

Quasiparticle band of antiferromagnetic semiconductors

— Single-site approximation for the s - f model —

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Abstract

For the s - f model in an antiferromagnetic semiconductor, the effect of the antiferromagnetic ordering of the localized spins on the conduction-electron state is investigated over a wide range of exchange strengths by combining the effective-medium approach with the Green's function in 2×2 sublattice Bloch function representation. The band splitting due to the reduced magnetic Brillouin zone occurs below the Néel temperature. There is a marked effect of the thermal fluctuation of the antiferromagnetically ordered localized spins on the conduction electron at the energies near the top (bottom) of the lower- (higher-) energy subband.

Key Word: antiferromagnetic semiconductor, s - f model, exchange interaction, coherent potential approximation (CPA)

1 Introduction

In the previous paper (hereafter referred to as Ref. 1), one of the present authors (M. T.) studied the electron state in an antiferromagnetic semiconductor by applying the effective-medium approach [2] for the s - f model [3, 4, 5]; Assuming the orthogonality of two eigenfunctions which were obtained for an electron moving in the effective medium, he calculated the density of states. The method, however, cannot be applied to the case of a strong interaction at finite temperatures. The cause of failure may be ascribed to the above-mentioned assumption of the orthogonality.

The other author (W. N.) and coworkers [6, 7, 8] independently calculated the temperature-dependent quasiparticle spectrum of a single conduction electron exchange coupled to an antiferromagnetically ordered localized-spin system using a momentum-conservation Green function technique.

In the self-energy approach treatment, they correctly derived the Green function in the 2×2 sublattice Bloch function representation.

In the present contribution we aim to devise an improved theory for the s - f model in antiferromagnetic semiconductors, that is applicable not only for weak interaction but also for strong interaction, as well as to a wide range of temperatures. For the purpose, we combine the two methods that were independently developed by the present authors.

2 Basic Consideration

Since the situation and notation examined here are the same as those in Ref. 1, we give here a brief summary of the effective-medium approach for the s - f model in an antiferromagnetic semiconductor. The currently accepted s - f model [2, 3, 4, 5] is used for describing the conduction (s) electron interacting with the localized (f) spins at each lattice site through the

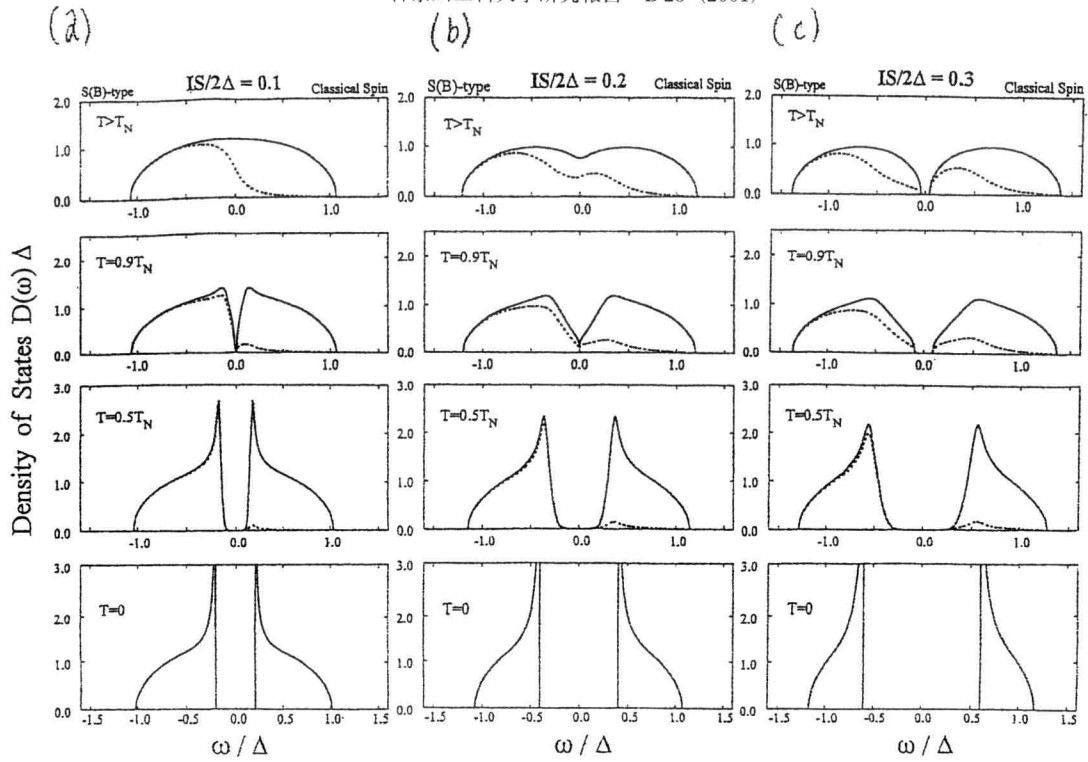


Figure 1: Density of states in an S(B)-type antiferromagnetic semiconductor with classical spins for $T \geq T_N$ and $T = 0.9T_N, 0.5T_N$, and 0; (a) $IS/2\Delta = 0.1$, (b) $IS/2\Delta = 0.2$, and (c) $IS/2\Delta = 0.3$. The solid line represents $D(\omega)\Delta$, the dotted line represents $D_p(\omega)\Delta$.

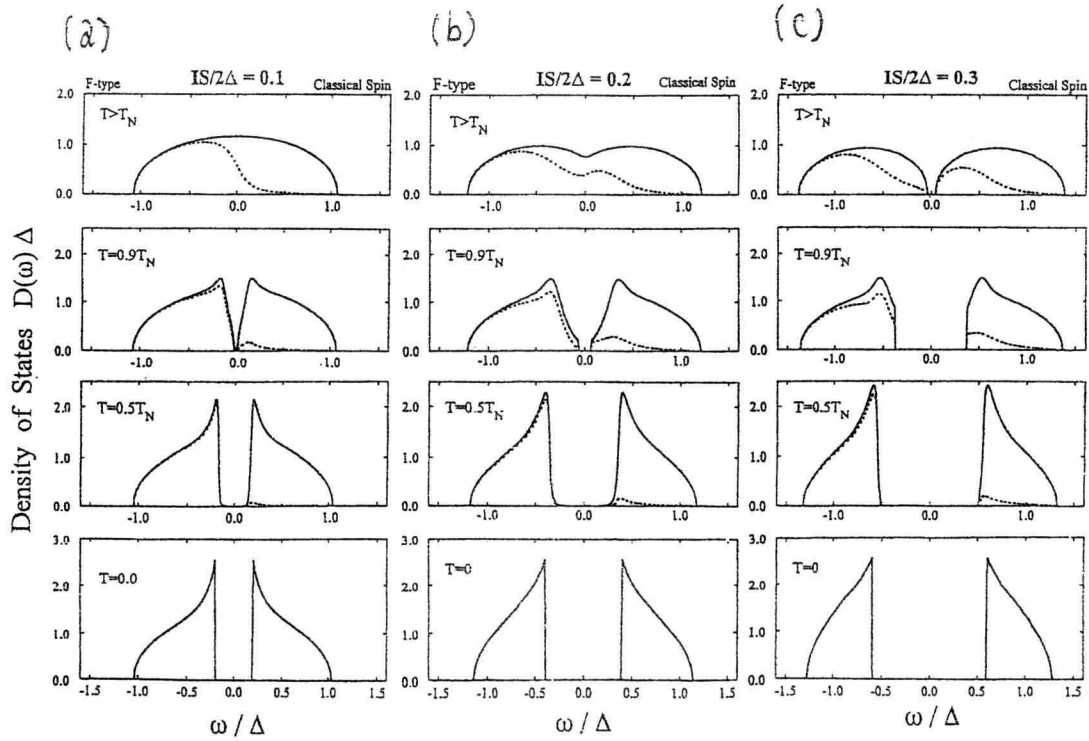


Figure 2: Same as Fig. 1, but for an F-type antiferromagnetic semiconductor with classical spins.

s - f exchange interaction.

In the case of an antiferromagnetic semiconductor [9], spontaneous magnetization develops in opposite orientations for different sublattices below the Néel temperature (T_N). Thus, when the spontaneous magnetization of sublattice A is $\langle S_z^A \rangle_{av}$ ($\equiv \langle S_z \rangle_{av}$), that of sublattice B is $\langle S_z^B \rangle_{av}$ ($= -\langle S_z \rangle_{av}$). Here, we assume that no external field is applied. When a single (s -) electron is injected into an otherwise empty conduction band, therefore, it moves in the crystal while being affected by the antiferromagnetically ordered f spins which are thermally fluctuating at $T < T_N$. In the effective-medium approach [1], the Hamiltonian for the s electron moving in the effective-medium is described by

$$K = \sum_{m,n,\mu} \varepsilon_{mn} a_{m\mu}^\dagger a_{n\mu} + \sum_{m,\mu} \Sigma(m,\mu) a_{m\mu}^\dagger a_{m\mu}, \quad (1)$$

where $\Sigma(m,\mu) = \Sigma_p$ for $\mu = \uparrow$ (\downarrow) and $\Sigma(m,\mu) = \Sigma_a$ for $\mu = \downarrow$ (\uparrow) when m belongs to sublattice A (B). In other words, Σ_p (Σ_a) stands for the majority- (minority-) spin electron; a majority-spin electron in the A sublattice becomes a minority-spin electron in the B sublattice and vice versa. It should be noted that the orientation of the spin of an electron moving in the effective medium remains unchanged because K includes a spin conserving term. Furthermore, the formula is symmetric for both \uparrow and \downarrow spins as long as no magnetic field is applied. In the sublattice Bloch function representation, K is represented by the 2×2 matrix: [1]

$$K = \begin{pmatrix} \varepsilon_1(k) + \Sigma_p & \varepsilon_2(k) \\ \varepsilon_2(k) & \varepsilon_1(k) + \Sigma_a \end{pmatrix}. \quad (2)$$

Here, $\varepsilon_1(k) [= \varepsilon^{AA}(k) = \varepsilon^{BB}(k)]$ and $\varepsilon_2(k) [= \varepsilon^{AB}(k) = \varepsilon^{BA}(k)]$ are the Bloch energies due to electron transfer between similar sublattice sites and between different sublattice sites, respectively. Thus, the matrix element of the reference propagator $(\omega - K)^{-1}$ is given by [6]

$$\frac{1}{\omega - K} = \frac{1}{(\omega - E_p)(\omega - E_a)} \times \begin{pmatrix} \omega - \varepsilon_1(k) - \Sigma_a & \varepsilon_2(k) \\ \varepsilon_2(k) & \omega - \varepsilon_1(k) - \Sigma_p \end{pmatrix}. \quad (3)$$

Here, E_p and E_a are the (complex) energy eigenvalues of K (see Eqs. (2.16) and (2.17) in Ref. 1). In the single-site approximation, Σ_p and Σ_a are so self-consistently determined that the average scattering of the s electron by a f spin located in the effective medium described by Σ_p and Σ_a is zero.

For the application of the single-site approximation using the t matrix formula [2], the diagonal matrix elements of $(\omega - K)^{-1}$ in the Wannier representation, or $F_\uparrow(\omega) = \langle Am \uparrow | (\omega - K)^{-1} | Am \uparrow \rangle = \langle Bm \downarrow | (\omega - K)^{-1} | Bm \downarrow \rangle$ and $F_\downarrow(\omega) = \langle Am \downarrow | (\omega - K)^{-1} | Am \downarrow \rangle = \langle Bm \uparrow | (\omega - K)^{-1} | Bm \uparrow \rangle$ (independent of site index m), are necessary. In the previous work [1], the energy eigenvalues of E_p and E_a and two eigenfunctions were first calculated by solving the secular equation for K . Then, assuming the orthogonalization of the two eigenfunctions, $F_\uparrow(\omega)$ and $F_\downarrow(\omega)$ were evaluated. The previous method, however, yielded nonphysical results for the cases of strong exchange interaction at antiferromagnetic temperatures ($T_N > T > 0$). The cause of the failure is ascribed to the assumption of orthogonality of the two eigenfunctions, which is incorrect when K is not Hermitian (or when $T_N > T > 0$). In the present work, without assuming the orthogonality of the two eigenfunctions, we calculate $F_\uparrow(\omega)$ and $F_\downarrow(\omega)$ directly using the matrix element of $(\omega - K)^{-1}$ shown in Eq. (3).

For numerical calculation, we introduce the semi-circular band with a half bandwidth of Δ , $\rho(\varepsilon)$, as an undisturbed (model) density of states (i.e., for $IS = 0$) [1]. Further, in order to replace the summation over k within the Brillouin zone by the integral of ε using $\rho(\varepsilon)$, we need the relationship between ε and the Bloch energy [or $\varepsilon_1(k)$ and $\varepsilon_2(k)$]. In this work, we proceed to perform calculation for two cases which are assumed as follows. (i) S(B)-type: when the nearest neighbors of each atom are from the other sublattice, we set $\varepsilon_1(k) \rightarrow 0$ and $\varepsilon_2(k) \rightarrow \varepsilon$. (ii) F-type: when the electron transfer between similar sublattice sites $\varepsilon_1(k)$ contributes to ε as much as that between different sublattice sites $\varepsilon_2(k)$, we set $\varepsilon_1(k) \rightarrow \varepsilon/2$ and $\varepsilon_2(k) \rightarrow \varepsilon/2$. (In Ref. 1, the above types were referred to as the sc (bcc) structure and fcc structure, but in this paper this is changed to

avoid misunderstanding. Note that $\rho(\varepsilon)$ used here is not related to a specific tight-binding system.)

Consequently, we calculate $F_\uparrow(\omega)$ and $F_\downarrow(\omega)$ by

$$F_\uparrow(\omega) = 2 \int_{-\Delta}^0 d\varepsilon \rho(\varepsilon) \frac{\eta_A}{\omega - E_p(\varepsilon)} + 2 \int_0^\Delta d\varepsilon \rho(\varepsilon) \frac{\eta_B}{\omega - E_a(\varepsilon)}, \quad (4)$$

$$F_\downarrow(\omega) = 2 \int_{-\Delta}^0 d\varepsilon \rho(\varepsilon) \frac{\eta_B}{\omega - E_p(\varepsilon)} + 2 \int_0^\Delta d\varepsilon \rho(\varepsilon) \frac{\eta_A}{\omega - E_a(\varepsilon)}, \quad (5)$$

with

$$\eta_A = \frac{\varepsilon_1(k) + \Sigma_a - E_p}{E_a - E_p}, \quad (6)$$

$$\eta_B = \frac{\varepsilon_1(k) + \Sigma_a - E_a}{E_p - E_a}. \quad (7)$$

Note that $\eta_A + \eta_B = 1$. The total density of states is estimated by $D(\omega) = -\frac{1}{\pi} \text{Im}[F_\uparrow(\omega) + F_\downarrow(\omega)]$. When we define $D_p(\omega)$ ($D_a(\omega)$) as the density of states for the P(A)-state that is the eigen state corresponding complex eigen value $E_p(E_a)$, $D(\omega) = D_p(\omega) + D_a(\omega)$. In the above expressions, the difference between the present approach and the previous one (Ref. 1) is that we replace $|c_A|^2$ and $|c_B|^2$ [which are defined by Eqs. (2.21) and (2.22) in Ref. 1] by η_A and η_B , which are defined by Eqs. (6) and (7), respectively. Next, we demonstrate how the present approach improves the unreasonable previous results.

3 Results and Discussion

3.1 S(B)-type antiferromagnetic semiconductors with classical spins

The result for density of states $D(\omega)$ in S(B)-type antiferromagnetic semiconductors with classical spins is shown in Fig. 1 for typical exchange strength cases: (a) weak interaction ($IS/2\Delta = 0.1$), (b) intermediate interaction ($IS/2\Delta = 0.2$), and (c) strong interaction ($IS/2\Delta = 0.3$). In the effective medium of the S(B)-type, a majority- (minority-) spin electron changes to a minority- (majority-) spin electron when the electron transfers from a site to another site, because the nearest neighbors of each atom are

from the other sublattice. The present study reveals how the conduction-electron states in an antiferromagnetic semiconductor are modified with the change in temperature or antiferromagnetic ordering of f spins over a wide range of exchange strengths. The present method reproduces the previous result [1] for both cases of $T \geq T_N$ and $T = 0$. When the exchange interaction is weak (see the case of (a) $IS/\Delta = 0.1$), the band, retaining a single band at paramagnetic temperatures ($T \geq T_N$), splits into two subbands below T_N ; this change is rather similar to that reported in Ref. 1. The band-splitting below T_N is caused by the reduction of the magnetic Brillouin zone, and is called ‘‘Slater splitting’’ [6]. When the exchange interaction is strong (see the case of (c) $IS/\Delta = 0.3$), there already exist two subbands at paramagnetic temperatures ($T \geq T_N$) which are characterized mainly by the coupling of the electron spin parallel or antiparallel to the orientation of f spins. Below T_N , each subband becomes narrower as the temperature approaches $T = 0$. The physical results for $IS/\Delta \geq 0.2$ are first obtained by the present improved approach. In Fig. 1 we also include the density of states of the P-state $D_p(\omega)$ for discussion. As long as the f spin is treated as a classical spin, at all temperatures $D(\omega) = D(-\omega)$ and $D_p(\omega) = D_a(-\omega)$. At $T = 0$, the entire lower- (higher-) energy subband consist of P-states (A-states); $D(\omega) = D_p(\omega)$ for $\omega \leq 0$ and $D(\omega) = D_a(\omega)$ for $\omega \geq 0$. With the increase in temperature from $T = 0$, particularly near the top of the lower-energy subband and/or the bottom of the higher-energy subband, the hybrid of the P-state and A-state begins, which suggests that the electron state is strongly disturbed due to the thermal fluctuation of f spins.

3.2 F-type antiferromagnetic semiconductors with classical spins

In Fig. 2, the change of the density of states for the F-type with temperature (or with antiferromagnetic ordering of f spins) is shown for three typical exchange strengths. The result for $T \geq T_N$ also agrees with that of the CPA, whereas the density of states

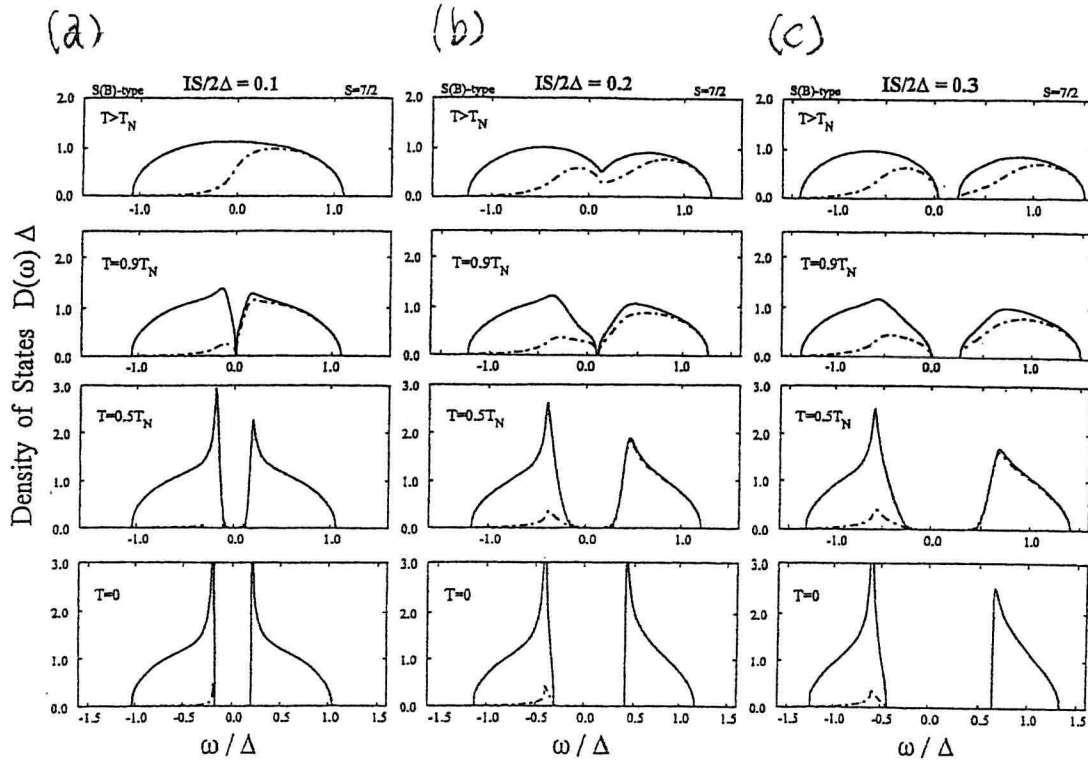


Figure 3: Same as Fig. 1, but for an S(B)-type antiferromagnetic semiconductor with $S = 7/2$. The solid line represents $D(\omega)\Delta$, the dotted line represents $D_a(\omega)\Delta$, rather than $D_p(\omega)\Delta$.

for $T = 0$ is given by

$$D(\omega)\Delta = \frac{4}{\pi} \left(\frac{\Delta}{\omega} \right)^2 \left[\left(\frac{\omega}{\Delta} \right)^2 + \left(\frac{IS}{\Delta} \right)^2 \right] \times \left\{ 1 - \left(\frac{\Delta}{\omega} \right)^2 \left[\left(\frac{IS}{\Delta} \right)^2 - \left(\frac{\omega}{\Delta} \right)^2 \right]^2 \right\}^{1/2}$$

for $IS < |\omega| < [\Delta + \sqrt{\Delta^2 + 4(IS)^2}]/2$ and 0 otherwise. (A misprint in Eq. (3.3) of Ref. 1 is corrected by Eq. (8) in this paper.) The difference in the results between the S(B)-type and the F-type arises from the distribution of ε into $\varepsilon_1(k)$ and $\varepsilon_2(k)$; for S(B)-type $\varepsilon_1 = 0$ and $\varepsilon_2 = \varepsilon$, while for F-type $\varepsilon_1 = \varepsilon_2 = \varepsilon/2$. Comparing Figs. 1 and 2, the variation in the density of states with temperature and/or with exchange strength is a common feature for both the S(B)-type and the F-type.

3.3 Effect of quantum spins

Here, we investigate how the quantum effect of the f spins modifies the s electron interacting with anti-

ferromagnetically ordered f spins through the s - f exchange interaction. In Fig. 3, we depict the density of states for an S(B)-type antiferromagnetic semiconductor with $S = 7/2$; the figure shows $D(\omega) \neq D(-\omega)$, as a consequence of quantum effect of f spins. When $T = 0$, in the classical-spin treatment we can set $\Sigma_p = -IS$ and $\Sigma_a = +IS$, while in the quantum-spin treatment we have to set $\Sigma_p = -IS$ and $\Sigma_a = +IS(1 + IF_\uparrow)/(1 - IF_\uparrow)$, where F_\uparrow is calculated self-consistently using Σ_p and Σ_a [see Eq. (4)]. This is, of course, due to the exchange scattering by the quantum fluctuation of the f spin. Even when f spins are completely antiferromagnetically ordered (or at $T = 0$), an s electron with down-spin on the A sublattice site can flip its spin while conserving the total spin ($= S - 1/2$). It should be emphasized that F_\uparrow (not F_p) is used for calculating Σ_a at $T = 0$ because s electron states with down-spin are occupied after spin flipping, F_\uparrow consists of F_p and F_a , as shown by Eq. (4).

4 Concluding remarks

In this study, we aimed to devise an improved theory for the s - f model in antiferromagnetic semiconductors that is applicable to a wide range of exchange strengths and temperatures. For this purpose, we improved the effective-medium approach for the s - f model [1, 2] using the corrected Green function in the 2×2 sublattice Bloch function representation [6, 7, 8]. The result revealed that the present improvement considerably extends the applicable range of temperatures and exchange strengths.

The numerical calculations were performed for three cases of antiferromagnetic semiconductors: the S(B)-type with classical spins, the F-type with classical spins, and S(B)-type with quantum spins ($S = \frac{7}{2}$). The S(B)-type and the F-type are classified according to their distribution of electron transfer energy to the transfer between similar and/or different sublattice sites. For each case, the results for the density of states exhibited "Slater splitting," that is, band-splitting due to the reduced magnetic Brillouin zone at $T < T_N$. The lower- (higher-) energy subband arises mainly from P- (A-) states which are composed of Wannier electron states in which the spin orientation is parallel (antiparallel) to the orientation of the f spin at each site. In particular, when $T = 0$, for classical f spins, the entire lower- (higher-) energy subband consists of P- (A-) states. The effect of the antiferromagnetic ordering of f spins on the s electron states is felt markedly at the energies near the top (bottom) of the lower- (higher-) energy subband. The electrons with the energies near the top (bottom) of the lower- (higher-) energy subband are strongly disturbed by the development in antiferromagnetic ordering through the s - f exchange interaction. Furthermore, the hybridization of the P-state and the A-state due to thermal fluctuation of f spins also occurs, especially near the top of the lower-energy subband and/or the bottom of the higher-energy subband. The s electron in an F-type antiferromagnetic semiconductor is more strongly affected than in an S(B)-type one due to the fluctuation of f spins because it transfers between similar and different sublattices. The quantum effect of f spins adds another complication because it

enables the spin-flip of a minority-spin electron even at $T = 0$. All these effects occur especially near the top of the lower-energy subband and/or the bottom of the higher-energy subband.

Throughout this study, calculation was performed only for the model density of states of semi-circular form. Calculation combining the present method with a realistic band structure of EuTe is desirable. We plan to examine these problems.

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