$$

where  $\chi_0^{-+}(q, \omega)$  is the dynamical susceptibility of non-interacting system and  $f(\epsilon)$  is the Fermi distribution function. The approximation (RPA) may be considered to be an extension of the HFA to the dynamical problem (dynamical HFA). The static limit of  $\chi^{-+}(q, \omega)$  is the wave vector dependent susceptibility and coincides with one obtained by the HFA. Its divergence denotes an instability toward a spin density wave (SDW) state whose wave vector is Q. From eq.(1.7) the condition is given by

$$1 = I \chi_0^{-+}(Q, 0). \quad (1.9)$$

When Q is zero, SDW reduces to ferromagnetism and to intrinsic antiferromagnetism, when Q is half the reciprocal lattice vector.

Originally the concept of SDW is proposed by Overhauser.<sup>19,20)</sup> He showed firstly that one dimensional system was unstable toward SDW with  $Q=2k_F$ , where  $k_F$  was the Fermi wave vector, and then showed that three dimensional electron gas with long range Coulomb interaction was also unstable in the HFA. However the instability of

the latter disappears when screening effect is taken into account.<sup>21)</sup> On the basis of Lomer's indication<sup>22)</sup> that electron and hole pockets near  $\Gamma$  and H points stabilize the antiferromagnetic structure of Cr, several authors investigated SDW by using idealized models for the band structure and short range electron-electron interaction. As is seen from eq.(1.9) what is necessary to discuss the instability is the wave vector dependent susceptibility of the non-interacting system. Fedders and Martin<sup>21)</sup> introduced spherical electron and hole Fermi surfaces of the same radius (perfect nesting), Shibatani, Motizuki and Nagamiya<sup>23)</sup> two octahedral Fermi surfaces of nearly the same size and Rice<sup>24)</sup> two spherical surfaces with different radii.

Although theories of this type, which assume electron and hole pockets of nearly the same size and may be called a nesting type, have such an advantage that the models are easily tractable mathematically, they are considered to be special ones. First of all, the nesting condition is considered to be satisfied only accidentally. Secondly, in the perfect nesting case,  $\chi_0^{-+}(q,0)$  at  $T=0$  shows a logarithmic divergence at  $q=Q$ ,  $Q$  being the wave vector spanning the electron and hole Fermi surfaces. In general the condition for antiferromagnetism is given by the inequality: the right hand side of eq.(1.9) is larger than the left hand side. Thirdly, in the ordered phase, the moment arises only from the electronic states which locate near the electron and hole Fermi surfaces in the nesting model. Even for Cr which is known to be the best candidate for the model to be applicable, electronic states in a much wider region in the  $k$  space contribute to the moment.

Tachiki and Nagamiya<sup>25)</sup> and Alexander and Horwitz<sup>26)</sup> have investigated an electron gas model with Umklapp processes. This model can describe intrinsic antiferromagnetism, where  $Q$  is half the reciprocal lattice vector. The model is considered to belong to a more general class than the nesting model in view of the above discussions. We use it for numerical calculations in the following sections.

### §§1.3. Physical Properties at Finite Temperatures

The band calculations have successfully reproduced the Fermi surfaces of 3d transition metals (Ni, Fe, Cr etc.) in their ordered phase.<sup>27-30)</sup> As the band calculation is considered to be a kind of HFA the above mentioned facts indicate that the HFA with the use of an effective interaction in place of the bare Coulomb repulsion is at least qualitatively a good approximation at zero temperature. However, as Asano have pointed out for Cr,<sup>29)</sup> if we adjust the parameters so as to reproduce the observed magnitude of magnetic moment at  $T=0$ , we obtain a too high Néel temperature  $T_N$  in HFA. Another drawback of the HFA appears in the temperature dependence of magnetization. It is well known that at low temperatures the deviation of the magnetization of ferromagnets is proportional to  $T^{3/2}$  due to the spin wave excitations. Of course RPA includes spin waves in the excitation spectrum, but the equilibrium state itself is nothing but the one obtained by HFA and does not contain the renormalization effect due to the spin waves. In the paramagnetic phase the defect of the HFA is typically seen by the temperature variation of susceptibility: it cannot explain the Curie-Weiss behaviors as observed not only in Fe, Co and Ni but in metals with small moments and low  $T_C$  such as  $ZrZn_2$ , which has been considered to be the best candidate for HFA to be applicable.

With respect to the Curie-Weiss type susceptibilities, it is seen that experimental data of itinerant ferromagnets are sometimes analyzed in a framework of the localized model. However, there are considerable differences between the Curie-Weiss laws obtained by assuming the localized model and those observed in

some itinerant ferromagnets. In the localized model the magnetic moment per atom deduced from saturation magnetization  $p_s$  and the one deduced from the paramagnetic Curie constant  $p_c$  are the same irrespective of  $T_C$ . Fig. 1 shows  $p_c/p_s$  versus  $T_C$  for various ferromagnetic materials.<sup>31)</sup> We see that  $p_c/p_s$  is much larger than 1 for itinerant ferromagnets with low  $T_C$ .

In Table 1 we collect experimental data of specific heat and electrical resistivity:  $\gamma$  is the coefficient of linear specific heat  $C=\gamma T$  and  $R_2$  is the coefficient of  $T^2$  term of the resistivity  $R=R_0+R_2T^2$ . It is seen that  $\gamma$  and  $R_2$  of materials with low  $T_C$  or  $T_N$  are generally greater than those of typical ferromagnetic metals, Fe, Co and Ni. As will be seen in later sections these quantities (especially electrical resistivity) are enhanced by the spin fluctuations. We may set up an operative category of weakly ferro- and antiferromagnetic metals which are defined as metals with low  $T_C(T_N)$  and small moments.

From the theoretical point of view weakly ferro- and antiferromagnetic metals are located at the opposite limit of the local moment case, where the intra atomic Coulomb interaction  $U$  dominates. In the latter case the degrees of freedom are only those of spin fluctuations and can be described by a spin hamiltonian. For weakly ferro- and antiferromagnetic metals, too, the spin fluctuations is expected to play a vital role to determine their thermodynamical properties and the above mentioned shortcomings of the HFA may be overcome by incorporating the effect of the spin fluctuations. Of course, characters of the spin fluctuations of the two limiting cases are different from each other. Then we may say that at finite temperatures the problem of magnetism, including a paramagnetic

case lying near the ferromagnetic or antiferromagnetic instability (nearly ferro- or antiferromagnetic case), is a problem of the spin fluctuations. In view of the electron correlation, the interaction term of the hamiltonian (1.1) may be rewritten in several ways. Among these, it can be expressed in terms of spin density operators [see eq.(2.5) below]. For magnetism, the problem of the electron correlation we may best grasp as the one of the spin fluctuations. To clarify the characters of the spin fluctuations in each case is a central problem of magnetism. In later sections we want to investigate the character in the weakly and nearly antiferromagnetic cases as far as possible.

## §2. The Self-Consistent Renormalization Theory of Spin Fluctuations

Theories which took account of the effect of spin fluctuations into magnetic properties were first given by Murata and Doniach<sup>32)</sup> and Moriya and Kawabata,<sup>2)</sup> independently. By using functional integral method, the former authors treated the spin fluctuations as a classical field. Since their treatment is classical its validity is limited to a considerable high temperature region and it generally overestimates the effect of the spin fluctuations. Furthermore, their theory predicts the first order phase transition. On the other hand the MK theory is a quantum mechanical one and its simplest approximation at high temperatures reduces to the Murata-Doniach theory. In this section we review first the MK theory and then its extension to antiferromagnetism developed by Hasegawa and Moriya.<sup>3)</sup> In the following sections we use the Hubbard hamiltonian [eq.(1.1)].

## §2.1. MK theory

Let us define free energy as a function of magnetization  $M$  and temperature  $T$  by

$$F(M, T) = \text{Tr} [P_M e^{-H/k_B T}] , \quad (2.1)$$

where  $P_M$  is the projection operator to a subspace with constant  $M$ . Magnetization  $M$  is measured in a unit of  $\mu_B$  and given by  $M = N_\downarrow - N_\uparrow$ , where  $N_\sigma$  is the number of electrons with spin  $\sigma$ . The equilibrium value of magnetization is obtained by

$$\frac{\partial}{\partial M} F(M, T) = 0 , \quad (2.2)$$

and the paramagnetic susceptibility in a unit of  $\mu_B^2$  is given by

$$\frac{1}{\chi} = \left[ \frac{\partial^2}{\partial M^2} F(M, T) \right]_{M=0} . \quad (2.3)$$

The Curie temperature is defined as the temperature where the susceptibility diverges;

$$\left[ \frac{\partial^2}{\partial M^2} F(M, T_C) \right]_{M=0} = 0 . \quad (2.4)$$

By rewriting the interaction term in terms of spin density operators,

$$\begin{aligned} H'(I) &= I \sum_{\mathbf{k}, \mathbf{k}', \mathbf{q}} a_{\mathbf{k}+\mathbf{q}\uparrow}^+ a_{\mathbf{k}'-\mathbf{q}\downarrow}^+ a_{\mathbf{k}'\downarrow} a_{\mathbf{k}\uparrow} \\ &= \frac{1}{2} N U - \frac{1}{2} I \sum_{\mathbf{q}} [s_+(\mathbf{q}), s_-(-\mathbf{q})]_+ , \end{aligned} \quad (2.5)$$

a part of the free energy due to the interaction term is given by

$$\begin{aligned}
 F_I(M, T) &= \int_0^I dI \frac{1}{I} \langle H'(I) \rangle_{M, I} \\
 &= \frac{1}{4} I (N^2 - M^2) + \Delta F(M, T),
 \end{aligned}
 \tag{2.6}$$

$$\begin{aligned}
 \Delta F(M, T) &= - \frac{1}{2} \sum_q \int_0^I dI \{ \langle [s_+(q), s_-(-q)]_+ \rangle_{M, I} \\
 &\quad - \langle [s_+(q), s_-(-q)]_+ \rangle_{M, 0} \}.
 \end{aligned}
 \tag{2.7}$$

Here  $\Delta F(M, T)$  is the correction to the Hartree-Fock free energy

$$F_{HF}(M, T) = F^{(0)}(M, T) + \frac{1}{4} I (N^2 - M^2)
 \tag{2.8}$$

and  $\langle \dots \rangle_{M, I}$  means the statistical average under fixed values of  $M$  and  $I$ . Eq.(2.7) may be expressed in terms of the dynamical susceptibility by using a fluctuation dissipation theorem;

$$\begin{aligned}
 \Delta F(M, T) &= - \frac{1}{2\pi} \int_{-\infty}^{\infty} d\omega \coth\left(\frac{\omega}{2k_B T}\right) \text{Im} \int_0^I dI \sum_q [\chi_{M, I}^{-+}(q, \omega) - \chi_{M, 0}^{-+}(q, \omega)] \\
 &= - k_B T \sum_n \sum_q \int_0^I dI [\chi_{M, I}^{-+}(q, i\omega_n) - \chi_{M, 0}^{-+}(q, i\omega_n)],
 \end{aligned}
 \tag{2.9}$$

where  $\chi_{M, I}^{-+}(q, \omega)$  is the dynamical susceptibility under given  $M$  and  $I$  and  $\omega_n$  is the Matsubara frequency of boson type;

$$\omega_n = 2\pi n k_B T.$$

The dynamical susceptibility is formally exactly expressed in terms of irreducible susceptibility  $\tilde{\chi}_{M,I}^{-+}(q, i\omega_n)$  which is defined by a set of bubble diagrams, each of which cannot be separated into two pieces, each having an external vertex, by removing an interaction vertex:

$$\chi_{M,I}^{-+}(q, i\omega_n) = \tilde{\chi}_{M,I}^{-+}(q, i\omega_n) / [1 - I\tilde{\chi}_{M,I}^{-+}(q, i\omega_n)] . \quad (2.10)$$

If one uses  $\chi_{M,0}^{-+}(q, i\omega_n)$  for  $\tilde{\chi}_{M,I}^{-+}(q, i\omega_n)$ , the RPA dynamical susceptibility is obtained.

The deviation of  $\tilde{\chi}_{M,I}^{-+}(q, i\omega_n)$  from  $\chi_{M,0}^{-+}(q, i\omega_n)$  which consists of second and higher order terms in  $I$  is to be incorporated in the following form

$$\tilde{\chi}_{M,I}^{-+}(q, i\omega_n) = \chi_{M,0}^{-+}(q, i\omega_n) / [1 + \lambda_{M,I}(q, i\omega_n)] , \quad (2.11)$$

and then the dynamical susceptibility is

$$\chi_{M,I}^{-+}(q, i\omega_n) = \chi_{M,0}^{-+}(q, i\omega_n) / [1 + \lambda_{M,I}(q, i\omega_n) - I\chi_{M,0}^{-+}(q, i\omega_n)] . \quad (2.12)$$

It should be noticed that this functional form is compatible with the spin conservation law<sup>33)</sup>  $[\chi_{M,I}^{-+}(0, \omega) = 0]$ . Owing to the isotropic nature of the hamiltonian [eq.(1.1)], we have the following important requirements. For  $T < T_C$ , the transversal static susceptibility should diverge:

$$1 + \lambda_{M,I}(0, 0) - I\chi_{M,0}^{-+}(0, 0) = 0 \quad (2.13)$$

For  $T > T_C$  the static limit of eq.(2.12) should coincide with the static susceptibility calculated from the free energy:

$$1 + \lambda_{0,I}(0,0) - I\chi_{0,0}^{-+}(0,0) = \chi^0/\chi \quad (2.13')$$

where  $\chi$  and  $\chi^0$  is the static susceptibility with and without the interaction  $I$ .

To proceed further we make some approximations. First we neglect  $\frac{\partial}{\partial I}\lambda_{MI}(q,i\omega_n)$  compared with  $\chi_{M0}^{-+}(q,i\omega_n)$  in a calculation of eq.(2.9) with a use of eq.(2.12). Then we have

$$\begin{aligned} \Delta F(M,I) = k_B T \sum_{nq} \{ \log[1 + \lambda_{M,I}(q,i\omega_n) - I\chi_{M,0}^{-+}(q,i\omega_n)] \\ + I\chi_{M,0}^{-+}(q,i\omega_n) \}. \end{aligned} \quad (2.14)$$

Secondly, we neglect  $q$ - and  $\omega$ -dependences of  $\lambda_{M,I}(q,i\omega_n)$  and further neglect  $\lambda_{M,I}(q,i\omega_n)$  and its derivatives with respect to  $M$  comparing with  $I\chi_{M,0}^{-+}(q,i\omega_n)$  and corresponding derivatives. However it is crucial to retain  $\lambda_{MI}(q,i\omega_n)$  in comparison with  $1 - I\chi_{M0}^{-+}(q,i\omega_n)$  for the reasons that the latter is very small in weakly and nearly ferromagnetic case and that without  $\lambda_{M,I}(q,i\omega_n)$  the requirements of eqs.(2.13) and (2.13') cannot be fulfilled. By using the approximations just mentioned the following equations are obtained. For  $T < T_C$  the equilibrium value of magnetization is given by

$$0 = \frac{\partial}{\partial M} F^{(0)}(M, T) - \frac{1}{2} IM - k_B T \Sigma K(i\omega_n)$$

$$= \frac{\partial}{\partial M} F^{(0)}(M, T) - \frac{1}{2} IM - \frac{1}{2\pi} \int_{-\infty}^{\infty} d\omega \coth\left(\frac{\omega}{2k_B T}\right) Im K(\omega),$$

$$K(i\omega_n) = I^2 \Sigma \left[ \frac{\partial}{\partial M} \chi_{M,0}^{-+}(q, i\omega_n) \right] \frac{\chi_{M,0}^{-+}(q, i\omega_n)}{I [\chi_{M,0}^{-+}(0,0) - \chi_{M,0}^{-+}(q, i\omega_n)]} \quad (2.15)$$

For  $T > T_C$  the static susceptibility is given by

$$\frac{1}{\chi} = \frac{1}{\chi_0} [1 + \lambda - I \chi_{0,0}^{-+}(0,0)] = \frac{1}{\chi_0} - \frac{1}{2} I - k_B T \Sigma G(i\omega_n),$$

$$= \frac{1}{\chi_0} - \frac{1}{2} I - \frac{1}{2\pi} \int_{-\infty}^{\infty} d\omega \coth\left(\frac{\omega}{2k_B T}\right) Im G(\omega)$$

$$G(i\omega_n) = I^2 \Sigma \left\{ \left[ \frac{\partial^2}{\partial M^2} \chi_{M,0}^{-+}(q, i\omega_n) \right]_{M=0} \frac{\chi_{0,0}^{-+}(q, i\omega_n)}{1 + \lambda - I \chi_{0,0}^{-+}(q, i\omega_n)} \right. \\ \left. + \left[ \frac{\partial}{\partial M} \chi_{M,0}^{-+}(q, i\omega_n) \right]_{M=0}^2 \frac{1}{[1 + \lambda - I \chi_{0,0}^{-+}(q, i\omega_n)]^2} \right\}$$

(2.16)

with

$$\lambda = \lambda_{MI}(0,0).$$

Since these equations are expressed in terms of the dynamical susceptibility of the non-interacting system, they can be calculated in principle for any band structure.\*)

Several authors have previously investigated the effect of spin fluctuations on the free energy by using RPA [neglect  $\lambda$  in eq.(2.14)] and discussed specific heat and susceptibility<sup>34-38)</sup>. However these treatments are not self-consistent. Above  $T_C$ , static limit of the dynamical susceptibility which is used to calculate the free energy differs from the one calculated from the resultant free energy. This inconsistency is easily seen if one drops  $\lambda$  in eq.(2.16). Below  $T_C$ , the magnetization used in RPA dynamical susceptibility to calculate  $K(i\omega_n)$  in eq.(2.15) is the HFA value which naturally disagrees with the one calculated from the renormalized free energy. So the validity of the above mentioned RPA calculations is limited to low temperatures only. On the other hand eqs.(2.15) and (2.16) are consistent and may be used continuously over the whole temperature range through  $T_C$ . Generally speaking, above mentioned inconsistency originates from the fact that RPA neglects couplings between different fluctuation modes. So RPA generally overestimates spin fluctuations. This

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\*) In eqs.(2.15) and (2.16) the contribution of the fluctuations may be divided into two parts by using an identity  $\coth(\frac{\beta\omega}{2}) = \text{sgn}\omega + 2 \text{sgn}\omega n(|\omega|)$ ,  $n(\omega)$  being the Bose factor  $[e^{\beta\omega} - 1]^{-1}$ . The first term gives a temperature independent contribution which may be considered as a renormalization of the interaction constant. We neglect the first term and discuss the temperature dependent term explicitly.

is illustrated by the fact that if one uses RPA in renormalizing the free energy the critical exponent of the specific heat in the vicinity of the fictitious  $T_C$  is too large.<sup>34)</sup> The self-consistent procedure to determine  $M$  in eq.(2.15) or  $\lambda$  in eq.(2.16) is regarded as an inclusion of couplings between uniform mode and modes with finite  $q$ . We may expect this mode-mode coupling leads to a suppression of the fluctuations themselves.

MK have solved self-consistent eqs.(2.15) and (2.16) by using an electron gas-like band. Their main conclusions are abridged as follows.

- 1)  $T_C$  is generally lowered from that calculated by HFA.
- 2) Paramagnetic susceptibility above  $T_C$  can obey the Curie-Weiss law. The Curie constant deduced from paramagnetic susceptibility is determined by the band structure and does not vary if one changes interaction constant  $I$ . So  $p_c/p_s$  defined in §§1.3 of weakly ferromagnetic metals are large in contrast to the local moment case. This fact gives a qualitative explanation of Fig.1.
- 3) For paramagnetic metals, if they lie near the ferromagnetic instability, their susceptibilities can show the Curie-Weiss behavior.
- 4) At low temperatures the deviation of magnetization is proportional to  $T^{3/2}$  as is well known from the spin wave theory. However the temperature range where the above statement holds is narrow in weakly ferromagnetic metals. Near  $T_C$  a relation  $M(T) \propto [T_C^{4/3} - T^{4/3}]^{1/2}$  holds in a considerably wide temperature range.

- 5) The amplitude of the spin fluctuations themselves are significantly suppressed owing to the interaction among them.

These conclusions show that the MK theory qualitatively improves the insufficiencies of HFA and RPA and that excitations which dominate thermodynamical properties of magnetic metals are not the single-particle excitations as in HFA but the collective spin fluctuation modes as many body excitations.

## §§2.2. HM Theory

[1] Although the staggered magnetization  $M_Q = -2\langle S_z(Q) \rangle$ ,  $Q$  being the antiferromagnetic wave vector, is not a constant of motion, we may define the free energy as a function of the macroscopic variable  $M_Q$  [see Appendix A of ref. 3)]:

$$F(M_Q, T) = F_{HF}(M_Q, T) + \Delta F(M_Q, T). \quad (2.17)$$

Here  $\Delta F(M_Q, T)$  is the correction to the Hartree Fock free energy

$$F_{HF}(M_Q, T) = F^{(0)}(M_Q, T) + \frac{1}{4}I(N^2 - M_Q^2). \quad (2.18)$$

The equilibrium value of the magnetization is obtained by

$$\frac{\partial}{\partial M_Q} F(M_Q, T) = 0, \quad (2.19)$$

and the paramagnetic staggered susceptibility  $\chi_Q$  is given by

$$\frac{1}{\chi_Q} = \left[ \frac{\partial^2}{\partial M_Q^2} F(M_Q, T) \right]_{M_Q=0}. \quad (2.20)$$

The Néel temperature is defined as the temperature where  $\chi_Q$  diverges;

$$\left[ \frac{\partial^2}{\partial M_Q^2} F(M_Q, T_N) \right]_{M_Q=0} = 0. \quad (2.21)$$

The free energy is calculable in the same manner as that in ferromagnetic case. The correction term of the free energy is expressed in terms of the dynamical susceptibility under fixed

values of  $M_Q$  and  $I$ ;

$$\begin{aligned}
\Delta F(M_Q, T) &= -k_B T \sum_{nq} \int_0^I dI [\chi_{M_Q, I}^{-+}(q, i\omega_n) - \chi_{M_Q, 0}^{-+}(q, i\omega_n)] \\
&= -k_B T \sum_{nq} \int_0^I dI [\chi_{M_Q, I}^{-+}(q, i\omega_n) + \chi_{M_Q, I}^{-+}(q+Q, i\omega_n) \\
&\quad - \chi_{M_Q, 0}^{-+}(q, i\omega_n) - \chi_{M_Q, 0}^{-+}(q+Q, i\omega_n)] . \quad (2.22)
\end{aligned}$$

Here  $\sum_q$  and  $\sum_q'$  stand for the summations in the first Brillouin zones of chemical and magnetic reciprocal lattice spaces, respectively. By introducing a matrix notation,

$$\chi_{M_Q, I}^{-+}(q, i\omega_n) = \begin{bmatrix} \chi_{M_Q, I}^{-+}(q, i\omega_n) & , \chi_{M_Q, I}^{-+}(q, -q-Q: i\omega_n) \\ \chi_{M_Q, I}^{-+}(q+Q, -q: i\omega_n) & , \chi_{M_Q, I}^{-+}(q+Q: i\omega_n) \end{bmatrix}, \quad (2.23)$$

we may rewrite eq.(2.22) as

$$\Delta F(M_Q, T) = -k_B T \sum_{nq} \text{Tr} \int_0^I dI [\chi_{M_Q, I}^{-+}(q, i\omega_n) - \chi_{M_Q, 0}^{-+}(q, i\omega_n)], \quad (2.24)$$

The dynamical susceptibility is formally exactly expressed in terms of irreducible susceptibility  $\tilde{\chi}_{M_Q, I}^{-+}(q, i\omega_n)$ ;

$$\begin{aligned}
\chi_{M_Q, I}^{-+}(q, i\omega_n) &= [1 - I \tilde{\chi}_{M_Q, I}(q, i\omega_n)]^{-1} \tilde{\chi}_{M_Q, I}(q, i\omega_n) \\
&= [1 + \lambda_{M_Q, I}(q, i\omega_n) - I \chi_{M_Q, 0}^{-+}(q, i\omega_n)]^{-1} \chi_{M_Q, 0}^{-+}(q, i\omega_n),
\end{aligned}
\tag{2.25}$$

where  $\lambda_{M_Q, I}(q, i\omega_n)$  defined by

$$\tilde{\chi}_{M_Q, I}(q, i\omega_n) = [1 + \lambda_{M_Q, I}(q, i\omega_n)]^{-1} \chi_{M_Q, 0}^{-+}(q, i\omega_n), \tag{2.26}$$

denotes the deviation of  $\tilde{\chi}_{M_Q, I}(q, i\omega_n)$  from  $\chi_{M_Q, 0}^{-+}(q, i\omega_n)$ , consisting of second and higher order terms in  $I$ .

Now we proceed further by making approximations appropriate for weakly and nearly antiferromagnetic metals.

$$\begin{aligned}
\Delta F(M_Q, T) &= k_B T \sum_{nq} \{ \log \det [1 + \lambda_{M_Q, 0}(q, i\omega_n) \\
&\quad - I \chi_{M_Q, 0}^{-+}(q, i\omega_n)] + I \text{Tr} \chi_{M_Q, 0}^{-+}(q, i\omega_n) \},
\end{aligned}
\tag{2.27}$$

$$\begin{aligned}
\frac{\partial}{\partial M_Q} \Delta F(M_Q, T) &= - k_B T \sum_{nq} \text{Tr} \left\{ \left[ \frac{\partial}{\partial M_Q} \chi_{M_Q, 0}^{-+}(q, i\omega_n) \right] \right. \\
&\quad \left. + [1 + \lambda_{M_Q, I}(q, i\omega_n) - I \chi_{M_Q, 0}^{-+}(q, i\omega_n)]^{-1} \chi_{M_Q, 0}^{-+}(q, i\omega_n) \right\},
\end{aligned}
\tag{2.28}$$

$$\begin{aligned}
\frac{\partial^2}{\partial M_Q^2} \Delta F(M_Q, T) &= - k_B T \sum_{nq} \text{Tr} \left\{ \left[ \frac{\partial^2}{\partial M_Q^2} \chi_{M_Q, 0}^{-+}(q, i\omega_n) \right] \right. \\
&\quad + [1 + \lambda_{M_Q, 0}(q, i\omega_n) - I \chi_{M_Q, 0}^{-+}(q, i\omega_n)]^{-1} \chi_{M_Q, 0}^{-+}(q, i\omega_n) \\
&\quad + \left[ \frac{\partial}{\partial M_Q} \chi_{M_Q, 0}^{-+}(q, i\omega_n) \right] [1 + \lambda_{M_Q, 0}(q, i\omega_n) - I \chi_{M_Q, 0}^{-+}(q, i\omega_n)]^{-1} \\
&\quad \times \left. \left[ \frac{\partial}{\partial M_Q} \chi_{M_Q, 0}^{-+}(q, i\omega_n) \right] [1 + \lambda_{M_Q, 0}(q, i\omega_n) - I \chi_{M_Q, 0}^{-+}(q, i\omega_n)]^{-1} \right\}.
\end{aligned}
\tag{2.29}$$

Owing to the isotropic nature of the hamiltonian [eq.(1.1)], we have important requirements. Below  $T_N$ , the transversal staggered susceptibility should diverge:

$$1 + \lambda_{M_Q, I}(Q, 0) - I\chi_{M_Q, 0}^{-+}(Q, 0) = 0. \quad (2.30)$$

Above  $T_N$ , the static limit of the staggered dynamical susceptibility should coincide with the susceptibility calculated by eq.(2.20):

$$1 + \lambda_{0, I}(Q, 0) - I\chi_{0, 0}^{-+}(Q, 0) = \chi_Q^0 / \chi_Q, \quad (2.31)$$

where  $\chi_Q$  and  $\chi_Q^0$  is the static staggered susceptibility with and without the interaction.  $\lambda_{M_Q, I}(q, i\omega_n)$  is considered to be generally small and important only for the staggered components  $\lambda_{M_Q, I}(q+Q, i\omega_n)$  with small  $q$  and  $\omega$ . We may approximate  $\lambda_{M_Q, I}(q, i\omega_n)$  by scalar function  $\lambda_{M_Q, I}(q+Q, i\omega_n)$  and further neglect  $q$ - and  $\omega$ -dependences. Then we have the following self-consistent equations. For  $T < T_N$  the equilibrium value of the staggered magnetization is given by

$$\begin{aligned} 0 &= \frac{\partial}{\partial M_Q} F^{(0)}(M_Q, T) - \frac{1}{2}IM_Q - k_B T \Sigma_K(i\omega_n) \\ &= \frac{\partial}{\partial M_Q} F^{(0)}(M_Q, T) - \frac{1}{2}IM_Q - \frac{1}{2\pi} \int_{-\infty}^{\infty} d\omega \coth\left(\frac{\omega}{2k_B T}\right) ImK_Q(\omega), \\ K_Q(i\omega_n) &= I^2 \sum_q \text{Tr} \left\{ \left[ \frac{\partial}{\partial M_Q} \chi_{M_Q, 0}^{-+}(q, i\omega_n) \right] \left[ I\chi_{M_Q, 0}^{-+}(Q, 0) \right. \right. \\ &\quad \left. \left. - I\chi_{M_Q, 0}^{-+}(q, i\omega_n) \right]^{-1} \chi_{M_Q, 0}^{-+}(q, i\omega_n) \right\}. \end{aligned} \quad (2.32)$$

For  $T > T_N$ , the static susceptibility is given by

$$\begin{aligned}
\frac{1}{\chi_Q} &= \frac{1}{\chi_Q^0} [1 + \lambda_Q - I \chi_{0,0}^{-+}(Q,0)] = \frac{1}{\chi_Q^0} - \frac{1}{2} I - k_B T \Sigma_Q(i\omega_n) \\
&= \frac{1}{\chi_Q^0} - \frac{1}{2} I - \frac{1}{2\pi} \int_{-\infty}^{\infty} d\omega \coth\left(\frac{\omega}{2k_B T}\right) \text{Im} G_Q(\omega), \\
G_Q(i\omega_n) &= I^2 \Sigma'_q \text{Tr} \left\{ \left[ \frac{\partial^2}{\partial M_Q^2} \chi_{M_Q,0}^{-+}(q, i\omega_n) \right]_{M_Q=0} \right. \\
&\quad \times [1 + \lambda_Q - I \chi_{0,0}^{-+}(q, i\omega_n)]^{-1} \chi_{0,0}^{-+}(q, i\omega_n) \\
&\quad + \left[ \frac{\partial}{\partial M_Q} \chi_{M_Q,0}^{-+}(q, i\omega_n) \right]_{M_Q=0} [1 + \lambda_Q - I \chi_{0,0}^{-+}(q, i\omega_n)]^{-1} \\
&\quad \times \left. \left[ \frac{\partial}{\partial M_Q} \chi_{M_Q,0}^{-+}(q, i\omega_n) \right]_{M_Q=0} [1 + \lambda_Q - I \chi_{0,0}^{-+}(q, i\omega_n)]^{-1} \right\}, \quad (2.33)
\end{aligned}$$

with

$$\lambda_Q = \lambda_{0,I}(Q,0).$$

These equations are self-consistent, eq.(2.32) is a self-consistent equation for  $M_Q$  and eq.(2.33) for  $\lambda_Q$ , and the approximation is one step beyond HFA and RPA. As eqs.(2.32) and (2.33) contain the dynamical susceptibilities of the non-interacting system only, they are calculable in principle, although the calculation of  $\chi_{M_Q,0}^{-+}(q, i\omega_n)$  in the ordered phase is a laborious task.

[2] To carry out the program of solving the self-consistent equations (2.32) and (2.33), the dynamical susceptibility under a fixed value of  $M_Q$  is necessary. Instead of taking the conditional statistical average, we take unconditional statistical average under a fictitious staggered magnetic field  $B_Q$  which generates  $M_Q$ . The staggered magnetic field  $B_Q$  reduces the first Brillouin zone into the half (magnetic first Brillouin zone) and results in a splitting of the electron band into two bands. The energy dispersions of the new bands can be calculated with a canonical transformation:

$$\begin{aligned}
H^{(0)}(B_Q) &= \sum_{\sigma k} \sum' \{ \epsilon_k a_{k\sigma}^+ a_{k\sigma} + \epsilon_{k+Q} a_{k+Q\sigma}^+ a_{k+Q\sigma} \\
&\quad + \sigma B_Q (a_{k+Q\sigma}^+ a_{k\sigma} + a_{k\sigma}^+ a_{k+Q\sigma}) \} \\
&= \sum_{\sigma k} \sum' ( \epsilon_{1k} a_{1k\sigma}^+ a_{1k\sigma} + \epsilon_{2k} a_{2k\sigma}^+ a_{2k\sigma} ), \tag{2.34}
\end{aligned}$$

with

$$\begin{aligned}
a_{1k\sigma} &= \cos\theta_k a_{k\sigma} - \sigma \sin\theta_k a_{k+Q\sigma} \\
a_{2k\sigma} &= \sigma \sin\theta_k a_{k\sigma} + \cos\theta_k a_{k+Q\sigma} \tag{2.35}
\end{aligned}$$

$$\tan 2\theta_k = \frac{\epsilon_{k+Q} - \epsilon_k}{2B}$$

and

$$\left. \begin{matrix} \epsilon_{1k} \\ \epsilon_{2k} \end{matrix} \right\} = \frac{1}{2}(\epsilon_{k+Q} + \epsilon_k) \pm \left[ \frac{1}{4}(\epsilon_{k+Q} - \epsilon_k)^2 + B_Q^2 \right]^{1/2}. \tag{2.36}$$

$B_Q$  is related to  $M_Q$  by

$$M_Q = 2 \sum_k' \frac{B_Q}{[\frac{1}{4}(\epsilon_{k+Q} - \epsilon_k)^2 + B_Q^2]^{\frac{1}{2}}} [f(\epsilon_{1k}) - f(\epsilon_{2k})], \quad (2.37)$$

where  $f(\epsilon)$  is the Fermi distribution function.

By using the canonical transformation the dynamical susceptibilities are given by

$$\begin{aligned} \chi_{M_Q,0}^{-+}(q+Q,\omega) = & \sum_k' \{ [\tau_{21}(k,q,\omega) + \tau_{12}(k,q,\omega)] \cos^2(\theta_k - \theta_{k+q}) \\ & + [\tau_{11}(k,q,\omega) + \tau_{22}(k,q,\omega)] \sin^2(\theta_k - \theta_{k+q}) \}, \end{aligned} \quad (2.38)$$

$$\begin{aligned} \chi_{M_Q,0}^{-+}(q,\omega) = & \sum_k' \{ [\tau_{21}(k,q,\omega) + \tau_{12}(k,q,\omega)] \cos^2(\theta_k + \theta_{k+q}) \\ & + [\tau_{11}(k,q,\omega) + \tau_{22}(k,q,\omega)] \sin^2(\theta_k + \theta_{k+q}) \}, \end{aligned} \quad (2.39)$$

$$\begin{aligned} \chi_{M_Q,0}^{-+}(q,-q-Q;\omega) = & \sum_k' \{ [\tau_{21}(k,q,\omega) - \tau_{12}(k,q,\omega)] \cos(\theta_k - \theta_{k+q}) \cos(\theta_k + \theta_{k+q}) \\ & + [\tau_{11}(k,q,\omega) - \tau_{22}(k,q,\omega)] \sin(\theta_k - \theta_{k+q}) \sin(\theta_k + \theta_{k+q}) \}, \end{aligned} \quad (2.40)$$

with

$$\tau_{ij}(k,q,\omega) = [f(\epsilon_{ik}) - f(\epsilon_{jk+q})] / (\epsilon_{jk+q} - \epsilon_{ik} - \omega). \quad (2.41)$$

By using symmetry relations, eq.(2.33) may be rewritten in a somewhat simpler form:

$$\begin{aligned}
G_Q(i\omega_n) = & I^2 \sum_q \left\{ \left[ \frac{\partial^2}{\partial M_Q^2} \chi_{M_Q,0}^{-+}(q, i\omega_n) \right]_{M_Q=0} \frac{\chi_{0,0}^{-+}(q, i\omega_n)}{1 + \lambda_Q - I \chi_{0,0}^{-+}(q, i\omega_n)} \right. \\
& + \left[ \frac{\partial^2}{\partial M_Q^2} \chi_{M_Q,0}^{-+}(q, i\omega_n) \right]_{M_Q=0} \frac{\chi_{0,0}^{-+}(q+Q, i\omega_n)}{1 + \lambda_Q - I \chi_{0,0}^{-+}(q+Q, i\omega_n)} \\
& + \left[ \frac{\partial}{\partial M_Q} \chi_{M_Q,0}^{-+}(q, -q-Q; i\omega_n) \right]_{M_Q=0}^2 \frac{1}{1 + \lambda_Q - I \chi_{0,0}^{-+}(q, i\omega_n)} \\
& \times \left. \frac{1}{1 + \lambda_Q - I \chi_{0,0}^{-+}(q+Q, i\omega_n)} \right\}. \quad (2.42)
\end{aligned}$$

Now we neglect the temperature independent part of the contribution of the spin fluctuations, which may be considered as a renormalization of the interaction constant, i.e., we replace  $\coth(\beta\omega/2)$  by  $2 \operatorname{sgn} \omega n(|\omega|)$  in eqs.(2.32) and (2.33).<sup>2,3)</sup> In other words, we take the Hartree-Fock ground state as a true ground state and focus our attention on the temperature dependence of the system. The temperature dependent part of the spin fluctuation contribution is dominated by low frequency modes. As  $\left[ \frac{\partial}{\partial M_Q} \chi_{M_Q,0}^{-+}(q, -q-Q; \omega) \right]_{M_Q=0}$  is proportional to  $\omega$  we may discard the last term in eq.(2.42). Further, in weakly and nearly anti-ferromagnetic case, the fluctuation modes have large amplitudes in a small region near  $Q$  in  $q$ -space. We may also discard the first term in eq.(2.42) and employ the following expansion form:

$$\begin{aligned}
& \chi_{0,0}^{-+}(q+Q, \omega) \\
& = \frac{\chi_Q^0}{2} [1 - A_{xx} q_x^2 - A_{yy} q_y^2 - A_{zz} q_z^2 - B\omega^2 + i C_0 \omega + \dots], \quad (2.43) \\
& \left[ \frac{\partial^2}{\partial M_Q^2} \chi_{M_Q,0}^{-+}(q+Q, \omega) \right]_{M_Q=0} = -F + \dots,
\end{aligned}$$

The expansion coefficients  $A_{ii}$  ( $i = x, y, z, \dots$ ),  $B$ ,  $C$  and  $F$  are calculated from a given band structure. Actually HM have used the electron gas model with Umklapp processes described in §§1.3,

$$\epsilon_k = \frac{1}{2m} k^2, \quad \epsilon_{k+Q} = \frac{1}{2m} (k - Q)^2 \quad (2.44)$$

and determined the coefficients. Then they have solved eq.(2.33) and discussed magnetic properties of itinerant antiferromagnets.

Now we survey the conclusions obtained by HM.

- 1) The leading term of the spin fluctuation spectrum  $G_Q(\omega)$  is proportional to  $\omega^{\frac{1}{2}}$  at  $T = T_N$ . By integrating with respect to  $\omega$ ,  $\lambda_Q$  at  $T = T_N$  is shown to be proportional to  $T_N^{3/2}$ . Therefore the fluctuations dominate over the contribution of the thermal single-particle excitations which is proportional to  $T^2$ . Thus the Néel temperature, when it is small, is given by

$$T_N \propto (\alpha_Q - 1)^{2/3}. \quad (2.45)$$

where  $\alpha_Q = \frac{1}{2} I \chi_Q^0$  is the dimensionless coupling constant.

This is generally small compared with the Hartree Fock value

$$T_N^{\text{HF}} \propto (\alpha_Q - 1)^{\frac{1}{2}}. \quad (2.46)$$

- 2) The staggered susceptibility  $\chi_Q$  shows a Curie-Weiss behavior for weakly and nearly antiferromagnetic metals. Instead, the uniform susceptibility has only weak temperature dependence. Recently, Usami and Moriya have investigated the case where both the uniform and staggered fluctuation components [the first and the second terms in eq.(2.42)] are important and

shown that the uniform susceptibility in this case can show a Curie-Weiss behavior.<sup>39)</sup>

- 3) Slightly below  $T_N$ , where  $M_Q$  is small and the free energy may be expanded for  $M_Q$ , the fluctuation is still characterized by the  $T^{3/2}$  behavior. Then the staggered magnetization is obtained as

$$M_Q \propto [T_N^{3/2} - T^{3/2}]^{1/2}, \quad (2.47)$$

instead of the Hartree-Fock value

$$M_Q^{HF} \propto [(T_N^{HF})^2 - T^2]^{1/2}. \quad (2.48)$$

- 4) Finally, as  $\lambda_Q$  is positive, the spin fluctuations themselves are significantly suppressed from the RPA values.

### §3. Physical Properties Related to the Spin Fluctuations

As is stated in §1.3, physical properties such as relaxation rate of nuclear magnetic resonance, specific heat and electrical resistivity etc. are closely related to the spin fluctuations. These are relatively well studied in ferromagnetic cases and the fact is known as the exchange enhancement. However for antiferromagnetism these quantities have hardly been well investigated so far even in the framework of RPA. In §2 we have seen that the self-consistent renormalization theory of spin fluctuations have qualitatively improved the conventional HFA and RPA. So our purpose of the present section is two fold. The first is to clarify the relation between the physical quantities and the spin fluctuations, especially for antiferromagnets. We note that RPA is valid in the low temperature limit. Secondly, we study the above mentioned renormalization effect which becomes important as temperature is raised. We expect to obtain qualitatively different temperature dependences of various quantities from those obtained by using RPA. To proceed our discussion let us bear in mind the corresponding results in the ferromagnetic case.

The most direct method observing the spin fluctuations is inelastic neutron scattering. As our approximation neglects  $q$ - and  $\omega$ -dependences of  $\lambda_{M_Q, I}(q, \omega)$ ,  $q$ - and  $\omega$ -dependences of  $\chi^{-+}(q, \omega)$  is essentially the same as those of RPA. However, even within RPA, there are several interesting points concerning with the spin wave spectrum; for an example the spin waves of the itinerant antiferromagnet decay into electron-hole pair excitations and have an intrinsic damping. We will also study the intensity of magnetic excitations at  $T=0$  by using RPA.

### §§3.1. NMR Relaxation Rate<sup>40,41)</sup>

The self-consistent renormalization theory of spin fluctuations is best applied to weakly and nearly ferro- and antiferromagnetic metals. In these substances the spin fluctuations provides a predominant relaxation mechanism of the nuclear magnetic resonance. As a resonance frequency of NMR is much smaller than the characteristic frequencies concerning electrons,  $T_1$  is one of the best physical quantities for us to detect the nature of low frequency components of the spin fluctuations which have been shown to play a vital role to the thermodynamical properties.

For brevity, let us consider only the Fermi contact type interaction between a nuclear spin  $\vec{I}$  and an electron spin  $\vec{s}$ :

$$A_{\text{hf}} \vec{I} \cdot \vec{s}, \quad (3.1)$$

where  $A_{\text{hf}}$  is the hyperfine coupling constant and is assumed to be constant for all the electronic states concerned. Then the nuclear spin-lattice relaxation rate is given by<sup>42)</sup>

$$1/T_1 = A_{\text{hf}}^2 k_B T \text{Im} \chi_{\text{loc}}^{-+}(\omega_0)/\omega_0, \quad (3.2)$$

where  $\omega_0$  is the nuclear magnetic resonance frequency and  $\chi_{\text{loc}}^{-+}(\omega)$  the transversal local dynamical susceptibility defined by

$$\chi_{\text{loc}}^{-+}(\omega) = i \int_0^\infty dt e^{i\omega t} \langle [s_-(r,t), s_+(r)] \rangle, \quad (3.3)$$

$r$  being the position of a nucleus under consideration. If there is a translational symmetry of the lattice (para- or ferromagnetic phase) the relaxation rate is given by the wave vector dependent dynamical susceptibility:

$$1/T_1 = A_{\text{hf}}^2 k_B T \sum_q \text{Im} \chi^{-+}(q, \omega_0) / \omega_0. \quad (3.4)$$

For weakly and nearly ferromagnetic metals, by using eq.(2.12) and an expansion form of  $\chi_{M,0}^{-+}(q, \omega)$  for small  $q$  and  $\omega$ , we obtain the following results. Above  $T_C$ , the relaxation rate is given as

$$T_{10}/T_1 \propto (\chi/\chi_0) \quad (3.5)$$

where  $1/T_{10} = \pi A_{\text{hf}}^2 [\rho(\epsilon_F)]^2 k_B T$  is the Korringa relaxation rate for the non-interacting electron system. Below  $T_C$ , we obtain

$$T_{10}/T_1 \propto [M(T)]^{-2}. \quad (3.6)$$

At  $T = 0K$ , as  $\chi_0/\chi$  is proportional to  $1-\alpha$  and  $M(T)$  to  $(\alpha - 1)^{1/2}$ , we see that the relaxation rate is enhanced by the factor  $|\alpha - 1|^{-1}$  near the critical boundary of ferromagnetism. For  $T > T_C$ , we see from eq.(3.5) that  $1/T_1$  is proportional to  $T\chi$  and when  $\chi$  obeys the Curie-Weiss law, as was shown in §2.1, we have

$$1/T_1 \propto T/(T - T_C). \quad (3.7)$$

It is well known that relaxation rate due to localized spins tends to a constant as temperature increases. The present result shows that the temperature independent  $T_1$  does not necessarily mean the existence of localized moments. Actually, Kontani, Hioki and Masuda confirmed that the present results, including the external magnetic field dependence also,<sup>43)</sup> hold experimentally for  $\text{ZrZn}_2$ <sup>44)</sup> and  $\text{Sc}_3\text{In}$ .<sup>45,46)</sup> On the other hand, HFA-RPA gives

$$1/T_1^{\text{RPA}} \propto T/(T^2 - T_C^2). \quad (3.8)$$

Let us turn to the antiferromagnetic metals.

[1] For antiferromagnetism, the fluctuations with wave vectors around antiferromagnetic wave vector  $Q$ , or equivalently staggered component of eq.(2.25) are important. Above  $T_N$ , we have

$$\chi_{0,I}^{-+}(q+Q,\omega) = \frac{\chi_{0,0}^{-+}(q+Q,\omega)}{1 + \lambda_Q - I\chi_{0,0}^{-+}(q+Q,\omega)} . \quad (3.9)$$

By using the expansion form eq.(2.43), the relaxation rate in the paramagnetic phase is given by

$$1/T_1 = A_{hf}^2 k_B T (\chi_Q^0 C_0 / \pi) (\alpha_Q A_{xx} A_{yy} A_{zz})^{-1/2} (\chi_Q / \chi_Q^0)^{1/2}. \quad (3.10)$$

$1/T_1$  is proportional to  $T\chi_Q^{1/2}$ . At  $T = 0$ , as  $\chi_Q$  is proportional to  $(1 - \alpha_Q)^{-1}$  for nearly antiferromagnetic metals, the relaxation rate is enhanced by the factor  $(1 - \alpha_Q)^{-1/2}$ . When the staggered susceptibility obeys the Curie-Weiss law as was shown in §2.2, we expect

$$1/T_1 \propto T/(T - T_N)^{1/2}. \quad (3.11)$$

In this case the relaxation rate does not tend to a constant as temperature goes up but increases as  $T^{1/2}$  in contrast with ferromagnetic case and with the localized moment case. On the other hand, RPA gives

$$1/T_1^{RPA} \propto T/(T^2 - T_N^2)^{1/2}. \quad (3.12)$$

Now we show some numerical examples based on the electron gas model with Umklapp processes:

$$\epsilon_k = k^2, \quad \epsilon_{k+Q} = (k - Q)^2. \quad (3.13)$$

Here and in what follows we use reduced units, which measure energy and momentum by  $Q$  and  $\epsilon_Q = k_B T_Q = Q^2/2m$ , respectively. For simplicity we take  $Q = (0,0,Q) = (\pi/a)(0,0,1)$ . Fig.2 and Fig.3 show the temperature dependence of the relaxation rates for anti-ferromagnetic metals ( $\alpha_Q > 1$ ) and for nearly antiferromagnetic metals ( $\alpha_Q \leq 1$ ). Solid lines represent the present results and dashed lines RPA results. In Fig. 2 we plot  $(T_{10}/T_1)(T/T_N)$  against  $(T/T_N)$  for various values of  $T_N$ . In Fig.3 we plot  $(T_{10}/T_1)(T/T_Q)$  against  $(T/T_Q)$  for various values of  $\alpha_Q$  (represented as  $\alpha$  in the figure).

[2] Below  $T_N$ , there exists a finite staggered magnetization  $M_Q$ , which gives rise to the non-diagonal part of the dynamical susceptibility  $\chi_{M_Q,I}^{-+}(q, -q-Q; \omega)$  and the formula (3.3) for  $T_1$  reduces to

$$\begin{aligned} 1/T_1 = A_{hf}^2 k_B T \sum_q' \frac{1}{\omega_0} \text{Im} [ & \chi_{M_Q,I}^{-+}(q, \omega_0) + \chi_{M_Q,I}^{-+}(q+Q, \omega_0) \\ & + \chi_{M_Q,I}^{-+}(q, -q-Q; \omega_0) + \chi_{M_Q,I}^{-+}(q+Q, -q; \omega_0) ] . \end{aligned} \quad (3.14)$$

From a symmetry consideration  $\text{Im}[\chi_{M_Q,I}^{-+}(q, -q-Q; \omega_0) + \chi_{M_Q,I}^{-+}(q+Q, -q; \omega_0)]$  is shown to be of the order  $\omega_0^2$  and may be neglected in discussing  $T_1$  of NMR. Further, with an exception that the substance locates not only near antiferromagnetic instability but also ferromagnetic one, we may discard the uniform component. By using eq.(2.25) and (2.30) and noticing that  $[\chi_{M_Q,0}^{-+}(q, -q-Q; \omega_0)]^2$  is of the order  $\omega_0^2$ , the following expression for  $T_1$  is obtained:

$$1/T_1 = A_{hf}^2 k_B T \sum_q \frac{1}{\omega_0} \text{Im} \frac{\chi_{M_Q,0}^{-+}(q+Q, \omega_0)}{i[\chi_{M_Q,0}^{-+}(Q, 0) - \chi_{M_Q,0}^{-+}(q+Q, \omega_0)]}. \quad (3.15)$$

For small reduced staggered magnetization  $\zeta_Q = M_Q/N$ , we may use the following expansion form for the real part of the dynamical susceptibility:

$$\text{Re } \chi_{M_Q,0}^{-+}(q+Q, \omega) = \frac{\chi_Q^2}{2} [1 + O(\zeta_Q^2) - A_{xx}q_x^2 - A_{yy}q_y^2 - A_{zz}q_z^2 + \dots] \quad (3.16)$$

where the expansion coefficients agree with those of eq.(2.43) up to the leading order of  $\zeta_Q$  and the deviation is of the order  $\zeta_Q^2$ . On the other hand, the imaginary part suffers a serious modification by an appearance of a finite staggered magnetization. The imaginary part generally has the following expansion form:<sup>47)</sup>

$$\text{Im } \chi_{M_Q,0}^{-+}(q+Q, \omega) = \frac{\chi_Q^0}{2} [c(q)\omega + d(q)\omega^3 + \dots]. \quad (3.17)$$

where the coefficient  $c(q)$  is given by line integrals in the  $k$ -space. To evaluate  $T_1$  we only need the first term whose calculation is performed in Appendix.

The relaxation rate is now calculated by inserting eqs.(3.16) and (3.17) with (A.11) into eq.(3.15). After a straightforward calculation we find a logarithmic divergence of the coefficient of  $T/M_Q$  in the expression for  $1/T_1$ . This arises from the intraband contribution of the dynamical susceptibility [ $\tau_{11}$  and  $\tau_{22}$  in eq.(2.38)] whose long wave and low frequency components survive to a certain extent in contrast with the cut off's at small wave vectors

as found in the interband contribution [ $\tau_{12}$  and  $\tau_{21}$  in eq.(2.38)] and in ferromagnetic case.

The long wave and low frequency intraband contributions which lead to the divergence of  $1/T_1$  may be easily suppressed by magnetic anisotropy which generally exists in the ordered phase. Though the anisotropy is usually small, it is sufficient to overcome the divergence since the divergence is very weak (logarithmic). Here we take account of the effect phenomenologically. Dealing with metals, we may fairly generally assume cubic symmetry. In weakly antiferromagnetic metals we may expand the free energy due to the anisotropy:

$$F_a = \frac{1}{2} K M_Q^4 (\alpha_x^2 \alpha_y^2 + \alpha_y^2 \alpha_z^2 + \alpha_z^2 \alpha_x^2), \quad (3.18)$$

where  $\alpha_x$ ,  $\alpha_y$  and  $\alpha_z$  are the directional cosines of the staggered magnetization vector with respect to the crystallographic axes.

The static transversal staggered susceptibility is given by

$$\chi_Q = 1/K M_Q^2. \quad (3.19)$$

The dynamical susceptibility  $\chi_{M_Q, I}^{-+}(q+Q, \omega)$  in the presence of the anisotropy should have the value in its static limit. We modify the dynamical susceptibility so that the above mentioned requirement is fulfilled:

$$\begin{aligned} & I[\chi_{M_Q, 0}^{-+}(Q, 0) - \chi_{M_Q, 0}^{-+}(q+Q, \omega)] \\ \rightarrow & I[\chi_{M_Q, 0}^{-+}(Q, 0) + \frac{1}{2} \chi_{Q, 0}^{0A} \chi_{Q, 0}^{0B} - \chi_{M_Q, 0}^{-+}(q+Q, \omega)] \end{aligned} \quad (3.20)$$

with

$$A_0 = K[2\chi_{M_Q,0}^{-+}(Q,0)]^3/\alpha_Q. \quad (3.21)$$

After a straightforward but rather lengthy calculation, the relaxation rate is given by

$$1/T_1 = A_{hf}^2 k_B T [\chi_{M_Q,0}^{-+}(Q,0) C_0 / (2\pi)^3 I] g[A_0] M_Q(T)^{-1}, \quad (3.22)$$

where  $g[A_0]$  is a function depending on the anisotropy constant  $K$  or  $A_0$  [the expression of  $g[A_0]$  is given by eq.(5.9) in Ref.41)]. As the dependence of  $g[A_0]$  on the magnetization is very weak, we may consider that  $g[A_0]$  is  $T$ -independent.  $g[A_0]$  diverges logarithmically as  $A_0$  becomes zero. Though the effect of anisotropy is important theoretically, the dependence of the relaxation rate on it is very weak. From eq.(3.22) we see

$$1/T_1 \propto T/M_Q(T) \quad (3.23)$$

in contrast to the ferromagnetic case [eq.(3.6)]. At  $T = 0$  K, as  $M_Q(T) \propto (\alpha_Q - 1)^{1/2}$ , the relaxation rate is enhanced by the factor  $|\alpha_Q - 1|^{-1/2}$  at both sides of the antiferromagnetic instability.

Near  $T_N$ , where  $M(T) \propto (T_N - T)^{1/2}$  hold, we obtain  $1/T_1 \propto T_N/(T_N - T)^{1/2}$  which shows a divergence of the same type as that above  $T_N$ .

In Fig.2, we also plot the relaxation rates below  $T_N$ , obtained by using eqs.(3.22) and (2.47).

Recently, Katayama, Akimoto and Asayama investigated the relaxation rates of  $\beta$  Mn metal and its alloys.<sup>48)</sup> Their results are shown in Fig.4. They observed the  $T^{1/2}$  behavior and concluded that pure

$\beta$  Mn is a nearly antiferromagnetic metal which lies very close to the antiferromagnetic instability.

### §§3.2. Specific Heat

Specific Heat is calculated from the free energy  $F(\Psi, T)$  where  $\Psi$  is an order parameter:

$$C(T) = - T \frac{d^2}{dT^2} F(\Psi^*(T), T) . \quad (3.23)$$

The suffix \* stands for the thermal equilibrium value defined by

$$\frac{\partial}{\partial \Psi^*} F(\Psi^*, T) = 0 . \quad (3.24)$$

Eq.(3.23) is rewritten by using eq.(3.24) as

$$C(T) = - T \left[ \frac{\partial^2}{\partial T^2} F(\Psi^*, T) + \frac{\partial^2 F(\Psi^*, T)}{\partial \Psi^* \partial T} \frac{d\Psi^*}{dT} \right] . \quad (3.25)$$

For ferromagnetism [antiferromagnetism], by taking  $M[M_Q]$  as  $\Psi$  and using the free energy of eq.(2.6) [(2.17)] with eq.(2.14) [(2.24)] and reinterpreting  $M[M_Q]$  as the equilibrium value determined by the self-consistent equation, we obtain the specific heat. This calculation is straightforward, although rather complicated.

Izuyama and Kubo<sup>34)</sup> investigated the critical anomaly of the specific heat near  $T_C$  in the paramagnetic side and obtained the critical exponent  $1/2$ , rather too large result. Berk and Schrieffer<sup>35)</sup> and Doniach and Engelsberg<sup>36)</sup> studied the specific heats of nearly ferromagnetic metals at low temperatures. They showed that the linear specific heat is enhanced by the factor  $-\log(1-\alpha)$ . Subsequently Brinkman and Engelsberg<sup>37)</sup> studied low temperature specific heats of weakly ferromagnetic metals and showed that the linear term is enhanced by the factor  $-\log(\alpha-1)$ . These

treatments are based on RPA. The free energy used for the calculation of the specific heat is a function of temperature only:

$$F_{\text{RPA}}(\Psi_{\text{HF}}^*(T), T), \quad (3.26)$$

where  $\Psi_{\text{HF}}^*(T)$  is the equilibrium value obtained from the Hartree-Fock free energy

$$\frac{\partial}{\partial \Psi_{\text{HF}}^*} F_{\text{HF}}(\Psi_{\text{HF}}^*, T) = 0 \quad (3.27)$$

Apparently,  $\Psi_{\text{HF}}^*(T)$  is not the equilibrium value of the free energy of eq.(3.26). Thus this type of theory shows an apparent inconsistency to perform the calculation through the transition point. The Curie point Izuyama and Kubo used is considered to be a fictitious one and the other authors' treatments are only valid at low temperatures. To discuss the specific heat due to fluctuations through the transition point the renormalization procedure discussed in §2. is indispensable.

The self-consistent calculations of the specific heats of nearly and weakly ferromagnetic metals are performed by Makoshi and Moriya<sup>49)</sup> in the framework of the MK theory. Their results may be abridged as follows.

1) Low temperature specific heat is enhanced by the factor  $-\log|\alpha-1|$ .

However, the temperature range where the linear specific heat is obtained becomes narrower as the ferromagnetic instability is approached. This trend is much more strong compared with RPA results.

2) The anomaly around the Curie point is rather small in contrast with the RPA results. Yet the self-consistent renormalization

theory gives an unphysical small dip just above  $T_C$ . This shows that the MK theory is still insufficient to describe critical phenomena.

For nearly antiferromagnetic metals Moriya have shown that the enhancement factor tends to a constant value at the antiferromagnetic instability.<sup>47)</sup> This originates from the fact that the imaginary part of the staggered dynamical susceptibility of the non-interacting system is proportional to  $\omega$  instead of the fact that the imaginary part of the uniform component is proportional to  $\omega/q$ . Hasegawa<sup>50)</sup> investigated the specific heats of both weakly and nearly antiferromagnetic metals in the framework of the HM theory. His conclusions may be abridged as follows.

- 1) The coefficient of the linear specific heat due to spin fluctuations ( $\Delta\gamma$ ) is enhanced by the factor

$$\Delta\gamma(1) - \Delta\gamma(\alpha_Q) \propto |\alpha_Q - 1|^{\frac{1}{2}}, \quad (3.28)$$

where  $\Delta\gamma(1)$  is the constant value obtained by Moriya for the antiferromagnetic instability ( $\alpha_Q = 1$ ). Combining the relation between  $\alpha_Q - 1$  and  $T_N$  [eq.(2.45)] with eq.(3.28) he got

$$\Delta\gamma(1) - \Delta\gamma(\alpha_Q) \propto T_N^{3/4}, \quad (3.29)$$

and showed that the experiments on  $(V_{1-x}Cr_x)B_2$  by Castaing et al.<sup>51)</sup> actually satisfied the relation. Recent experiments on  $Cr_{1-x}Mo_x$  by Mamiya and Masuda<sup>52)</sup> also support the relation.

- 2) As the temperature increases the enhancement factor decreases rapidly. This trend is generally strong when the substance

lies near the instability and is stronger in the self-consistent theory than in RPA.

### §§3.3. Magnetic Excitations<sup>53)</sup>

[1] The most direct method of observing the spin fluctuations is an inelastic neutron scattering experiment, which essentially measures the imaginary part of the dynamical susceptibility. As our approximation scheme neglects the  $q$ - and  $\omega$ -dependences of  $\lambda_{M_Q, I}(q, \omega)$ ,  $q$ - and  $\omega$ -dependences of the dynamical susceptibility is the same as those of the RPA dynamical susceptibility. Nevertheless, the excitation spectrum includes some interesting points compared with those of ferromagnetic case. In this subsection, we will study the magnetic excitations in the antiferromagnetic phase, especially spin waves, in some detail.

To discuss the spin waves of an itinerant antiferromagnet some authors introduced, implicitly or explicitly, nesting type band.<sup>21, 54-57)</sup> They obtained well defined spin waves with a high velocity determined by the Fermi velocity. It should be mentioned here that the nesting model is a rather special one in the following sense. The ordered state of the model is insulating, i.e. there is no Fermi surface. In this connection we comment on two points. First, in the nesting model,  $1/T_1$  has no direct process if anisotropy or external field lifts up the spin wave spectrum. Second, in the model there is no linear specific heat in the ordered phase. Fisher investigated also the case where the Fermi level is not located within the gap and concluded that the velocity of the spin waves had no imaginary part even in this case.<sup>57)</sup> However, as Gillan has correctly indicated,<sup>58)</sup> Fisher's conclusion is based on an erroneous assumption that the dynamical susceptibility of the non-interacting system is analytic in the long wave and low frequency region. Taking care of this point Gillan calculated

the velocity as a complex number and obtained a damping proportional to  $q$ . Very recently, Cade and Young calculated numerically the transversal magnetic susceptibility by using the band structure of  $\gamma$ -Mn.<sup>59)</sup> Although, they also have obtained a considerable damping, we cannot distinguish whether the damping originates from many band effects or an intrinsic nature of antiferromagnetism.

It is instructive to compare the situation with that of a ferromagnetic metal. In the ferromagnet electrons suffer a uniform exchange field and the size of the Fermi surfaces are different for up and down spin electron bands. As a result there is a Stoner gap in the particle-hole pair excitation spectrum and we have undamped spin waves below the Stoner gap. In an antiferromagnet whose wave vector is  $Q$  and the staggered magnetization is along the  $z$ -axis, electrons suffer a staggered exchange field and an electron with momentum  $k$  couples with the electrons of the same spin and momentum  $k \pm Q$ . We have two bands with a splitting in the reduced Brillouin zone for each spin component. Therefore there are spin flip excitations with zero frequency in the long wave region so far as the antiferromagnetic state is metallic. So the damping of the spin waves into electron-hole pairs may be expected in the single band model and this is a unique feature of itinerant antiferromagnets.

[2] The dynamical susceptibility in RPA is given by eq.(2.25) and (2.30) with neglecting  $\lambda_{M_{Q,I}}(q,\omega)$ . The explicit form is

$$\chi^{-+}(q, \omega) = \frac{1}{\Delta(q, \omega)} \{ [1 - I\chi_{B_Q}(q+Q, \omega)] \chi_{B_Q}(q, \omega) + I[\chi_{B_Q}(q, -q-Q: \omega)]^2 \}, \quad (3.30)$$

$$\chi^{-+}(q+Q, \omega) = \frac{1}{\Delta(q, \omega)} \{ [1 - I\chi_{B_Q}(q, \omega)] \chi_{B_Q}(q+Q, \omega) + I[\chi_{B_Q}(q, -q-Q: \omega)]^2 \}, \quad (3.31)$$

with

$$\Delta(q, \omega) = [1 - I\chi_{B_Q}(q, \omega)] [I\chi_{B_Q}(Q, 0) - I\chi_{B_Q}(q+Q, \omega)] - I^2 [\chi_{B_Q}(q, -q-Q: \omega)]^2. \quad (3.32)$$

Here we suppressed the under suffix  $M_Q, I$  and denoted  $\chi_{M_Q, I}^{-+}(p, p': \omega)$  as  $\chi_{B_Q}(p, p': \omega)$ . The dynamical susceptibility of the non-interacting system  $\chi_{B_Q}(q+Q, \omega)$ ,  $\chi_{B_Q}(q, \omega)$  and  $\chi_{B_Q}(q, -q-Q: \omega)$ , are given in eqs.(2.38), (2.39) and (2.40), respectively. The components  $\chi^{-+}(q, \omega)$  and  $\chi^{-+}(q+Q, \omega)$  express the magnetic excitations around the chemical and magnetic reciprocal lattice points, respectively. As the intensity of the former is small we investigate the latter [note that the numerator of eq.(3.30) is zero for  $q=0$  and  $\omega=0$ ].

If the low lying elementary excitations are exhausted by the spin waves they can be treated phenomenologically. An equation of motion of the magnetization density under an external field varying in space and time,  $\vec{H}(q, \omega)$ , is given by

$$F = \sum_p \frac{1}{2\chi_p} \vec{M}_p \cdot \vec{M}_{-p} + \dots - \vec{M}_{-q} \cdot \vec{H}(q, \omega), \quad (3.33)$$

$$\vec{H}_{\text{eff}}(p) = \frac{\partial F}{\partial \vec{M}_{-p}} = \frac{1}{\chi_p} \vec{M}_p + \dots - \vec{H}(q, \omega) \delta_{p,q}, \quad (3.34)$$

$$\frac{d}{dt} \vec{M}_p = \sum_{p'} \vec{M}_{p-p'} \times \vec{H}_{\text{eff}}(p'). \quad (3.35)$$

By linearizing the torque equation we obtain the dynamical susceptibilities.<sup>60)</sup> We get for ferromagnets

$$[\chi^{-+}(q, \omega)]_{\text{sw}} = \frac{M_q^{-}(\omega)}{H^{-}(q, \omega)} = [(\chi_q^{-1} - \chi_0^{-1}) - (\omega/M)]^{-1}, \quad (3.36)$$

and

$$\begin{aligned} [\chi^{-+}(q+Q, \omega)]_{\text{sw}} &= \frac{M_{q+Q}^{-}(\omega)}{H^{-}(q+Q, \omega)} \\ &= [\chi_q^{-1} - \chi_Q^{-1}] / [(\chi_q^{-1} - \chi_Q^{-1})(\chi_{q+Q}^{-1} - \chi_Q^{-1}) - (\omega/M_Q)^2], \end{aligned} \quad (3.37)$$

for antiferromagnets. The spin wave dispersion is given by

$$\omega_q = M(\chi_q^{-1} - \chi_0^{-1}), \quad (3.38)$$

for ferromagnets and for antiferromagnets

$$\omega_q^2 = M_Q^2(\chi_q^{-1} - \chi_Q^{-1})(\chi_{q+Q}^{-1} - \chi_Q^{-1}). \quad (3.39)$$

It is noteworthy here that if one replaces  $\chi_q$  by  $J(q)$ , the Fourier  $q$ -component of the inter atomic exchange  $J_{ij}$ , eqs.(3.36)-(3.39) give correct results for the localized model.

For ferromagnetic metals the microscopic result based on RPA,

$$[\chi_{M,I}^{-+}(q,\omega)]_{\text{RPA}} = \frac{\chi_{M,0}^{-+}(q,\omega)}{I[\chi_{M,0}^{-+}(0,0) - \chi_{M,0}^{-+}(q,\omega)]}, \quad (3.40)$$

is easily shown to coincide with the phenomenological one by using an expansion

$$\chi_{M,0}^{-+}(q,\omega) = \chi_{M,0}^{-+}(q,0) + \frac{\omega}{2B} \chi_{M,0}^{-+}(0,0), \quad (3.41)$$

where B is the exchange field which produce the magnetization M.

The same is not true for antiferromagnetic metals. In order to compare the microscopic results with the phenomenological ones we tentatively assume that we may expand the susceptibilities of the non-interacting system for small  $(\omega/B_Q)$  and  $(q/B_Q)$ ;

$$\begin{aligned} \chi_{B_Q}(q+Q,\omega) &= \chi_{B_Q}(q+Q,0) + \left(\frac{\omega}{2B_Q}\right)^2 \chi_{B_Q}^I(0,0) + \dots, \\ \chi_{B_Q}(q,-q+Q;\omega) &= -\left(\frac{\omega}{2B_Q}\right) \chi_{B_Q}^I(0,0) + \dots, \end{aligned} \quad (3.42)$$

with

$$\chi_{B_Q}(p,\omega) = \chi_{B_Q}^I(p,\omega) + \chi_{B_Q}^{II}(p,\omega)$$

where the suffix I represents the part of the interband contribution and II that of the intraband contribution [see eqs.(2.38) and (2.39) and (2.40)]. Then we have

$$\begin{aligned}
& \chi^{-+}(q+Q, \omega) \\
& \cong I^{-1} [\chi_{B_Q}(Q, 0) - \chi_{B_Q}(q, 0)] \chi_{B_Q}(q+Q, 0) \{ [\chi_{B_Q}(Q, 0) - \chi_{B_Q}(q+Q, 0)] \\
& \times [\chi_{B_Q}(Q, 0) - \chi_{B_Q}(q, 0)] - (\omega/2B_Q)^2 \chi_{B_Q}^I(0, 0) [\chi_{B_Q}(Q, 0) - \chi_{B_Q}^{II}(0, 0)] \}^{-1}.
\end{aligned}
\tag{3.43}$$

Equation (3.43) coincides with eq.(3.37) if the intraband contributions vanish. The nesting model just belongs to this case and by expanding  $\chi_{B_Q}(q+Q, 0)$  for small  $q/B_Q$  we obtain the well known dispersion relation

$$\omega_q = \frac{1}{3} \bar{v}_F q, \tag{3.44}$$

where  $\bar{v}_F$  is the geometric mean of the Fermi velocities of the electron and hole bands.

In a general case where the Fermi surfaces exist, eqs.(3.37) and (3.43) do not agree because of the non-vanishing intraband contribution. As will be seen in the later paragraphs, we generally have the intraband particle-hole pair excitations with small momentum transfer whenever the Fermi surfaces exist. In this case the expansion for  $(\omega/B_Q)$  and  $(q/B_Q)$  [eq.(3.42)] is not valid and  $\chi_{B_Q}^{II}(q+Q, \omega)$  etc. depend on  $(q/\omega)$ . In other words  $\chi_{B_Q}^{II}(q+Q, \omega)$  etc. are not analytic functions of  $q$  and  $\omega$  even in the region of small  $(q/B_Q)$  and  $(\omega/B_Q)$ . The physical meaning of the above mentioned discrepancy is considered to be as follows. The phenomenological equation of motion which is a classical torque equation of the macroscopic magnetization density takes no account of the incoherent particle-hole pair excitations.

[3] To investigate the magnetic excitations in more detail we introduce a specific model, the electron gas model with Umklapp processes, in the same manner as the other sections. In this subsection we use reduced units which measure energy and momentum by the Fermi energy and Fermi momentum in the paramagnetic phase, respectively. We take  $Q = (0,0,Q)$ .

The static properties  $\chi_{B_Q}(Q,0)$ ,  $\chi_{B_Q}(0,0)$ ,  $\chi_{B_Q}^I(0,0)$ , the normalized staggered magnetization  $\zeta_Q = M_Q/N$  and the radius of the Fermi surface in the  $Q$  direction of the upper band  $q_1$  are plotted in Fig.5 as functions of the staggered exchange field  $B_Q$ . We take  $k_F = 0.8 Q$  in this figure and in the following numerical calculations. The staggered magnetization is related to  $\chi_{B_Q}(Q,0)$  by

$$\zeta_Q = \frac{2}{3} B_Q \frac{1}{\rho} \chi_{B_Q}(Q,0), \quad (3.45)$$

where  $\rho$  is the density of states in the paramagnetic phase.

$\chi_{B_Q}^I(0,0)$  is given by

$$\chi_{B_Q}^I(0,0) = \rho \frac{B_Q}{Q} \left[ \tan^{-1} \frac{Q^2}{2B_Q} + \tan^{-1} \frac{Qq_1}{B_Q} \right] + \dots, \quad (3.46)$$

for small  $B_Q$ . It is seen from eq.(3.43) that the deviation from the phenomenological theory is large for weakly antiferromagnetic metals ( $B_Q$  small). In the following we consider the case  $B_Q = 0.1$ .

Imaginary part of  $\chi_{B_Q}(q+Q, \omega)$  is shown in Fig.6 as a function of  $q$  [ $q = (0,0,q)$ ] and  $\omega$ . Dashed lines I, II, III are the boundaries separating the regions where the excitations between the bands 1 and 1, 2 and 2, and 1 and 2, respectively, exist. For small  $q$  these lines are given by

$$\omega = a_I(B_Q)q \quad (I),$$

$$\omega = a_{II}(B_Q)q \quad (II),$$

$$\omega = 2B_Q + a_{III}(B_Q)q^2 \quad (III). \quad (3.47)$$

The coefficients in the small  $B_Q$  limit are

$$a_I(B_Q) = Q, \quad a_{II}(B_Q) = 2, \quad a_{III}(B_Q) = Q^2/2B_Q. \quad (3.48)$$

Line II tends to the boundary in the paramagnetic phase continuously as  $B_Q$  becomes 0. Lines I and III are characteristic of the anti-ferromagnetic state and the imaginary part diverges as  $|\omega - \omega^*|^{\frac{1}{2}}$  when  $\omega$  approaches the line ( $\omega^*$ ) for a fixed  $q$ . In the low frequency region below the line I, the imaginary part is proportional to  $\omega q[\text{eq.}(3.17)]$ . The large imaginary part suggests that the exchange-enhanced dissipative modes of spin fluctuations are expected to be dominant in this region.

Real parts of  $\chi_{B_Q}(q, \omega)$  and  $\chi_{B_Q}(q+Q, \omega)$  are illustrated in Fig.7 by solid lines as a function of the  $\omega$  for a fixed  $q$  ( $q/B_Q=0.5$ ). The dashed line is  $\chi_0(q, \omega)$  in the paramagnetic phase. The arrows indicate the position of the boundaries I, II, III. We can see characteristic structures associated with the new boundaries I and III in addition to the one associated with II which also exists in the paramagnetic phase. In our model, the singularities at the boundaries I and III are rather strong and the real part has finite discontinuities. These strong singularities as well as those of the imaginary part result from the fact that the energy denominator of eq.(2.41) in our case becomes zero on a line, instead of a point, on the Fermi surface as  $\omega$  approaches the boundary value  $\omega^*$ .

The magnetic excitations  $[Im \chi^{-+}(q+Q, \omega)]$  are shown in Fig.8 as a function of  $q$  and  $\omega$ . In the low frequency region we have two structures. The lower frequency peak is due to diffusive electron-hole pair excitations and the higher one is due to spin wave like modes. This assignment is confirmed by considering an anisotropy [see also Fig.9]. The spin waves decay into electron-hole pairs and have an intrinsic  $q$ -dependent width. The intrinsic width is a unique feature of the itinerant antiferromagnets in contrast with the ferromagnetic and local moment cases.

Now we consider the effect of anisotropy in a phenomenological way [eqs.(3.18)-(3.21)]. Figure 9 shows the magnetic excitations in the presence of the anisotropy [a case of a fairly strong anisotropy  $A(\chi_Q^0/2\rho) = 1.0$ ]. The effect of the anisotropy is two fold. Firstly, the dissipative low frequency modes are suppressed by the effect. We see that the low frequency peak in Fig.8 disappears in Fig.9. Secondly, the spin wave modes are lifted up and in the long wave limit become good modes which do not decay into electron-hole pairs. The spin wave frequency dispersion has a finite gap  $\omega_G$ . By using eq.(3.46) in eq.(3.43) with the above mentioned modification [eq.(3.20)], we get

$$\omega_G = \left\{ \frac{4AQ}{\pi\rho} [\chi_{B_Q}(Q,0) - \chi_{B_Q}(0,0)] \right\}^{1/2} B_Q^{3/2}, \quad (3.49)$$

for small  $B_Q$ .

We have seen unique features of the spin waves of itinerant antiferromagnets: intrinsic damping and importance of the anisotropy. The excitations of electron-hole pair type have also large amplitude especially in the case without anisotropy and contribute considerably

to the physical properties such as specific heat, NMR relaxation rate and resistivity, as discussed in the other subsections.

Because of rather academic nature of our model for the numerical calculations, detailed comparison with experiments is beyond our scope. However, we may gain a better understanding of the neutron scattering experiments in the light of our results. The alloy system  $\gamma$ -FeMn is known to be an antiferromagnetic metal system where the band nesting plays a minor role in contrast with Cr.<sup>30)</sup> Tajima, Ishikawa, Endoh and Noda have studied the magnetic excitations of the system by neutron scattering.<sup>61)</sup> Their results show that the spin waves have a significant damping which is almost proportional to  $q$ . Sato and Maki investigated the excitations theoretically.<sup>62)</sup> To explain the noncollinear spin structure of  $\gamma$ -FeMn system,<sup>63)</sup> they considered several Fermi surfaces near  $\Gamma$  and X points and concluded that the multi spin density wave state is the most stable one. Then they studied the excitation and obtained the damping proportional to  $q^2$  in contrast with the experiment. Tajima et. al. have also obtained the energy gap  $\omega_Q$  proportional to  $3/2$  power of the magnetization, in accordance with eq.(3.49). Sato and Maki have also studied the gap by considering the dipole spin interaction and obtained the result that the gap is proportional to  $B_Q$ . These facts suggest that the neutron scattering experiment on  $\gamma$ -FeMn exhibits the general characters of magnetic excitations of standard antiferromagnetic metals and not those of a rather special antiferromagnet of the nesting type.

### §§3.4. Electrical Resistivity<sup>64)</sup>

[1] As has been seen in Table 1 in §§1.3, electrical resistivity of magnetic metals is characterized by a large term proportional to  $T^2$  at low temperatures. This resistivity is considered to be due to the scatterings by spin fluctuations. This last subsection is devoted to a study of the resistivity. After Mills and Lederer<sup>65)</sup> let us introduce a simple model consisting of s- and d-band electrons. Only the s-electrons contribute to the conductivity and the d-electrons play a role of scatterers, i.e. the conduction electrons are scattered by the spin fluctuations of the d-band electrons via an s-d exchange interaction. The model hamiltonian of the system is

$$H = H_s + H_d + H_{s-d}, \quad (3.50)$$

$$H_s = \sum_{k, \sigma} \xi_k c_{k\sigma}^+ c_{k\sigma}, \quad (3.51)$$

$$H_{s-d} = J \sum_{qk} [c_{k+q\uparrow}^+ c_{k\downarrow} s_-(q) + c_{k+q\downarrow}^+ c_{k\uparrow} s_+(q) + (c_{k+q\uparrow}^+ c_{k\uparrow} - c_{k+q\downarrow}^+ c_{k\downarrow}) s_z(q)], \quad (3.52)$$

where  $c_{k\sigma}$  is the annihilation operator of the s-electron of momentum  $k$  and spin  $\sigma$ ,  $J$  the coupling constant of the s-d interaction and  $s_\alpha(q)$  [ $\alpha = +, -, z$ ] the spin density operator for the d-band defined by eq.(1.6).

When the antiferromagnetic ordering, whose wave vector is  $Q$ ,<sup>\*)</sup> sets in, s-electrons suffer a periodic exchange field via the s-d exchange interaction:

$$B_s = J \langle s_z(Q) \rangle = J \langle s_z(-Q) \rangle. \quad (3.53)$$

The periodic field reduces the first Brillouin zone into the half and results in a splitting of the conduction band. The canonical transformation to describe the new bands is the same as eqs.(2.34)-(2.36):

$$\left. \begin{array}{l} \xi_{1k} \\ \xi_{2k} \end{array} \right\} = \frac{1}{2}(\xi_{k+Q} + \xi_k) \mp \left[ \frac{1}{4}(\xi_{k+Q} - \xi_k)^2 + B_s^2 \right]^{1/2}, \quad (3.54)$$

$$\tan 2\psi_k = (\xi_{k+Q} - \xi_k)/2B_s. \quad (3.55)$$

By the transformation, the distortion of the Fermi surface of the conduction band is taken account of. By using Born approximation, transition probabilities due to the s-d interaction can be calculated:

$$\begin{aligned} & \omega_{s-d}(1 k \sigma \rightarrow 1 k+q \sigma) \\ &= (2/\hbar) J^2 [n(\omega_{1k,1k+q}) + 1] \{ \cos^2(\psi_k - \psi_{k+q}) \text{Im} \chi^{zz}(q, \omega_{1k,1k+q}) \\ & \quad - 2\sigma \cos(\psi_k - \psi_{k+q}) \sin(\psi_k + \psi_{k+q}) \text{Im} \chi^{zz}(q, -q-Q; \omega_{1k,1k+q}) \\ & \quad + \sin^2(\psi_k + \psi_{k+q}) \text{Im} \chi^{zz}(q+Q, \omega_{1k,1k+q}) \} \text{ etc}, \end{aligned} \quad (3.56)$$

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\*) For brevity let us consider the single  $Q$  antiferromagnet as the same manner in the other subsections. We take the  $z$ -axis along  $Q$  and consider the case where the current flows parallel to  $Q$ .

where  $\omega_{ik,jk'}$  is the energy change of the scattered electron and  $n(\omega)$  the Bose function.

As we deal with the anisotropic and inelastic scattering, we have recourse to variational principle.<sup>66)</sup> We choose  $\nabla \xi_{ik}$  as a trial function. The actual distribution of the electrons deviates from the one described by the trial function owing to the anisotropic nature of the s-d scattering. Although an estimation of the deviation is practically impossible, we may consider the deviation is not so serious from the following reasons. Firstly, in the actual substance, impurity scattering and phonon scattering which are isotropic have a tendency to reduce the deviation. Especially, at low temperatures the s-d scattering is dominated over by the impurity scattering and it can be shown that the trial function is exact up to the first order of  $B_s$  in this case [see Appendix I of Ref. 64)]. Secondly, the contribution of the deviation to the resistivity is proportional to the square of the deviation [eq.(A.5) in Ref.64)]. Above  $T_N$  our procedure is equivalent to introducing a relaxation time averaged over the conduction electrons. Below  $T_N$  we can take account of the effect of the gap of the conduction bands resulting from the ordering of the d-band. Therefore we may expect that our trial function describes well qualitative features of the resistivity due to the spin fluctuations, although it generally overestimates the resistivity to some extent.

After straightforward calculations the following expression for the electrical resistivity is obtained:

$$\begin{aligned}
R = & \left[ \hbar J / n e (1 - g B_s) \right]^2 \frac{1}{k_B T} \sum_q' \int d\omega n(\omega) [n(\omega) + 1] \\
& [2\Gamma^{zz}(q, \omega) \operatorname{Im} \chi^{zz}(q, \omega) + \Gamma^{+-}(q, \omega) \operatorname{Im} \{ \chi^{+-}(q, \omega) + \chi^{-+}(q, \omega) \} \\
& + 2\Gamma^{zz}(q+Q, \omega) \operatorname{Im} \chi^{zz}(q+Q, \omega) + \Gamma^{+-}(q+Q, \omega) \\
& \operatorname{Im} \{ \chi^{+-}(q+Q, \omega) + \chi^{-+}(q+Q, \omega) \} ] , \tag{3.57}
\end{aligned}$$

with  $g = 3\pi Q/4k_F^* \epsilon_F^*$ ,  $k_F^*(\epsilon_F^*)$  being Fermi momentum (energy) of the s-band. As the resistivity is expressed in terms of the dynamical susceptibilities, the expression is applicable for both itinerant and localized models for the d-electrons.  $\Gamma^{\alpha\beta}(q, \omega)$  takes care of the dependence on the nature of the s-band, particularly its splitting in the ordered phase. Their explicit forms are

$$\begin{aligned}
\Gamma^{zz}(q, \omega) = & \sum_k' [\sin^2(\psi_k - \psi_{k+q}) \{ \eta_{12}(k, q, \omega) + \eta_{21}(k, q, \omega) \} \\
& + \cos^2(\psi_k - \psi_{k+q}) \{ \eta_{11}(k, q, \omega) + \eta_{22}(k, q, \omega) \} ] , \\
\Gamma^{zz}(q+Q, \omega) = & \sum_k' [\sin^2(\psi_k + \psi_{k+q}) \{ \eta_{12}(k, q, \omega) + \eta_{21}(k, q, \omega) \} \\
& + \cos^2(\psi_k + \psi_{k+q}) \{ \eta_{11}(k, q, \omega) + \eta_{22}(k, q, \omega) \} ] , \\
\Gamma^{+-}(q, \omega) = & \sum_k' [\cos^2(\psi_k + \psi_{k+q}) \{ \eta_{12}(k, q, \omega) + \eta_{21}(k, q, \omega) \} \\
& + \sin^2(\psi_k + \psi_{k+q}) \{ \eta_{11}(k, q, \omega) + \eta_{22}(k, q, \omega) \} ] , \\
\Gamma^{+-}(q+Q, \omega) = & \sum_k' [\cos^2(\psi_k - \psi_{k+q}) \{ \eta_{12}(k, q, \omega) + \eta_{21}(k, q, \omega) \} \\
& + \sin^2(\psi_k - \psi_{k+q}) \{ \eta_{11}(k, q, \omega) + \eta_{22}(k, q, \omega) \} ] , \tag{3.58}
\end{aligned}$$

with

$$\begin{aligned} \eta_{ij}(k, q, \omega) = & [f(\xi_{jk+q}) - f(\xi_{ik})] \delta(\xi_{ik} - \xi_{jk+q} - \hbar\omega) \\ & \times [q_z + \frac{1}{2} Q \{ (-1)^j \sin 2\psi_{k+q} - (-1)^i \sin 2\psi_k \}]^2. \end{aligned} \quad (3.59)$$

In the paramagnetic phase  $\Gamma^{\alpha\beta}(q, \omega)$  is proportional to the dynamical susceptibility of the conduction band  $\chi_{(c)}^{\alpha\beta}(q, \omega)$

$$\Gamma^{\alpha\beta}(q, \omega) = \frac{1}{\pi} q^2 \text{Im} \chi_{(c)}^{\alpha\beta}(q, \omega) \quad (\text{paramagnetic phase}). \quad (3.60)$$

The factor  $1-gB_s$  in eq.(3.57) denotes a change of effective carrier number or effective mass resulting from the gap of the conduction band and is the origin of the hump in the resistivity observed just below  $T_N$ . Miwa<sup>67)</sup> and Elliott and Wedgwood<sup>68)</sup> investigated the distortion of the Fermi surface of the conduction band in consequence of the screw-type ordering of localized 4f-electrons. Using the relaxation time obtained by the molecular field approximation they gave an explanation of strong anomalies observed in heavy rare earth metals at the temperature where the magnetic ordering changed. The factor is consistent with their result.

To discuss the resistivity of antiferromagnets, we may disregard the contribution of the uniform components of the spin fluctuations [first two terms of the last brace in eq.(3.57)] because (1)  $\Gamma^{\alpha\beta}(q, \omega)$  represents small angle scattering compared with  $\Gamma^{\alpha\beta}(q+Q, \omega)$  and (2)  $\text{Im} \chi^{\alpha\beta}(q+Q, \omega)$  has a larger amplitude than  $\text{Im} \chi^{\alpha\beta}(q, \omega)$  in antiferromagnets. Further simplification may

be possible because  $q_z$  in eq.(3.59) gives only a weak dependence of  $\Gamma^{\alpha\beta}(q+Q, \omega)$  on  $q$ . Neglecting this term and making the following expansion for small  $\omega$

$$\Gamma^{\alpha\beta}(q+Q, \omega) = \frac{1}{2} \rho_c(\epsilon_F^*) Q^2 [(k_F^*/Q)(\hbar\omega/\epsilon_F^*) \gamma^{\alpha\beta}(q) + \dots], \quad (3.61)$$

where  $\rho_c(\epsilon_F^*)$  is the density of states of the conduction band, we obtain

$$R = \frac{m}{ne^2} \frac{9\epsilon_Q}{4\hbar} J^2 \rho_c(\epsilon_F^*) \chi_Q^0 \left(\frac{Q}{k_F^*}\right)^4 \bar{R}(T), \quad (3.62)$$

$$\bar{R}(T) = \frac{1}{(1 - gB_s)^2} \frac{1}{T} \int_0^r q^2 dq \int d\omega \omega n(\omega) [n(\omega) + 1] F(q, \omega), \quad (3.63)$$

$$F(q, \omega) = \frac{2}{3\chi_Q^0} [2\gamma^{zz}(q) \text{Im} \chi^{zz}(q+Q, \omega) + \gamma^{+-}(q) \text{Im} \{ \chi^{+-}(q+Q, \omega) + \chi^{-+}(q+Q, \omega) \}], \quad (3.64)$$

where  $m$  is the effective mass and  $n$  the electron number of the conduction band. The cut off parameter  $r$  is indicative of the extent around  $Q$  in the  $q$ -space where the spin fluctuations are effective on the resistivity and therefore depends on the band structure. The function  $\gamma^{\alpha\beta}(q)$  denotes the influence of the gap  $B_s$  on  $s$ - $d$  scattering and is normalized to unity in the paramagnetic state. The explicit form of  $\gamma^{\alpha\beta}(q)$  is given in Appendix.  $\bar{R}(T)$  which is a dimensionless quantity represents the  $T$  dependence of the resistivity. In eqs.(3.63) and (3.64) and in what follows reduced units which measure energy and momentum by  $\epsilon_Q$  and  $Q$  are again used unless otherwise stated.

[2] The expression of resistivity of ferromagnetic metals is given by neglecting  $B_s$ , keeping uniform components only and taking the summation on  $q$  over the whole first Brillouin zone in eq.(3.57).<sup>69)</sup> As for  $\Gamma^{\alpha\beta}(q, \omega)$  we may use eq.(3.60). Of course in the ferromagnetic state, conduction electrons suffer a uniform exchange field but the field does not play any essential role.

Mills and Lederer<sup>65)</sup> introduced the s-d model and calculated the resistivity due to RPA spin waves in itinerant ferromagnets. Subsequently the same model as applied to nearly ferromagnetic metals has been studied by employing RPA for the spin fluctuations. Schindler and Rice<sup>70)</sup> investigated the resistivity with the use of a simple model function for the RPA dynamical susceptibility. Their result shows that the resistivity of nearly ferromagnetic metals at low temperatures is proportional to  $T^2$  and its coefficient diverges at the critical boundary of ferromagnetism. In the extreme vicinity of and at the critical boundary Mathon<sup>71)</sup> showed that the resistivity at low temperatures was proportional to  $T^{5/3}$ . Mills<sup>72)</sup> discussed the resistivity of nearly ferromagnetic metals in a whole temperature range of interest using an expansion form of the RPA dynamical susceptibility. His calculation shows that the resistivity varies as  $T^2$  at low temperatures and is proportional to  $T$  at sufficiently high temperatures.

The resistivity was investigated on the basis of the MK theory by Moriya and the present author.<sup>69)</sup> The calculation is performed in the whole temperature range of interest for both weakly and nearly ferromagnetic metals. The main results of the calculation are summarized as follows.

- 1) At low temperatures the electrical resistivity is proportional to  $T^2$  for both ferromagnetic and paramagnetic metals. The coefficient of the term is large and diverges at the critical boundary as  $|\alpha - 1|^{-\frac{1}{2}}$ .
- 2) In the vicinity of the boundary the  $T^2$  behavior holds only in narrow temperature range and  $T^{5/3}$  behavior takes over as the temperature is raised. This trend is stronger in the self-consistent calculation than in RPA. In a substance lying just at the critical boundary the low temperature resistivity behaves as  $T^{5/3}$ .
- 3) The temperature derivative of the resistivity is discontinuous at  $T_C$ . The change of slope at  $T_C$  is proportional to the square of the magnetization at  $T = 0\text{ K}$  and is small for weak ferromagnets.
- 4) The resistivity is generally suppressed from that calculated with the use of the RPA spin fluctuations. This effect can be seen typically by saturation tendency of the resistivity at high temperatures.

These characteristics are consistent with experiments on typical weakly ferromagnetic metals  $\text{ZrZn}_2$ ,<sup>73,74)</sup>  $\text{Sc}_3\text{In}$ <sup>46)</sup> and a typical nearly ferromagnetic metal  $\text{HfZn}_2$ .<sup>75)</sup> Recent experiment on  $\text{Ni}_3\text{Al}$  by Sato also supports the results.<sup>76)</sup>

[3] In the paramagnetic phase,  $B_s = 0$  and  $\gamma^{\alpha\beta}(q) = 1$  hold and the three dynamical susceptibilities are connected with each other by the rotational invariance. By using the dynamical susceptibility discussed in §§2.2 and the expansion form eq.(2.43), the resistivity is obtained. At low temperatures the resistivity does not depend on the cut off parameter  $r$ . Performing the  $q$ -integral in eq.(3.63) we get

$$\begin{aligned}\bar{R}(\delta, \omega) &= \int q^2 dq F(q, \omega) \\ &= \frac{\pi C_0 (1+\delta) \omega}{\alpha_Q [2A_{xx} A_{yy} A_{zz}]^{\frac{1}{2}}} [\delta + \sqrt{\delta^2 + (C_0 \omega)^2}]^{-\frac{1}{2}},\end{aligned}\quad (3.65)$$

with  $\delta = \chi_Q^0 / \alpha_Q \chi_Q$ .

There are two limiting cases:

$$\bar{R}(T) = \frac{\pi C_0 (1+\delta)}{2\alpha_Q [A_{xx} A_{yy} A_{zz}]^{\frac{1}{2}}} \frac{T^2}{\sqrt{\delta}} Z(2) \quad (\delta \gg T), \quad (3.66)$$

$$\bar{R}(T) = \frac{\pi C_0 (1+\delta)}{\alpha_Q [2A_{xx} A_{yy} A_{zz}]^{\frac{1}{2}}} T^{3/2} Z(2) \quad (\delta \ll T) \quad (3.67)$$

where

$$Z(n) = \int_0^\infty d\omega \omega^n n(\omega) [n(\omega) + 1] = \Gamma(n+1) \zeta(n). \quad (3.68)$$

At high temperatures expanding the Bose factor as

$$n(\omega) [n(\omega) + 1] = \left(\frac{T}{\omega}\right)^2 \left[1 - \frac{1}{12} \left(\frac{\omega}{T}\right)^2 + \dots\right], \quad (3.69)$$

and performing  $\omega$ -integral first in eq.(3.63), we get

$$\bar{R}(T) = \frac{\pi(1+\delta)}{2\alpha_Q A^{3/2} \sqrt{\delta}} T \left[ \tan^{-1} \kappa - \frac{\kappa}{1+\kappa^2} \right], \quad (3.70)$$

with  $\kappa = r\sqrt{A/\delta}$ . In eq.(3.70) we have assumed  $A_{xx} = A_{yy} = A_{zz} = A$  for simplicity.

It should be noted that the imaginary part of  $\chi_{M_Q,0}^{-+}(q+Q,\omega)$  is generally small ( $\propto \omega$ ) compared with that of the ferromagnet ( $\propto \frac{\omega}{q}$ ). Equation (3.67) corresponds to the  $T^{5/3}$  law at the critical boundary of ferromagnetism. Because of the above mentioned nature of the antiferromagnetic fluctuations eq.(3.67) is applicable in a small temperature range and at higher temperatures the resistivity is suppressed from this value significantly. Another consequence is that  $\bar{R}(\delta,\omega)$  has a long tail in the region of large  $\omega$ . As a result, the situation where eq.(3.70) is applicable is hardly realized in the temperature region of our interest.

Now we show some numerical examples based on an electron gas model with Umklapp processes for the d-band, whose Fermi wave vector  $k_F$  is  $0.8 Q$ . Figures 10, 11 and 12 show  $\bar{R}(T)$  versus  $T$  in the paramagnetic state for some values of the cut off parameter  $r$ , 0.6, 1.2 and 1.8, respectively. Solid lines show the calculation based on the HM theory for several values of  $\alpha_Q$  or  $T_N$ . For comparison RPA results are shown by dashed lines.

From these analytical and numerical results we may draw the following conclusions.

(A) Nearly antiferromagnetic metals

(1) The resistivity at low temperatures is proportional to  $T^2/\sqrt{\chi_Q}$ .

As  $\chi_Q$  is proportional to  $1-\alpha_Q$  at  $T = 0$  K, the coefficient

of the term diverges as  $(1-\alpha_Q)^{-1/2}$  when the critical boundary of antiferromagnetism is approached. Recent experiments on the temperature and pressure dependences of the resistivity of 7 at % Co doped  $\text{NiS}_2$ <sup>77)</sup> show that the coefficient diverges as  $(P-P_0)^{-1/2}$ , where  $P_0$  is the critical pressure. This is consistent with our theory.

- (2) If the substance lies very near the critical boundary, the  $T^2$  law of the resistivity holds only in a small temperature range and the  $T^{3/2}$  law takes over as the temperature is slightly raised. Especially, just at the critical boundary  $R$  at low temperatures is proportional to  $T^{3/2}$ .
- (3) However, the temperature region where  $T^{3/2}$  law holds is also very narrow and  $R$  becomes almost  $T$ -linear. This is due to the smallness of the imaginary part of  $\chi_{M_Q,0}^{-+}(q+Q,\omega)$ . Ogawa<sup>78)</sup> observed linear  $T$  dependence in  $\beta$ -Mn at low temperatures. As  $\beta$ -Mn is considered to lie very near the critical boundary<sup>48)</sup> this linear  $T$  dependence may be attributed to this mechanism.
- (4) At high temperatures the resistivity is strongly suppressed from the RPA value and show a tendency of saturation.

(B) Antiferromagnetic metals in the paramagnetic state

At  $T_N$  the resistivity is expressed by eq.(3.67), but it deviates from the value expressed by eq.(3.67) immediately above  $T_N$ . As a result  $R$  becomes almost  $T$ -linear (Fig.11 and 12) or even make a dip for small  $r$  (Fig.10). At high temperatures the resistivity of the antiferromagnetic metal has a common feature with that of the nearly antiferromagnetic metal.

[4] Now we consider the resistivity in the antiferromagnetic phase. Below  $T_N$  we confine ourselves to low temperatures ( $T \ll T_N$ ). In this temperature region the spin fluctuations may be divided into two groups. One group consists of collective spin waves and the other paramagnon type spin fluctuation modes. Let us study the characteristics of the resistivity due to both of these types of spin fluctuations by examining the transversal components.

The resistivity due to the paramagnon type modes is proportional to  $T^2$ . This term is easily calculated by using the expansion forms:

$$\frac{3}{2} \bar{R}_1^{sf}(T) = \left[ \frac{2\chi_{M_{Q,0}}^{-+}(Q,0)C_0}{\chi_Q \alpha_Q} \right] Z(2) h(B_Q/B_S) \frac{T^2}{B_Q} . \quad (3.71)$$

The factor  $h(B_Q/B_S)$ , whose explicit form is given by eq.(4.8) in Ref.64), denotes the effect of the gap of the conduction band.  $h(B_Q/B_S)$  shows logarithmic divergence as  $B_S \rightarrow 0$  in the same manner as  $g[A_0]$  in the expression for  $T_1$ . The resistivity is proportional to  $T^2/B_Q$ . Because  $B_Q^2$  is proportional to  $\alpha_Q - 1$  at  $T = 0$  K, the coefficient of  $T^2$  is large and diverges as  $(\alpha_Q - 1)^{-1/2}$  when the critical boundary of antiferromagnetism is approached from the antiferromagnetic side.

The resistivity due to the spin waves have been investigated by several authors by using the localized moment model.<sup>79,80)</sup> Unfortunately, their results contradict with each other. We have investigated the spin waves in §3.3 and seen that the spin waves of itinerant antiferromagnets have an intrinsic width and the phenomenological treatments is insufficient for the itinerant case. However, the contribution of the spin waves to the resistivity

is considered to be small in the itinerant case and important for the local moment case. So we study the resistivity by using the phenomenological theory for the spin waves. By using eq.(3.37) the resistivity due to the spin waves is given by

$$\frac{3}{2} \bar{R}(T)_{sw} = \frac{1}{T} \int q^2 dq \int d\omega \omega n(\omega) [n(\omega) + 1] \gamma^{+-}(q) \left(1 - \frac{\chi_0}{\chi_Q}\right) \frac{\pi B_Q^2}{\omega_Q} \delta(\omega - \omega_q). \quad (3.72)$$

we may fairly generally assume that  $B_s \lesssim B_Q$ . In the temperature region where  $T$  is greater than the gap energy of the conduction band ( $T \gg B_s$ ),  $\gamma^{+-}(q)$  may be replaced by unity and we have

$$\frac{3}{2} \bar{R}(T)_{sw}^0 = \pi \left(1 - \frac{\chi_0}{\chi_Q}\right) \frac{B_Q^2}{v^3} T^2 Z(2) \quad (B_s \ll T \ll B_Q), \quad (3.73)$$

where  $v$  is the velocity of the spin wave  $\omega_q = v_q$ , which is assumed to be isotropic. The resistivity is proportional to  $T^2$  similarly to the contribution of the paramagnon type modes. At low temperatures where  $T \ll B_s$  holds the effect of the gap of the s-band is important. The resistivity at low temperatures is proportional to  $T^5$  owing to the extra factor  $(q_z/B_s)^3$  [eq.(A.12)] which originates from the fact that the scattering around  $Q$  is suppressed by the gap. To see this gap effect and the continuous change of the resistivity through the region  $T \sim B_s$ , let us show the results of eq.(3.72) in Fig.13. The figure shows  $\bar{R}(T)_{sw}/\bar{R}(T)_{sw}^0 (\propto \bar{R}(T)_{sw}/T^2)$  versus  $T/B_Q$ . The effect of the gap is indicated by the parameter

$$\bar{V} = 2V(B_s/B_Q).$$

The curves show how the resistivity changes its behavior from the  $T^5$  dependence to the  $T^2$  dependence.

#### §4. Summary and Discussions

In the preceding sections we have investigated the properties of the itinerant antiferromagnets. For weakly and nearly antiferromagnetic metals, which have been the main objects of our study, the spin fluctuations whose wave vectors are near the antiferromagnetic wave vector play a predominant role. The self-consistent renormalization theory of our scheme treats properly the spin fluctuations which have a local character in  $q$ -space. In the present article we have seen that the theory qualitatively improves the conventional HFA-RPA theory and that the physical properties closely related to the spin fluctuations are well understood by the framework of the theory. Many experiments also support the results. Further systematic experiments are highly desired. This type of theory may be extended to the cases of more general magnetic structures, for example helical spin structures<sup>60,81)</sup> and coexistence of ferro- and antiferromagnetism.<sup>82)</sup>

Through our study we have used the electron gas model with Umklapp processes as a model for the non-interacting system. This is because that the nesting-type models are considered to be rather special ones as we have seen in the preceding sections. However, in the band type model, where all the portions of the band is responsible for the antiferromagnetism, the calculation of the dynamical susceptibility is a laborious task and we have confined ourselves to low temperatures in the antiferromagnetic phase. To set up a band type model, which is easily tractable mathematically in the ordered phase, is an important problem awaiting solution.

The self-consistent theory we have reviewed is a theory suitable for weak magnetism. To acquire a unified understanding of magnetism, it is indispensable to proceed to the theory of strong magnetism. This implies to treat the case with large amplitude of magnetization and/or the spin fluctuations in a wider region in  $q$ -space. From the point of view of the electron correlation, our theory have made some approximations suitable for relatively weak electron-electron interaction. The theory of strong magnetism naturally includes the problem of stronger correlation.

Experiments on  $\text{NiS}_{2-x}\text{Se}_x$  show that the system exhibits the metal-insulator (Mott) transition and that the metallic side of the transition is also antiferromagnetic.<sup>83)</sup> To discuss the Mott transition, too, the theory of antiferromagnetism with large amplitude is important. We may gain a clearer conception of the transition in terms of charge fluctuations. It is noteworthy here that conductivity is related to the dielectric constant. In this case we should grasp the electron correlation as the problem of not only the spin fluctuations but also of the charge fluctuations and should clarify the connection between the two.

In the case of the strong electron correlation, our Hartree-Fock ground state with a use of the effective electron-electron interaction may encounter a serious criticism, although no definite experimental fact against the Hartree-Fock ground states of the transition metals has been reported so far. In any case, it will be a matter of great significance to describe not only the excited states but also the ground state more accurately.

These problems, we believe, are fundamental and fascinating ones still to be solved in the theory of magnetism and also in many body problems.

## Acknowledgments

The author dedicates sincere gratitudes to Professor Tôru Moriya, who guided him to the field of solid state physics, for enlightening discussions and encouragements during the course of the study and for critical reading of the manuscript. His thanks also go to Dr. H. Hasegawa and Dr. K. Makoshi for many stimulating and useful discussions. He also appreciates stimulating discussions with the other members of the research group under Professor T. Moriya, Mr. K. Usami, Mr. Y. Takahashi and Mr. M. Isoda. Many exciting discussions with Professor H. Yasuoka on experimental results, particularly on NMR experiments, are gratefully acknowledged. Thanks are also due to Miss. A. Hiraide for typing the manuscript.

## Appendix

The expansion coefficients  $c(q)$  and  $\gamma^{+-}(q)$  of the  $\omega$  linear terms of  $\chi_{M_Q,0}^{-+}(q+Q,\omega)$  and  $\Gamma^{+-}(q+Q,\omega)$ , respectively, are expressed by the line integrals in the  $k$ -space.<sup>41,64)</sup>

$$c(q) = c_{11}(q) + c_{22}(q) + c_{12}(q) + c_{21}(q), \quad (A.1)$$

$$\gamma^{+-}(q) = \gamma_{11}^{+-}(q) + \gamma_{22}^{+-}(q) + \gamma_{12}^{+-}(q) + \gamma_{21}^{+-}(q), \quad (A.2)$$

$$c_{ij}(q) = \frac{1}{2\chi_Q^0} \frac{1}{8\pi^2} \int_L dk \{ |\nabla \epsilon_{ik}|^2 |\nabla \epsilon_{jk+q}|^2 - (\nabla \epsilon_{ik} \cdot \nabla \epsilon_{jk+q})^2 \}^{-\frac{1}{2}} \begin{cases} \sin^2(\theta_k - \theta_{k+q}) & (i = j) \\ \cos^2(\theta_k - \theta_{k+q}) & (i \neq j), \end{cases} \quad (A.3)$$

$$\gamma_{ij}^{+-}(q) = \frac{1}{\pi} \int_L dk \{ |\nabla \xi_{ik}|^2 |\nabla \xi_{jk+q}|^2 - (\nabla \xi_{ik} \cdot \nabla \xi_{jk+q})^2 \}^{-\frac{1}{2}} \begin{cases} \sin^4(\psi_k - \psi_{k+q}) \cos^2(\psi_k + \psi_{k+q}) & (i = j) \\ \cos^4(\psi_k - \psi_{k+q}) \cos^2(\psi_k + \psi_{k+q}) & (i \neq j). \end{cases} \quad (A.4)$$

The integral contour  $L$  is given by the line of intersection of the surfaces defined by  $\epsilon_{ik} = \epsilon_F$  and  $\epsilon_{jk+q} = \epsilon_F$  or  $\xi_{ik} = \epsilon_F^*$  and  $\xi_{jk+q} = \epsilon_F^*$ . The terms in eqs.(A.1) and (A.2) may be divided into two groups:

$$\left. \begin{aligned} c_{intra}(q) &= c_{11}(q) + c_{22}(q), \\ c_{inter}(q) &= c_{12}(q) + c_{21}(q), \end{aligned} \right\} \quad (A.5)$$

$$\left. \begin{aligned} \gamma_{\text{intra}}^{+-}(q) &= \gamma_{11}^{+-}(q) + \gamma_{22}^{+-}(q), \\ \gamma_{\text{inter}}^{+-}(q) &= \gamma_{12}^{+-}(q) + \gamma_{21}^{+-}(q). \end{aligned} \right\} \quad (\text{A.6})$$

Here we call them intra and interband contributions, respectively.

In the paramagnetic state eqs.(A.3) and (A.4) give essentially the same results, although  $c(q)$  is referred to the d-band and  $\gamma^{+-}(q)$  to the s-band:

$$\begin{aligned} c_{\text{intra}}(q) &= c^{\text{I}}(q) \\ &= c_0 \begin{cases} (2/\pi) \sin^{-1}(q_z/2r_0 q_{\perp}) & (q_z/q_{\perp} \leq 2r_0) \\ 1 & (q_z/q_{\perp} > 2r_0), \end{cases} \quad (\text{A.7}) \end{aligned}$$

$$c_{\text{inter}}(q) = c^{\text{II}}(q) = c_0 - c^{\text{I}}(q), \quad (\text{A.8})$$

$$\begin{aligned} \gamma_{\text{intra}}^{+-}(q) &= \gamma^{\text{I}}(q) \\ &= \begin{cases} (2/\pi) \sin^{-1}(q_z/2r_0 q_{\perp}) & (q_z/q_{\perp} \leq 2r_0^*) \\ 1 & (q_z/q_{\perp} > 2r_0^*), \end{cases} \quad (\text{A.9}) \end{aligned}$$

$$\gamma_{\text{inter}}^{+-}(q) = \gamma^{\text{II}}(q) = 1 - \gamma^{\text{I}}(q), \quad (\text{A.10})$$

where  $q_{\perp} = (q_x^2 + q_y^2)^{1/2}$  is the wave vector perpendicular to  $Q$ ,  $r_0 = [k_F^2 - 1/4]^{1/2}$  is the radius of the circle of intersection of the Fermi surface and the magnetic zone boundary plane and  $r_0^*$  that of the s-band.

In the ordered phase the gap  $B_Q$  or  $B_S$  has different influence on intra- and interband contributions. For the interband contribution

the most important effect is a limitation of the region in the  $q$ -space where the contribution exists. For the intraband contribution of the matrix elements  $[\sin^2(\theta_k - \theta_{k+q})$  etc.] are the most important. Performing the line integral by taking account of the above mentioned facts, we obtain

$$\left. \begin{aligned} c_{\text{intra}}(q) &= c^{\text{I}}(q) [q_z / \sqrt{q_z^2 + B_Q^2}], \\ c_{\text{inter}}(q) &= c^{\text{II}}(q) \theta(q_{\perp} - q_L), \end{aligned} \right\} \quad (\text{A.11})$$

$$\left. \begin{aligned} \gamma_{\text{intra}}^{+-}(q) &= \gamma^{\text{I}}(q) [q_z / \sqrt{q_z^2 + B_S^2}]^3, \\ \gamma_{\text{inter}}^{+-}(q) &= \gamma^{\text{II}}(q) (1 - B_S / q_{\perp} r_0^*) \theta(q_{\perp} - q_L^*), \end{aligned} \right\} \quad (\text{A.12})$$

where  $\theta(x)$  is the step function and  $q_L^2 = (B_Q / r_0)^2 + (q_z / 2r_0)^2$  and  $q_L^{*2} = (B_S / r_0^*)^2 + (q_z / 2r_0^*)^2$ .

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	$T_C(T_N)$	$\gamma$	$R_2$
Sc <sub>3</sub> In (F)	$\sim 6$	11.5	0.048
ZrZn <sub>2</sub> (F)	$\sim 25$	30.4 $\sim$ 37.4	0.025
Fe (F)	1043	5	$1.3 \times 10^{-5}$
Co (F)	1388	5	$1.3 \times 10^{-5}$
Ni (F)	627	7.3	$1.6 \times 10^{-5}$
HfZn <sub>2</sub> (P)	—	15.8	0.002
CrB <sub>2</sub> (AF)	$\sim 85$	13.6	0.0015
$\alpha$ -Mn (AF)	95	11.8	0.15

Table 1. Transition temperatures, coefficients of linear specific heat  $\gamma$  (mJ/mole K<sup>2</sup>) and coefficients of T<sup>2</sup> term of resistivity  $R_2$  ( $\mu\Omega\text{cm}/\text{K}^2$ ) of various materials. F, P and AF stand for ferromagnet, paramagnet and antiferromagnet, respectively.

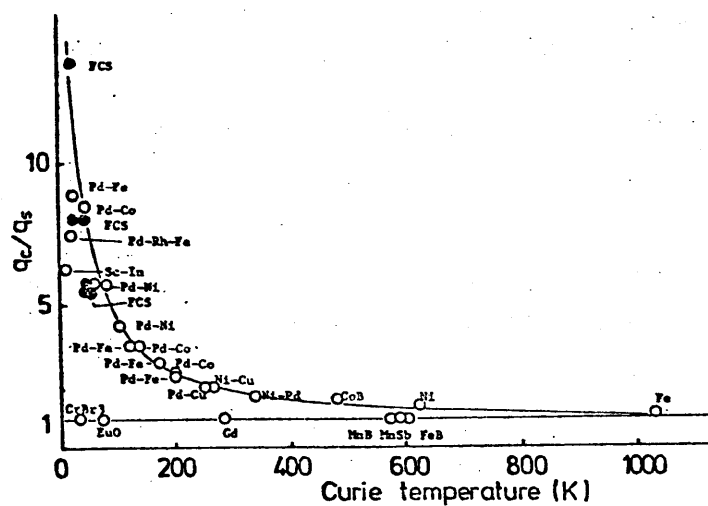


Fig. 1. The ratios  $p_c/p_s$  (denoted as  $q_c/q_s$  in the figure) of various ferromagnets as a function of Curie temperature.<sup>31)</sup>

FCS stands for  $(\text{Fe}_{1-x}\text{Co}_x)\text{Si}$ .

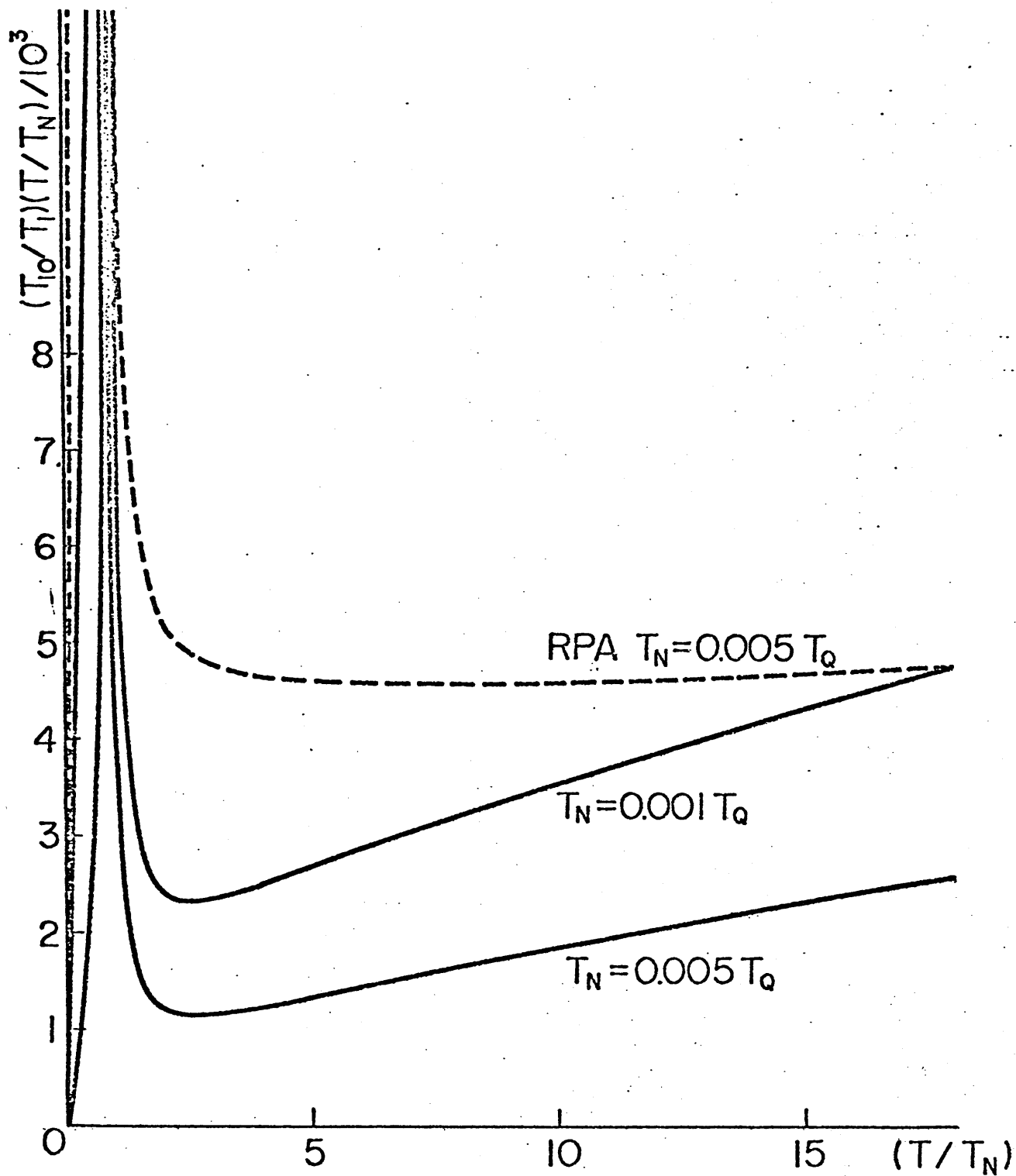


Fig. 2. Temperature dependences of the nuclear spin-lattice relaxation rates of weakly antiferromagnetic metals for the electron gas model with Umklapp processes.  $T_{10}$  is the Korringa relaxation rate. The dashed lines are the RPA results.

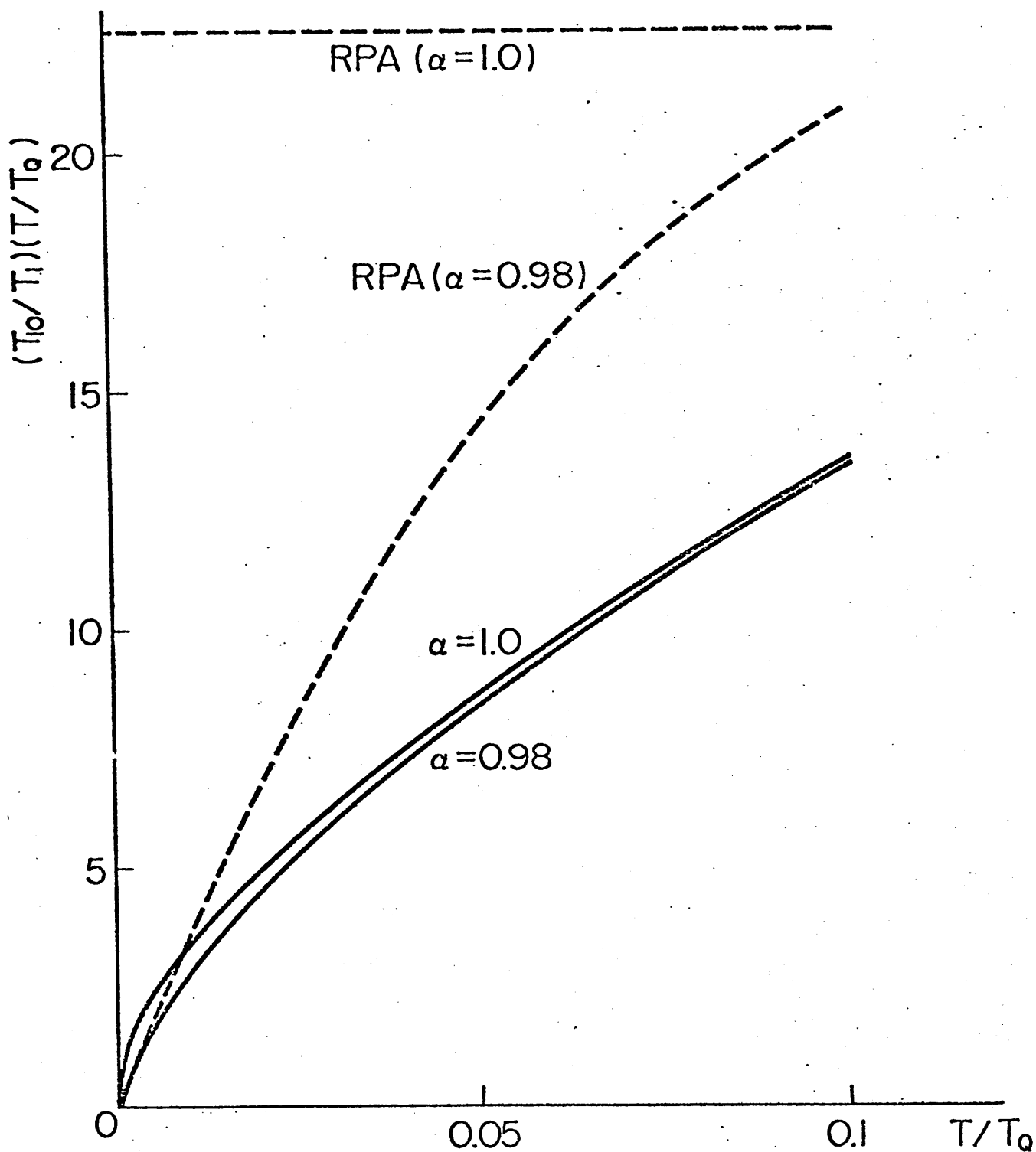
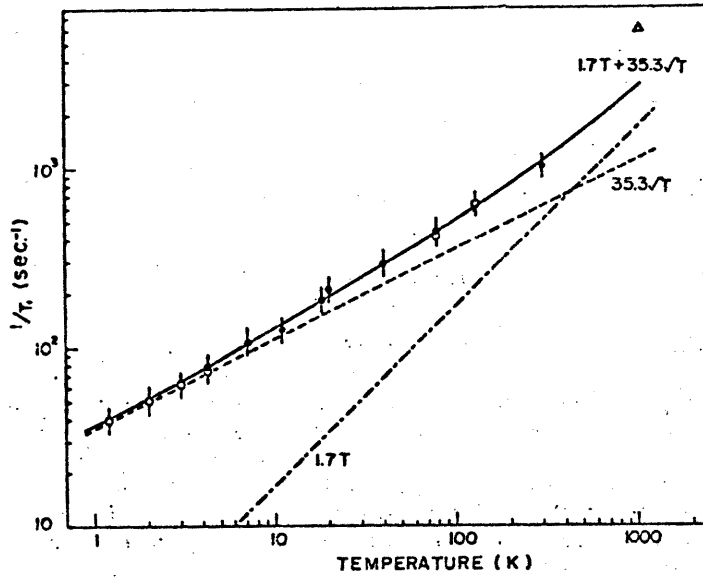
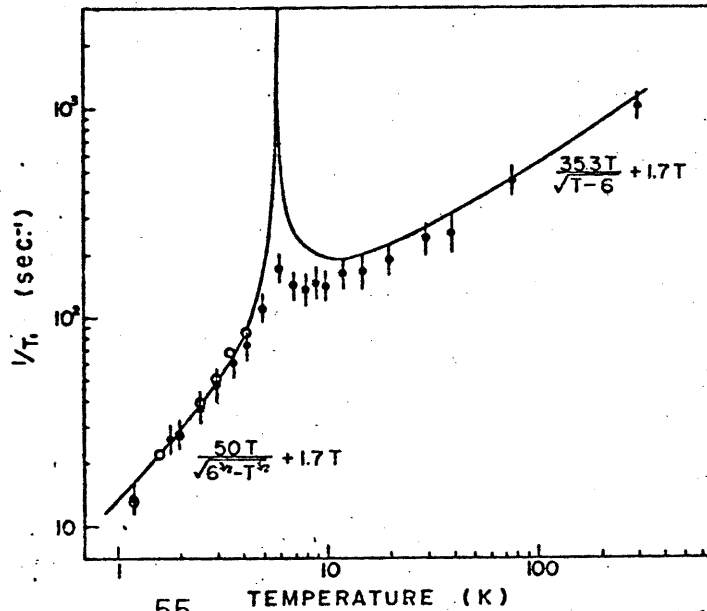


Fig. 3. Temperature dependences of the nuclear spin-lattice relaxation rates of nearly antiferromagnetic metals for the electron gas model with Umklapp processes. The dimensionless coupling constant  $\alpha_Q$  is denoted as  $\alpha$  in the figure. The notation is the same as in Fig. 2.



a)  $1/T_1$  of  $\text{Mn}^{55}$  in pure  $\beta\text{Mn}$  metal is plotted against temperature. The dashed line indicates the spin part,  $1/T_1 = 35.3/T \text{ sec}^{-1}$ . The dash dotted line indicates the orbital part  $1/T_1 = 1.7 T \text{ sec}^{-1}$ . The solid line shows the relation  $1.7 T + 35.3 T \text{ sec}^{-1}$ .



b)  $1/T_1$  of  $\text{Mn}^{55}$  in  $\beta\text{Mn}$  alloy with Ge 1.0% is plotted against temperature. The solid line indicates the relation  $1/T_1 = 1.7 T + 35.3 T / \sqrt{T-6} \text{ sec}^{-1}$  above 6K  $1/T_1 = 1.7 T + 50 T / \sqrt{6^{3/2} - T^{3/2}} \text{ sec}^{-1}$  below 6K.

Fig. 4.  $1/T_1$  of  $\text{Mn}^{55}$  in  $\beta\text{Mn}$  metal and its alloy. [Katayama, Akimoto and Asayama.<sup>48)</sup>]

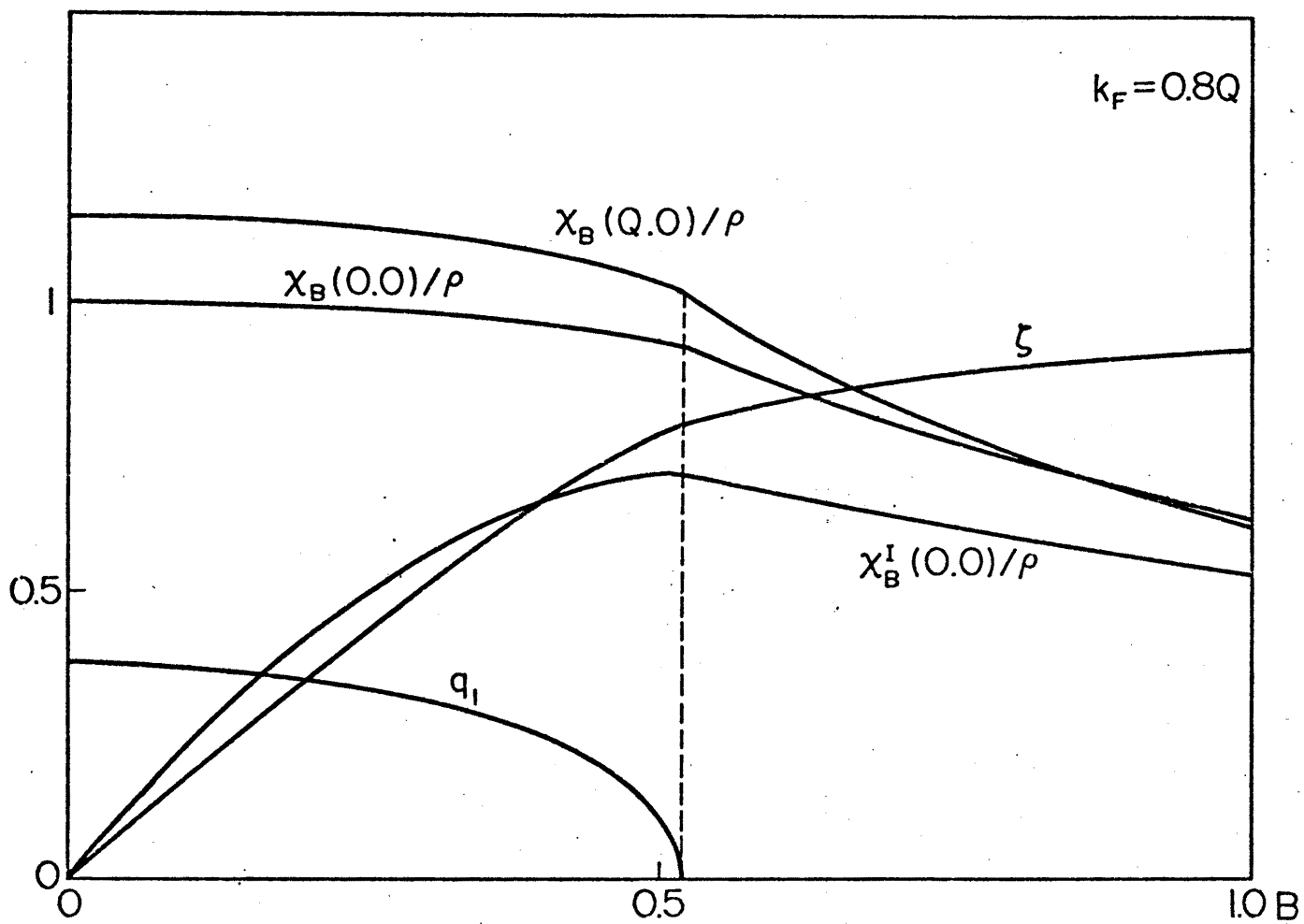


Fig. 5. The static properties  $\chi_{B_Q}(Q,0)$ ,  $\chi_{B_Q}(0,0)$ ,  $\chi_{B_Q}^I(0,0)$ ,  $z$  and  $q_1$  as functions of the staggered exchange field  $B_Q$ . In figures  $B_Q$  is represented by the symbol  $B$ .

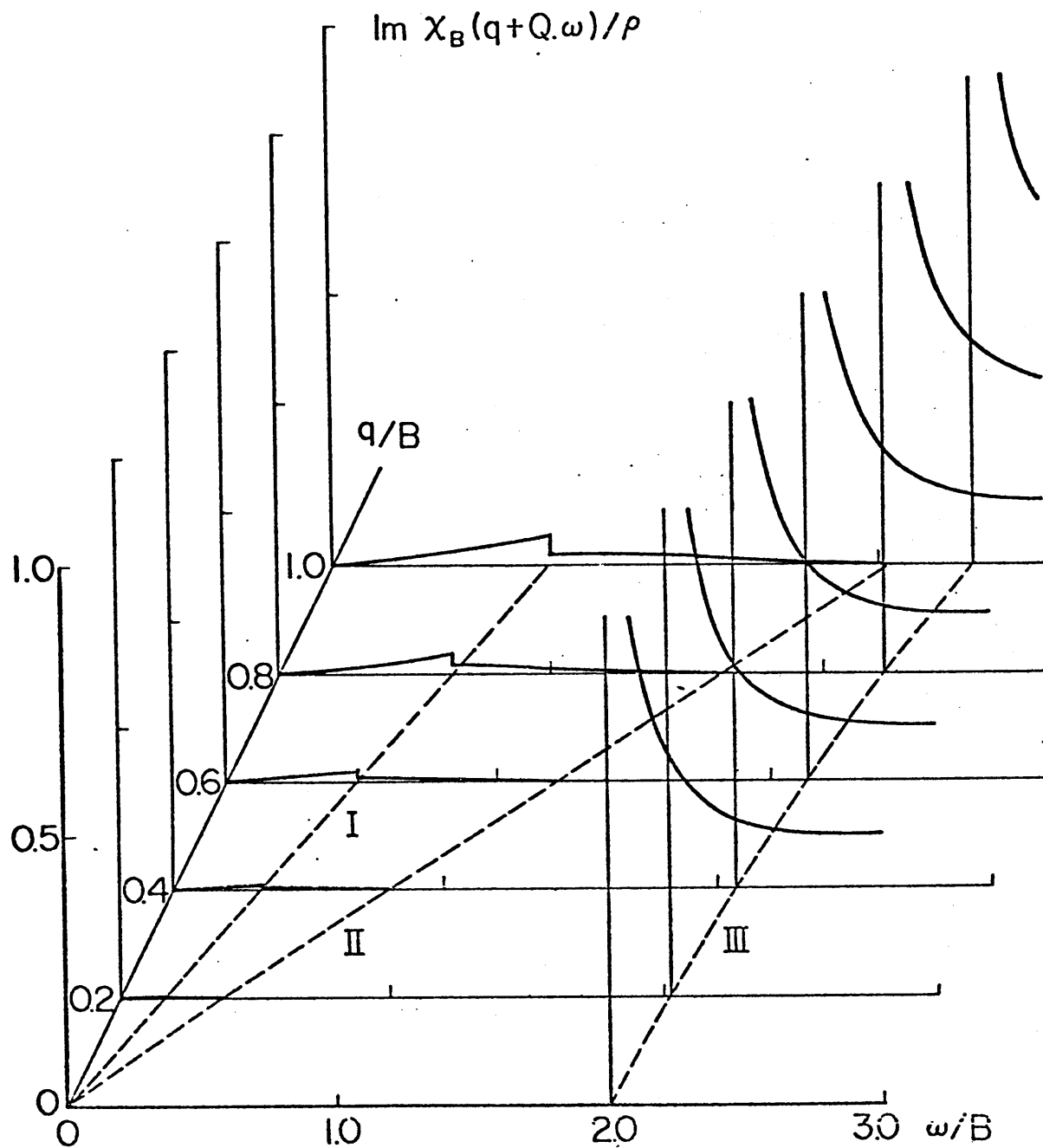


Fig. 6. Imaginary part of  $\chi_{B_Q}(q+Q, \omega)$ . Dashed lines I, II, III are boundaries where the excitations between bands 1 and 1, 2 and 2 and 1 and 2, respectively, exist.

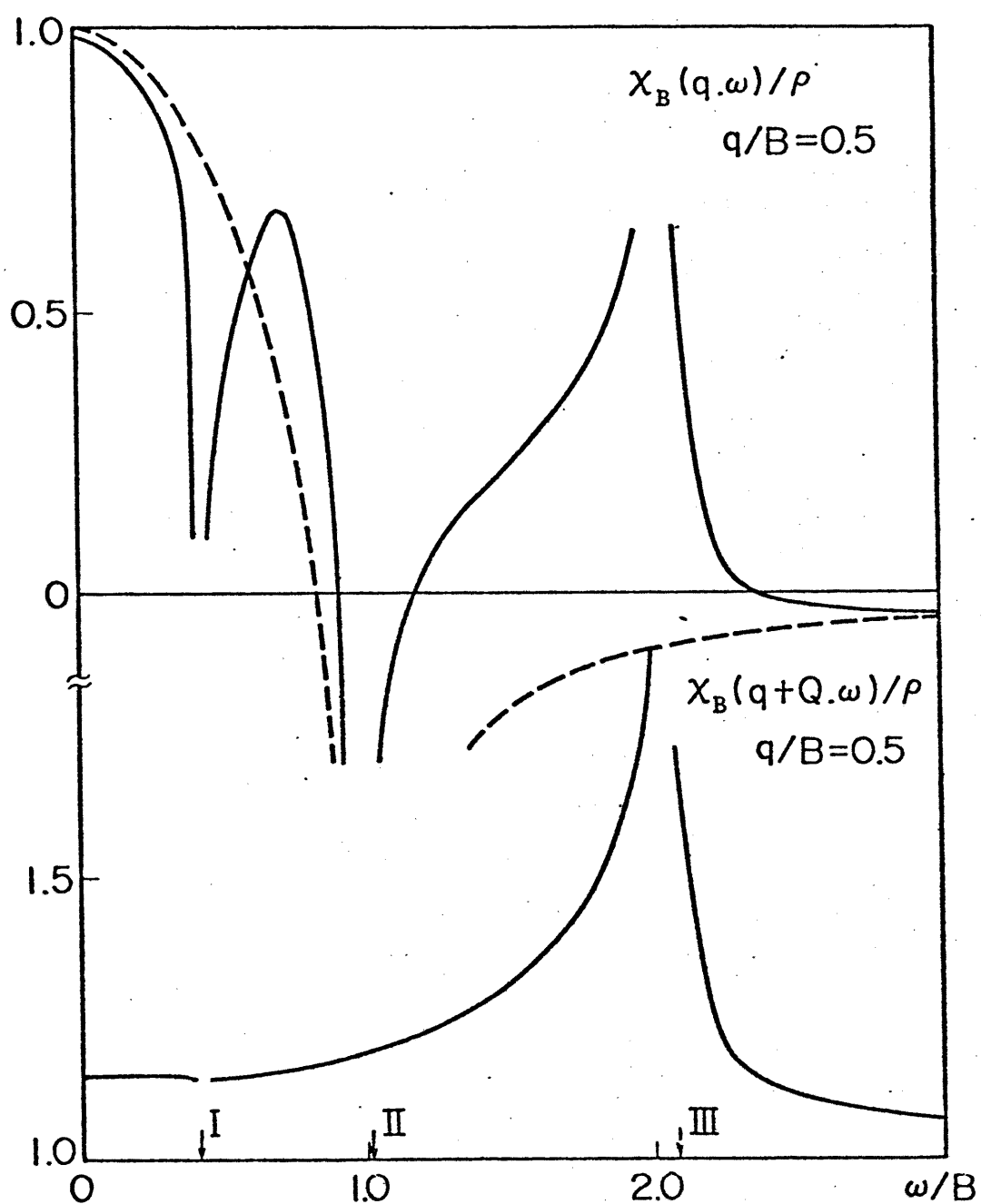


Fig. 7. Real parts of  $\chi_{B_Q}(q, \omega)$  and  $\chi_{B_Q}(q+Q, \omega)$ . For comparison  $\text{Re } \chi_0(q, \omega)$  in the paramagnetic phase is shown by dashed line.

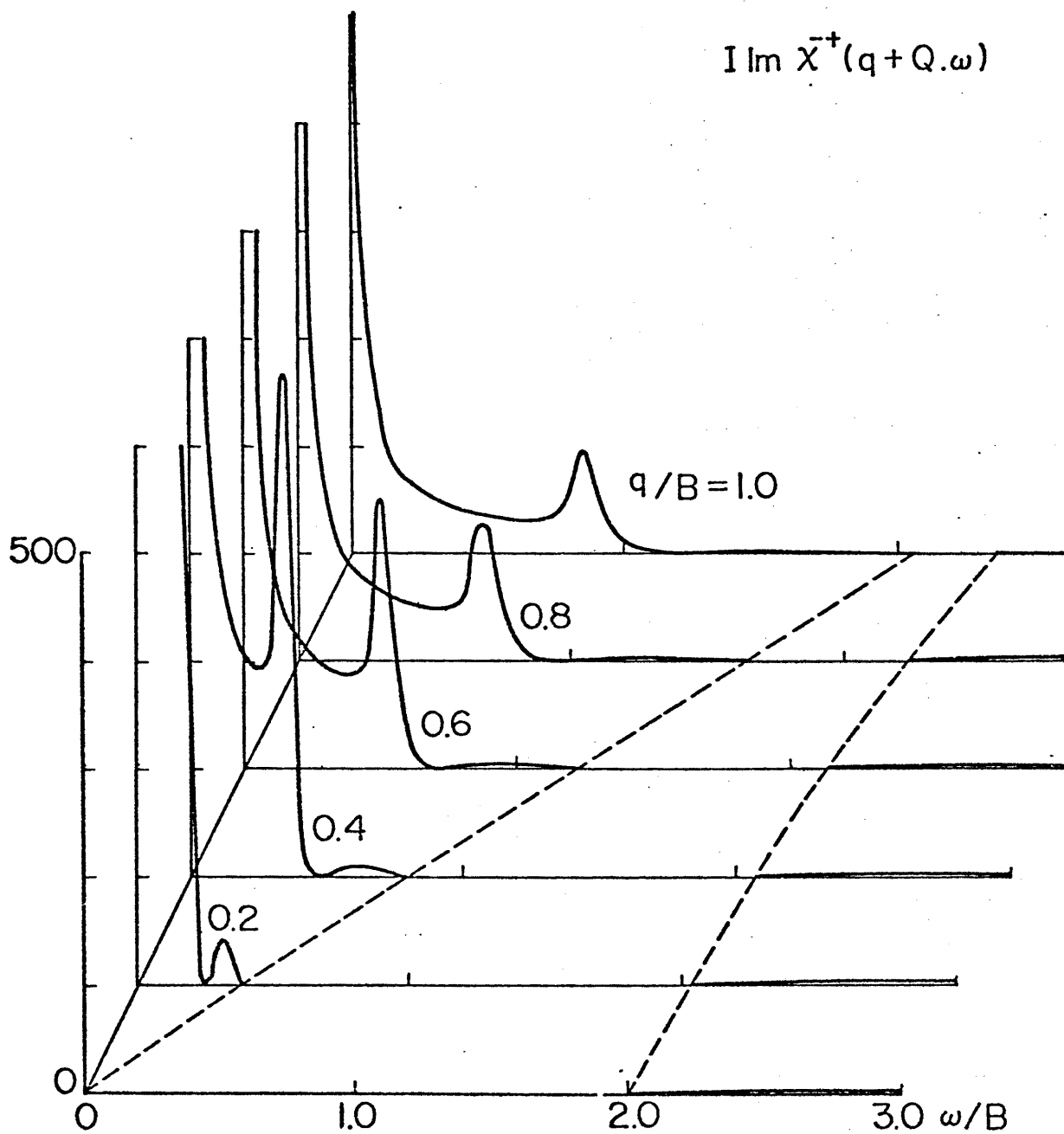


Fig. 8. Magnetic excitations around the magnetic reciprocal lattice point. The vertical axes denote dimensionless quantity  $I \text{Im } \bar{\chi}^{+}(q+Q, \omega)$ . We take  $B_Q = 0.1$  in this figure and Fig. 9.

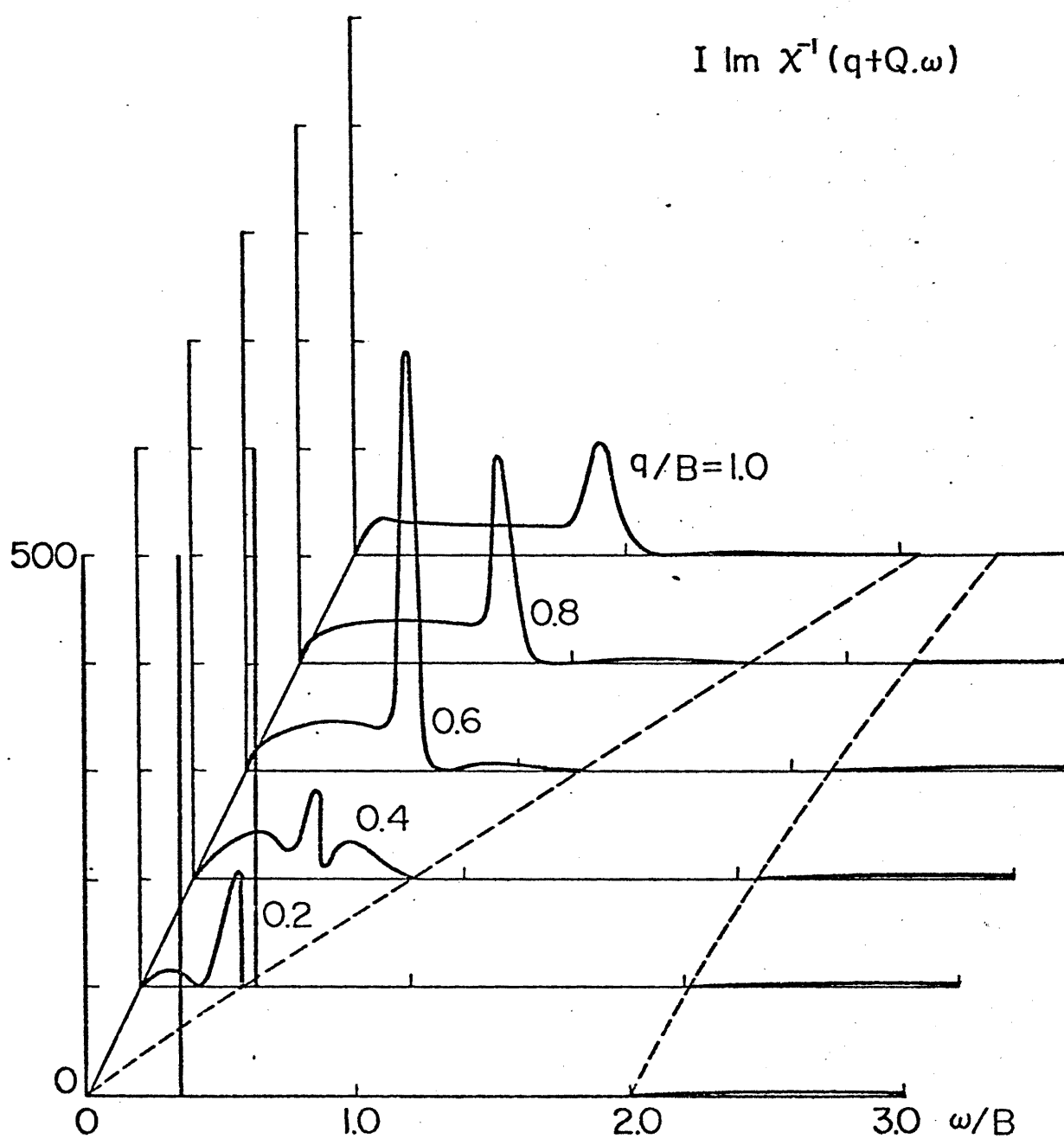


Fig. 9. Magnetic excitations in the presence of the anisotropy. The notations are the same as those of Fig. 8.

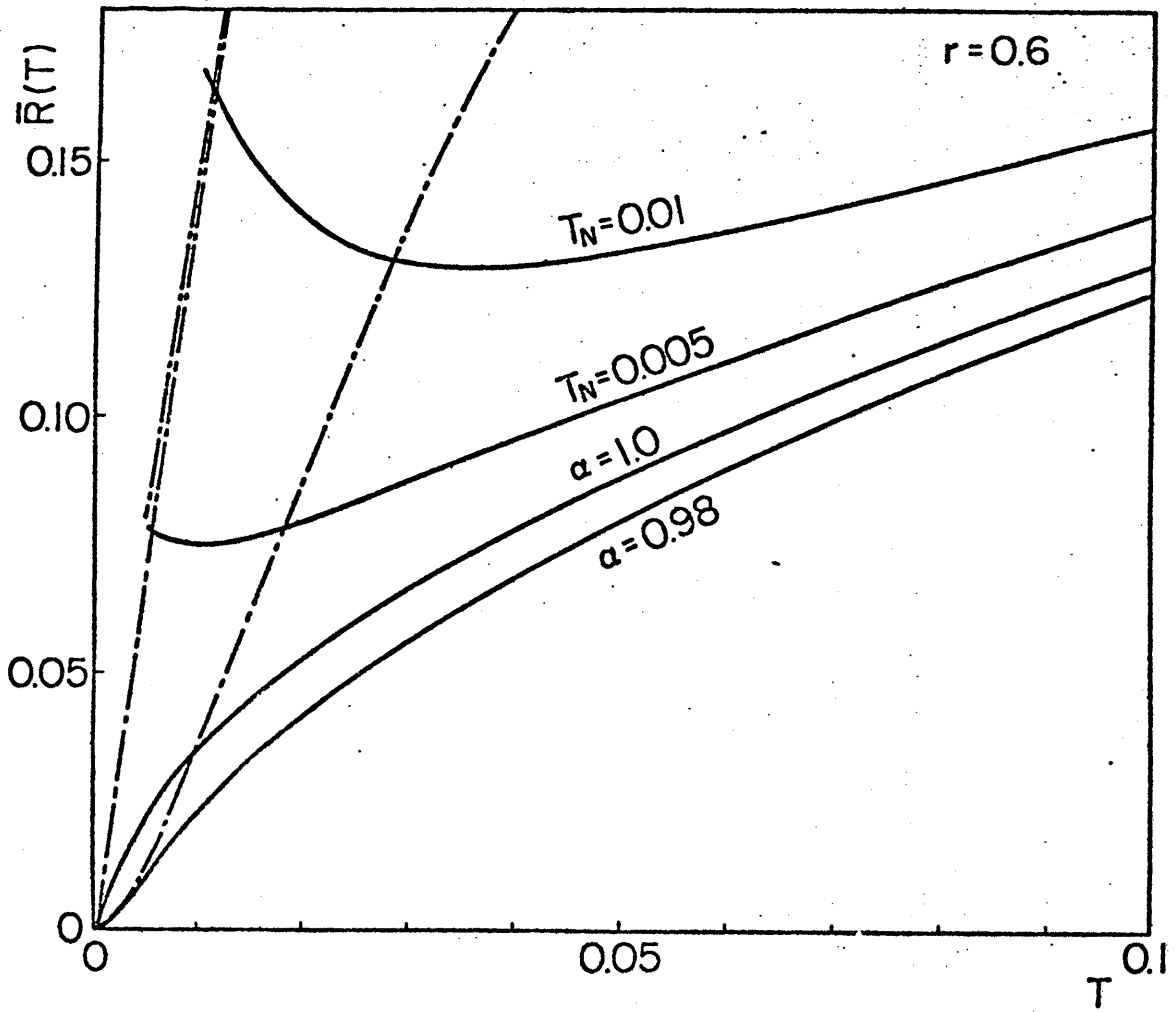


Fig. 10. The electrical resistivity of weakly and nearly antiferromagnetic metals for the cut off parameter  $r = 0.6Q$ . The RPA results are shown by dashed lines for the same values of  $T_N$  or  $\alpha_Q$  (denoted as  $\alpha$  in the figure).

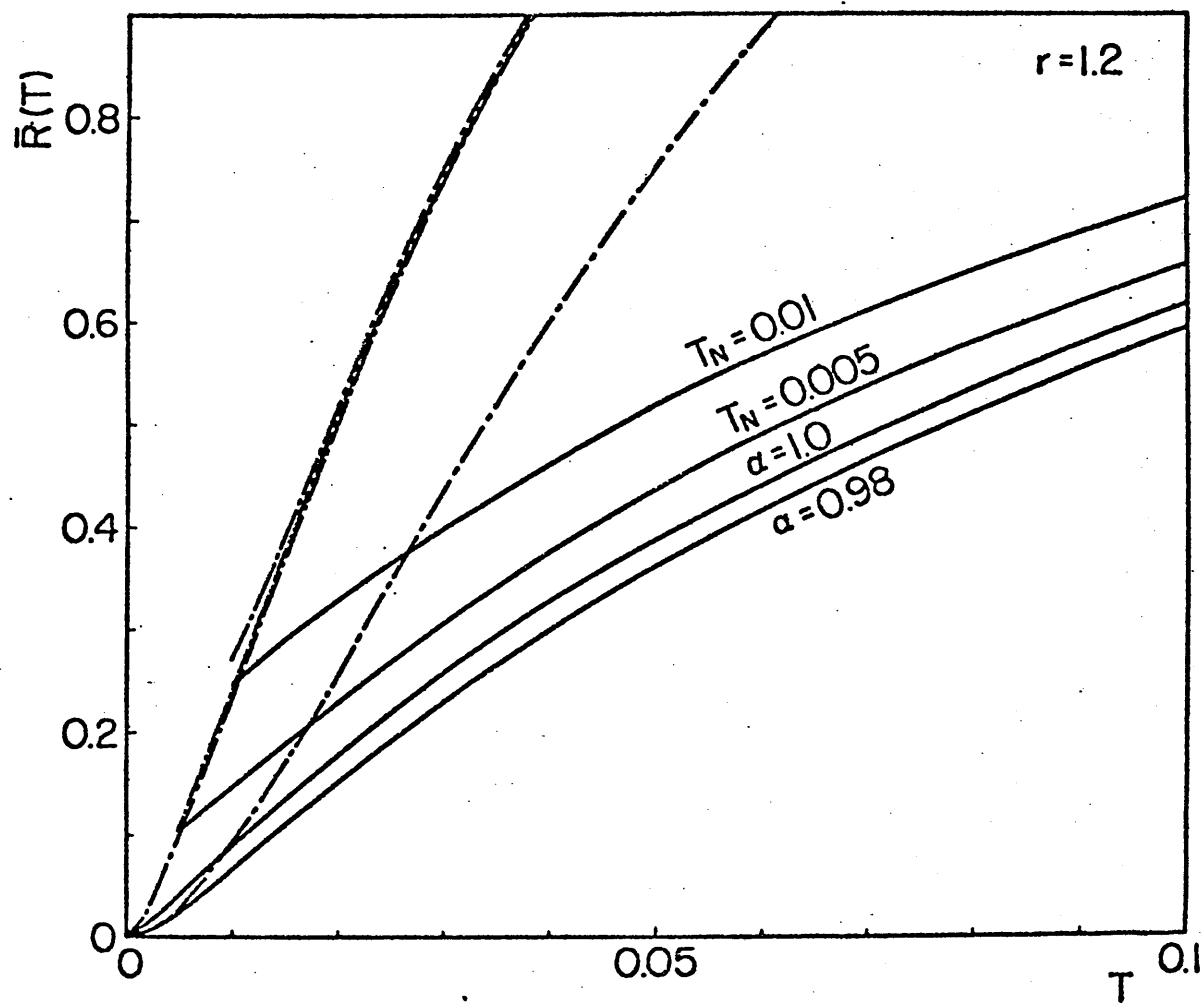


Fig. 11.  $\bar{R}(T)$  versus  $T$  for  $r = 1.2Q$ . Other notations are the same as in Fig. 10.

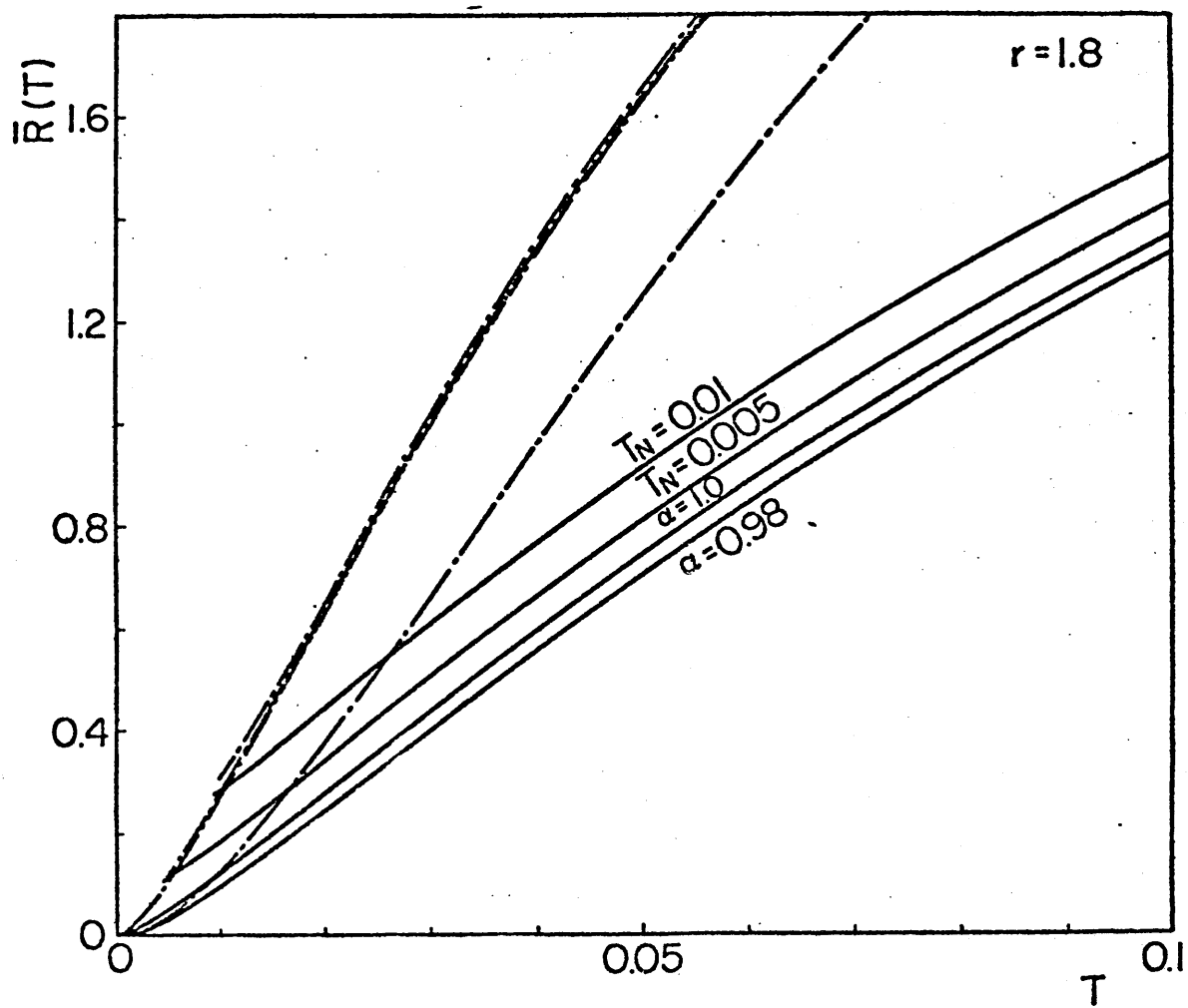


Fig. 12.  $\bar{R}(T)$  versus  $T$  for  $r = 1.8Q$ . Other notations are the same as in Fig. 10.

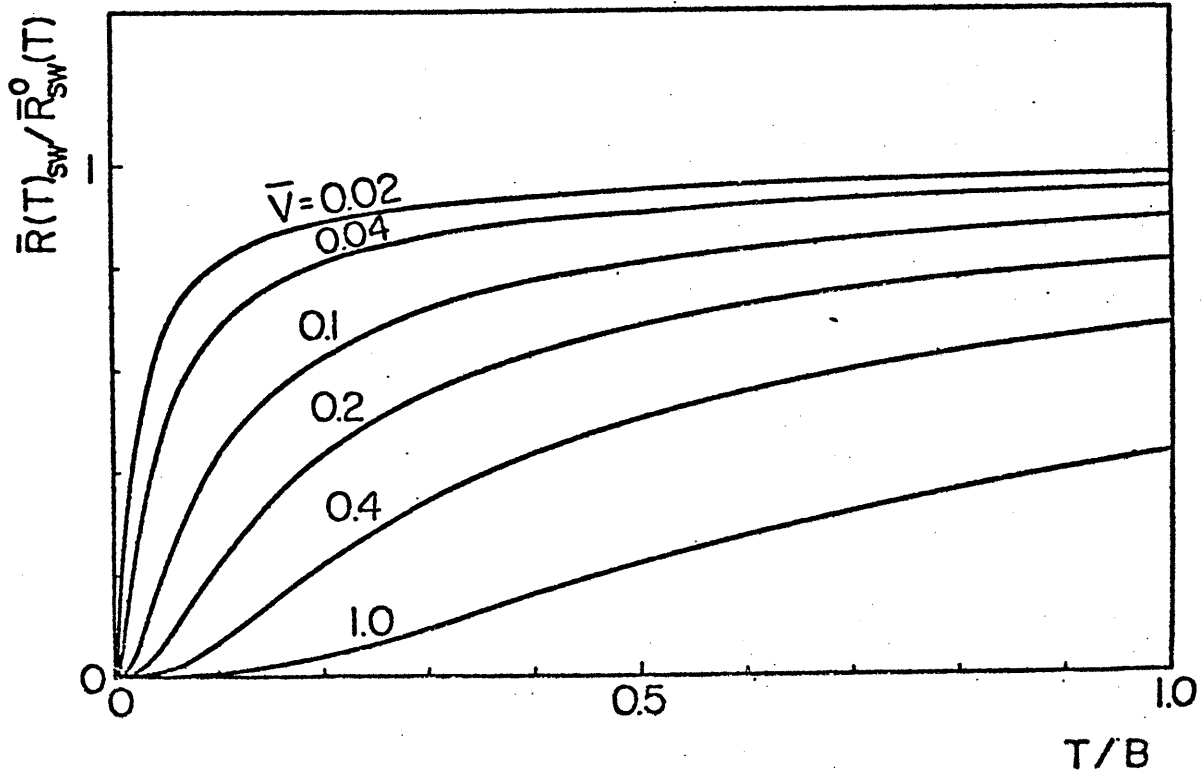


Fig. 13. The electrical resistivity due to spin waves. The vertical axis  $[\bar{R}_{sw}(T)/\bar{R}^0_{sw}(T)]$  is proportional to  $\bar{R}_{sw}(T)/T^2$ . This figure shows the effect of the gap of the conduction band on the resistivity. The effect is characterized by the parameter  $\bar{v} = 2v(B_s/B_Q)$ .