Electrical resistivity due to s-f exchange interaction in degenerate ferromagnetic semiconductors

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Applying the single-site approximation to the s-f model, the electrical resistivity in a degenerate ferromagnetic semiconductor is studied theoretically. It is revealed that in the weak exchange-interaction limit, the resistivity of the up-spin electron agrees with that obtained by the Born approximation, while the resistivity of the down-spin electron retains a finite value even at $T = 0$, which is due to the spin-flip scattering process. The density of states and electrical resistivity for the strong exchange-interaction limit are also calculated. The results of electrical resistivity show a similar temperature and magnetic field dependence for a wide range of exchange-interaction strengths.

KEYWORDS: s-f model, electrical resistivity, magnetoresistance, magnetic semiconductor, EuS, double exchange interaction

Electron scattering by thermally fluctuating localized spins has been studied by several authors. Assuming that the (s-f) exchange interaction energy (IS) between the conduction (s-) electron and localized (f-) spins is weak compared with the conduction bandwidth (W), Kasuya,[1] de Gennes and Friedel,[2] and Haas[3] calculated the electrical resistivity using the perturbation theory. On the other hand, under the assumption that the exchange interaction is infinitely strong, Kubo and Ohata studied the resistivity using the virtual crystal approximation (VCA) together with the theory of Brownian motion, in connection with the double exchange interaction.[4] However, as far as we know, no theory for resistivity is available for a wide range of exchange-interaction strengths, although the reality lies between these two limiting cases. In this work, on the basis of the single-site approximation to the s-f model, we intend to develop an improved theory for the resistivity of a degenerate ferromagnetic semiconductor, which is applicable in wide ranges of IS/W and temperature.

In the s-f model, the Hamiltonian for an s electron interacting with f spins through the s-f exchange interaction is

$$H = \sum_{k,\mu} \varepsilon_k a^\dagger_{k\mu} a_{k\mu} - I \sum_{m,\mu,\nu} a^\dagger_{m\mu} \boldsymbol{\sigma} \cdot \boldsymbol{S}_m a_{m\nu} \, . \tag{1}$$

The total Hamiltonian, H_t, consists of H and H_f, where H_f represents the Heisenberg-type exchange interaction between f spins.

In a previous work,[5)] we studied the electron state in an effective medium where an s electron is subjected to a complex potential (or coherent potential), $\Sigma_\uparrow$ or $\Sigma_\downarrow$, according to the orientation of its spin. Therein, an s electron moving in this effective medium was described by the reference Hamiltonian K:

$$K = \sum_{k,\mu} (\varepsilon_k + \Sigma_\mu)\, a^\dagger_{k\mu} a_{k\mu} \,. \tag{2}$$

Then, we determined $\Sigma_\uparrow$ and $\Sigma_\downarrow$ under the condition that the total scattering by a single f spin embedded in the medium is zero, to calculate the spin-polarized density of states, $D_\uparrow(\omega)$ and $D_\downarrow(\omega)$. Hence, when the concentration of s electrons, n, is given, the Fermi energy ε_F is obtained for degenerate electrons under the condition that all the electron states with energy less than the Fermi energy are full. For the purpose of the numerical calculation, the energy of the undisturbed (model) band is assumed as $\varepsilon_k = W(k/q_D)^2$ for $0 \leq k \leq q_D$, and the summation over the wave number vector k in the first Brillouin zone is replaced by the integration within the Debye sphere q_D.

In this work, applying the Velicky theory[6)] to the s-f model, we study electron scattering due to the fluctuating f spin. The Velicky theory was first applied successfully to disordered alloys, and its extension to the s-f model is straightforward. When the s electron moves in the effective medium mentioned above, the spin flip does not occur, so that the spin-up and spin-down electrons become separate systems. Therefore, the conductivity for electrons with spin μ is expressed as

$$\sigma_\mu = \frac{1}{A} \int_0^1 dx \left\{ \mathrm{Im} \, \frac{x^2}{x^2 - (\varepsilon_F - \Sigma_\mu)/W} \right\}^2 . \tag{3}$$

Here, A is a constant defined by $A = 3\pi^3 h / 2e^2 q_D$. Thus, once Σ_μ and ε_F are known, the resistivity $\rho = 1/(\sigma_\uparrow + \sigma_\downarrow)$ can be calculated.

First, we point out that when the exchange interaction is weak, the present result for the resistivity at the high-temperature limit, ρ_∞, agrees with that of the Born approximation (BA),[1)]

$$\rho_\infty = 3A \left(\frac{2}{x}\right)^{\frac{2}{3}} \left(\frac{IS}{W}\right)^2 \left(1 + \frac{1}{S}\right) , \tag{4}$$

where x $(= n/N)$ is the number of s electrons per site. When magnetization arises, the present theory gives different results depending on the orientation of the electron spin. In a weak exchange-interaction limit, the ratios of the resistivity of the electron with up and down spin, $\rho_\uparrow (= 1/\sigma_\uparrow)$ and $\rho_\downarrow (= 1/\sigma_\downarrow)$, to that of the high-temperature limit, $2\rho_\infty$, are expressed as a function of normalized magnetization $M (=< S_z >_{\mathrm{av}} / S)$:

$$\frac{\rho_\uparrow}{2\rho_\infty} = \frac{(1 - M)(1 + 1/S + M)}{1 + 1/S} , \tag{5}$$

$$\frac{\rho_\downarrow}{2\rho_\infty} = \frac{(1 + M)(1 + 1/S - M)}{1 + 1/S} . \tag{6}$$

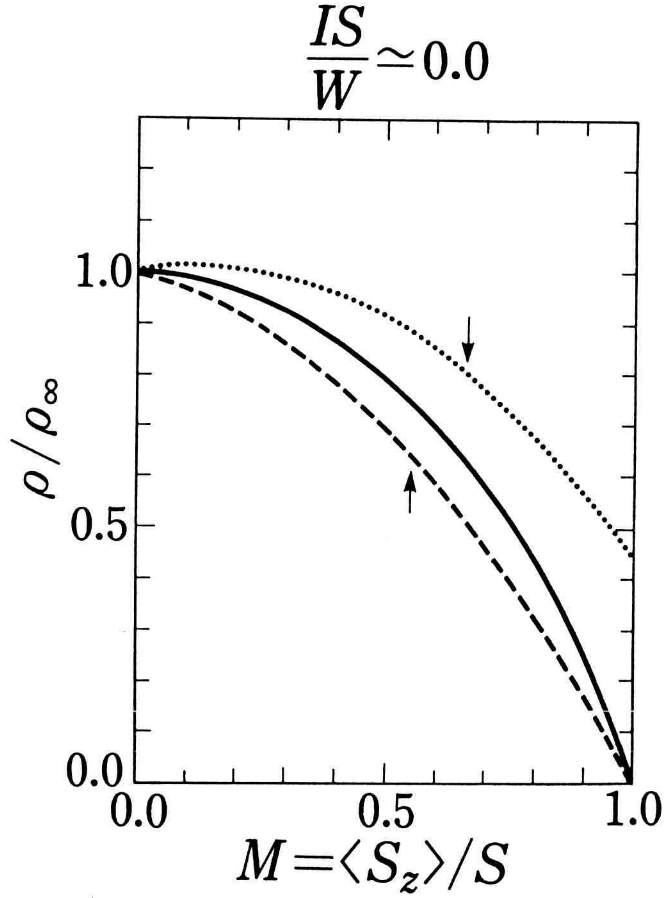

Fig. 1. Resistivity as a function of M; dashed line (↑) is for eq. (5), dotted line (↓) for eq. (6), and solid line for eq.(7).

It should be pointed out that replacing M by $-M$ in the expression for $\rho_\uparrow$ leads to an expression for $\rho_\downarrow$. At paramagnetic temperatures, $M = 0$ and $\rho_\uparrow = \rho_\downarrow = 2\rho_\infty$; as the temperature is decreased from T_C (i.e., as M is increased), $\rho_\uparrow$ drops sharply, and reaches 0 at $T = 0$ ($M = 1$). On the other hand, $\rho_\downarrow$ decreases gradually while maintaining a value somewhat higher than $\rho_\uparrow$, and reaches $2\rho_\infty/(S+1)$ at $T = 0$; when $M = 1$, $\rho_\downarrow/2\rho_\infty = 0.44$ for $S = 7/2$. The result is interpreted as follows. The s electron is scattered due to the thermal fluctuation of f spins. As the magnetization develops, the amplitude of f spin fluctuation decreases, so that the resistivity also decreases. In particular, for the completely ferromagnetic case (i.e., $T = 0$), the states of s electrons with up spin only shift $-IS$ with no damping. On the other hand, the electron states with down spin are damped because they can flip their spin under the condition that the total spin ($= S - 1/2$) is conserved if the density of states with up spin is not zero therein. Consequently, $\rho_\downarrow$ retains a finite

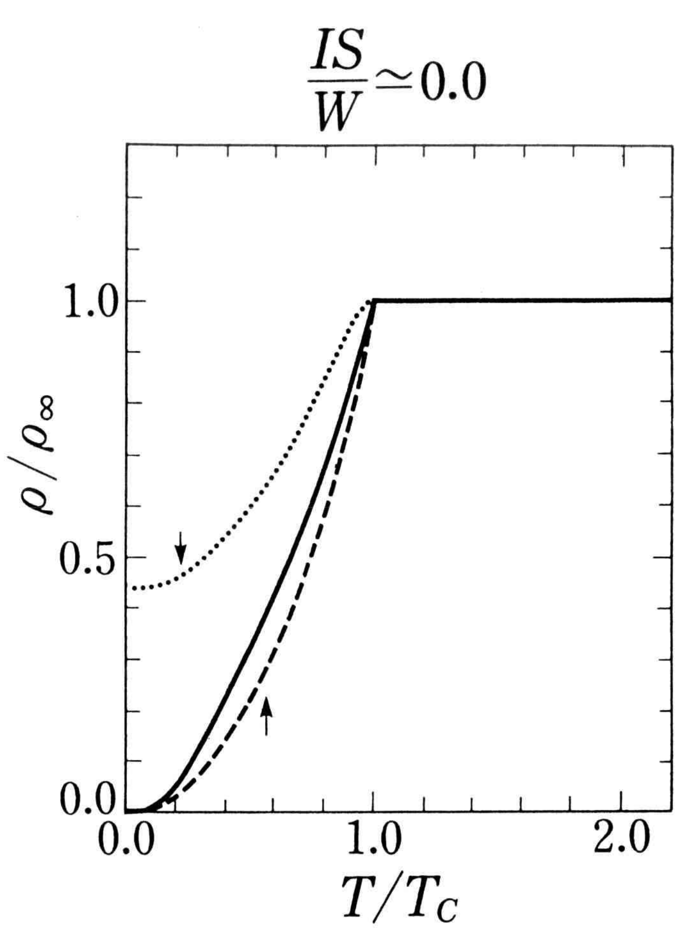

Fig. 2. Resistivity as a function of T/T_C ; dashed line (↑) is for $\rho_\uparrow/2\rho_\infty$, dotted line (↓) for $\rho_\uparrow/2\rho_\infty$, and solid line for ρ/ρ_∞.

value even at $T=0$. This spin-flip process of the s electron with down spin is a quantum effect due to the finiteness of the f spin value. Thus, in the classical spin limit (i.e., $1/S \rightarrow 0$), $\rho_\downarrow$ reaches 0 at $T=0$. Note that the BA[1] results in $\rho_\uparrow = \rho_\downarrow$, which is equal to that expressed in eq. (5), or $\rho_\uparrow$ in this study. That is, the BA does not give an accurate result for the resistivity of the electrons with down spin at ferromagnetic temperatures.

In the weak exchange-interaction limit, the change in the density of states is so negligible that the number of electrons which occupy the up-spin band is assumed to be equal to that occupying the down-spin band (or $n_\uparrow = n_\downarrow$). Then, the (total) resistivity $\rho = \rho_\uparrow\rho_\downarrow/(\rho_\uparrow + \rho_\downarrow)$ is expressed, for the weak exchange-interaction limit, as

$$\frac{\rho}{\rho_\infty} = \frac{(1-M^2)[(1+1/S)^2 - M^2]}{(1+1/S)(1+1/S-M^2)} \,. \tag{7}$$

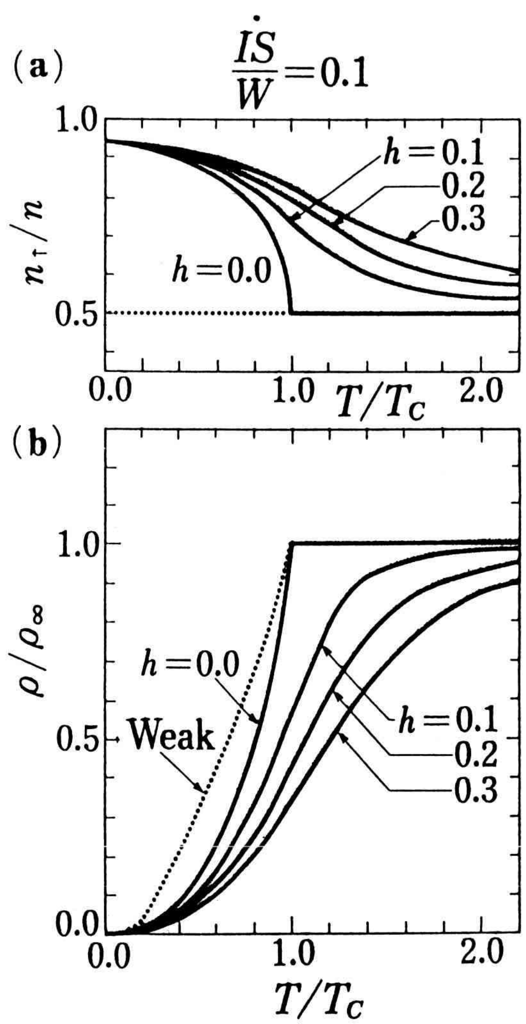

Fig. 3. Result for $IS/W = 0.1$ and $S = 7/2$. (a) The ratio of $n_\uparrow$ to n, and (b) the normalized electrical resistivity, ρ/ρ_∞, as a function of the normalized temperature, T/T_C, under the normalized external magnetic field, h. The dotted line is for the weak exchange-interaction limit or eq. (7)

Thus, as the temperature is decreased from paramagnetic temperatures ($M = 0$), ρ decreases from ρ_∞, and reaches 0 at $T = 0$ ($M = 1$). The overall feature of ρ at ferromagnetic temperatures is similar to $\rho_\uparrow$, while $\rho_\uparrow \leq 2\rho \leq \rho_\downarrow$. The resistivity in the weak exchange interaction limit is shown as a function of M in Fig. 1, and as a function of T/T_C in Fig. 2.

For a finite value of IS/W, the change in the density of states is so efficient that the proportion of the up-spin electron, $n_\uparrow/n$, becomes larger than 0.5 at ferromagnetic temperatures. This makes ρ tend toward $\rho_\uparrow/2$. In addition, terms such as $I^2[< S_z^2 >_{\rm av} - < S_z >_{\rm av}^2]{\rm Im}(F_\uparrow - F_\downarrow)$ are recovered in the expression of ρ, where $F_\mu =< m\mu|(\omega - K)^{-1}|m\mu >$ (independent of site index m). Note also that within the approximation up to the second order of IS/W, we may set $F_\uparrow = F_\downarrow$. In Fig. 3, we show the result for $IS/W = 0.1$ with $n = 0.1$, as an example. For comparison, the normalized resistivity of the weak exchange-interaction limit is included.

We also studied the effect of the external magnetic field. In magnetic semiconductors, a magnetic field changes the f spin ordering, so that the density of states, and hence the resistivity, is affected. In this work, we simply assume that the external magnetic field H_z affects only the f spins; that is, the external field is taken into account when the thermal average over the f spin states is performed. The figures show results for various normalized magnetic fields, h, defined by

$$h = \frac{(S+1)g\mu_B H_z}{3k_B T_C} . \tag{8}$$

The results suggest a large magnetoresistance around the Curie temperature (T_C).

When $I(2S+1) > W$, the conduction band has two subbands which are characterized by the coupling way of the electron spin parallel or antiparallel to the orientation of f spins. As IS/W increases further, Σ_μ becomes divergent as $-IS$ in the parallel-coupling band, and as $+I(S+1)$ in the antiparallel-coupling band. However, even when $IS/W \to \infty$, our theory is applicable (see Appendix). In Fig. 4, we show the result for the density of states with $IS/W = \infty$, for various temperatures. The overall feature is similar to that with $IS/W = 0.5$ reported in a previous paper,[5] except that the energy difference between the two the subbands is infinite. The total density of states is confirmed to be 1.0 for both up- and down-spin bands, respectively. Throughout all temperatures, the total density of states is maintained as $2(S+1)/(2S+1)$ for the parallel-coupling subband (lower-energy subband) and $2S/(2S+1)$ for the antiparallel-coupling subband (higher-energy subband).

In Fig. 5, we show the present result for the resistivity of $IS/W = \infty$ with $n = 0.1$. We also include the result of virtual crystal approximation (VCA) that is obtained by ignoring the correlation between successive hopping of an electron (hole).[4] In the entire temperature region below T_C, the present result shows lower values of resistance than that of the VCA.

Figure 6 shows ρ_∞/A with $n = 0.1$ as a function of IS/W. The Born approximation (BA) predicts that ρ_∞ is proportional to $(IS/W)^2$. From Fig. 6, we estimate the range of application of BA to be $IS/W < 0.1$. A rough estimation using BA [or eq. (6)] together with the experimental data[7,8] predicts $IS/W = 0.11$ for EuS and 0.091 for EuO. Figure 6 also indicates that EuS and EuO lie at the limit of the range of application of BA, and that the real values of IS/W may be somewhat larger than that obtained above. Nevertheless, at first glance, BA seems to sufficiently explain the experimental results for Gd-doped EuS and EuO, when the doping level is high enough to produce a degenerate semiconductor.[7] This is because ρ/ρ_∞ tends toward $\rho_\uparrow/2\rho_\infty$ (or the result of BA) for a finite value of IS/W and shows a similar temperature and magnetic field dependence for a wide range of IS/W, as clarified in this study.

To summarize, on the basis of the single-site approximation for the s-f model, we devised an improved theory for the resistivity of a degenerate ferromagnetic semiconductor. The present theory gives reasonable results for both weak and strong exchange-interaction limits, and hence seems to be applicable over entire ranges of IS/W and temperature, except near T_C. Near T_C, scattering due to the correlation of f spins becomes significant,[9] but is ignored throughout this work. The incorporation of the effect of the f spin correlation will be the theme for future study.

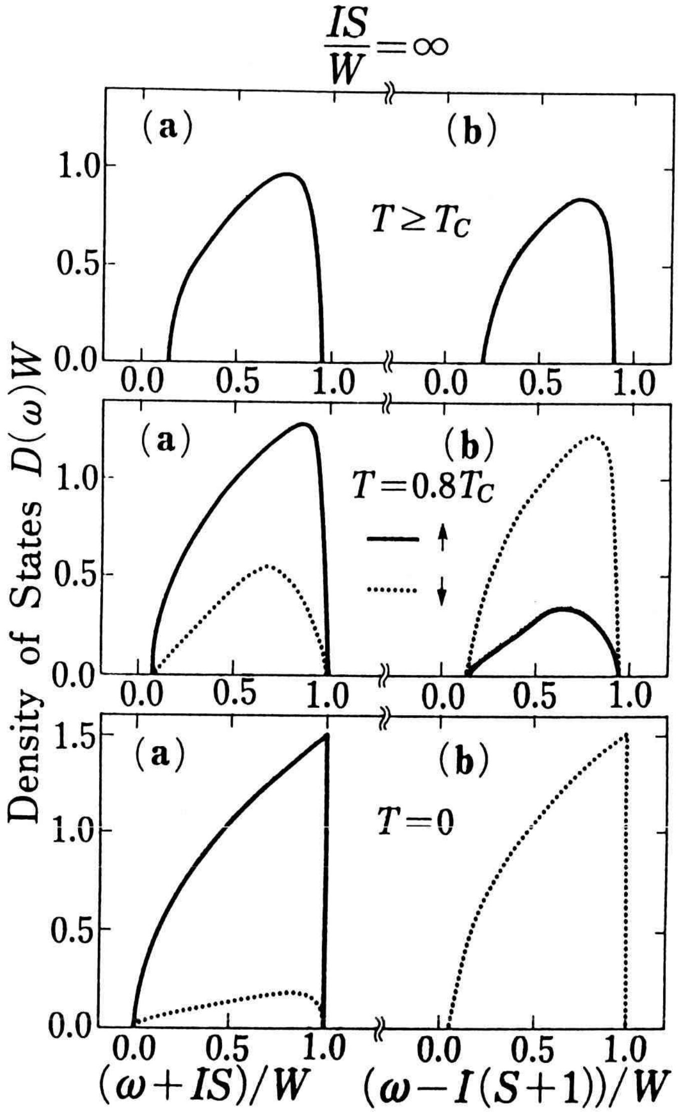

Fig. 4. The density of states of $IS/W = \infty$ with $S = 7/2$ for $T \geq T_C, T = 0.8T_C$, and $T = 0$: (a) parallel coupling band as a function of $(\omega + IS)/W$ and (b) antiparallel coupling band as a function of $[\omega - I(S + 1)]/W$.

Recently, Furukawa[10)] studied the double-exchange model in the limit $S = \infty$ as the strong coupling limit of the Kondo lattice model, to explain the colossal magnetoresistance (MR) with a negative sign observed in the experiment of $La_{1-x}Sr_xMnO_3$.[11)] The present theory can be applied straightforwardly to that problem; detailed results will be reported elsewhere.

Appendix: Expression for $IS/W \to \infty$ limit

We must treat the parallel-coupling band and antiparallel-coupling band separately. Here, we set $W = 1$ for simplicity.

(a) Parallel-coupling subband: Since $\Sigma_\mu \to -IS$ as IS increases, we set $u_\mu = IS + \Sigma_\mu$, and

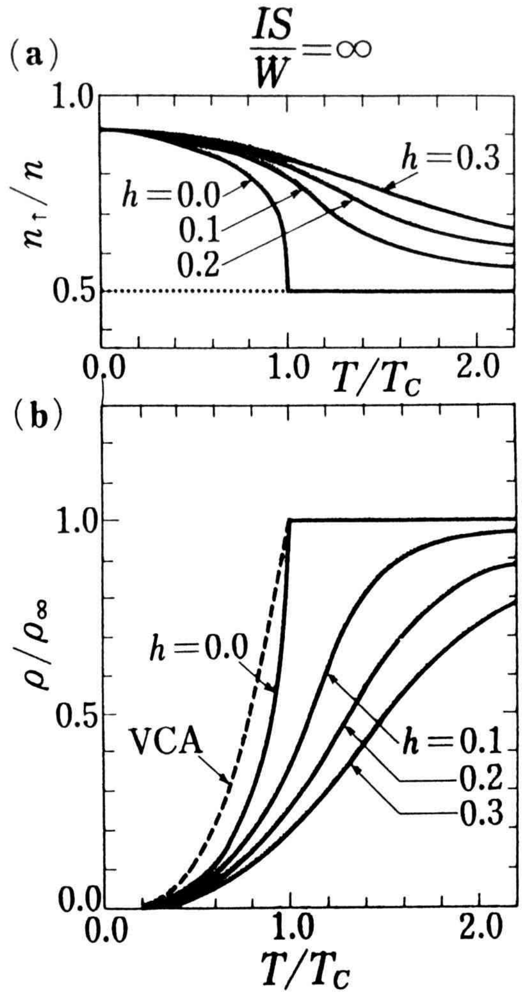

Fig. 5. Result for $IS/W = \infty$. (a) The ratio of $n_\uparrow$ to n, and (b) the normalized electrical resistivity, ρ/ρ_∞, as a function of the normalized temperature, T/T_C, under the normalized external magnetic field, h. The dashed line indicates the result of VCA.

$z = \omega + IS$. Then, the coherent potential approximation (CPA) condition[5] for $IS/W \to \infty$ limit is written as

$$u_\uparrow = -\frac{(F_\downarrow^{-1} + u_\downarrow)(1 - c_\uparrow)}{1 + 1/S + c_\uparrow}, \tag{A·1}$$

$$u_\downarrow = -\frac{(F_\uparrow^{-1} + u_\uparrow)(1 + c_\downarrow)}{1 + 1/S - c_\downarrow}, \tag{A·2}$$

where a complex number $c_\mu = A_\mu/B_\mu$ is defined in terms of A_μ and B_μ in the Appendix of ref. 5.

(b) Antiparallel-coupling subband: Since $\Sigma_\mu \to I(S+1)$ as IS increases, we set $u_\mu = -I(S+$

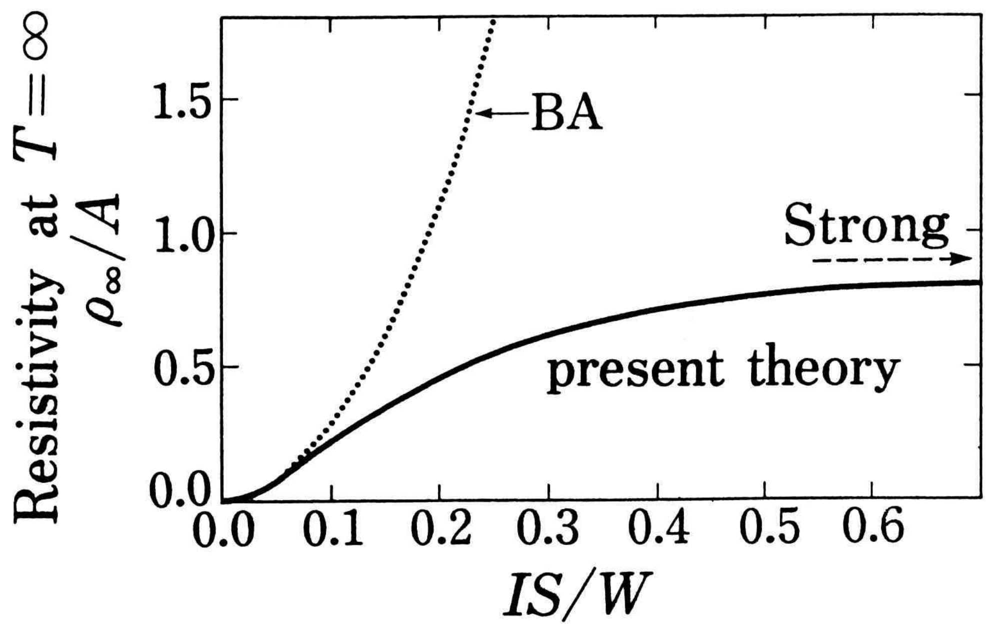

Fig. 6. The (reduced) electrical resistivity for $n=0.1$ with $S=7/2$ at $T=\infty$, ρ/A, as a function of IS/W. Solid line: present theory. Dotted line: the Born approximation (BA). The dashed arrow marks to the limit of strong exchange interaction.

1) $+\Sigma_\mu$ and $z=\omega-I(S+1)$. Then, the CPA condition for $IS/W\to\infty$ limit is rewritten as

$$u_\uparrow=-\frac{(F_\downarrow^{-1}+u_\downarrow)(1+1/S+c_\uparrow)}{1-c_\uparrow}, \tag{A·3}$$

$$u_\downarrow=-\frac{(F_\uparrow^{-1}+u_\uparrow)(1+1/S-c_\downarrow)}{1+c_\downarrow}. \tag{A·4}$$

When $T\to 0$ (or $c_\uparrow\to 1$), $u_\uparrow\to\infty$, while $F_\uparrow^{-1}+u_\uparrow\to z-\omega_G$, where the average band energy is $\omega_G=0.6$ for the model band. Hence, at $T=0$ in the antiparallel-coupling band, the density of states with up spin is 0, while the density of states with down spin has a definite value with

$$u_\downarrow=-\frac{1}{2S}(F_\uparrow^{-1}+u_\uparrow)=-\frac{1}{2S}(z-0.6). \tag{A·5}$$

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