# Dynamical coherent potential approach for the *s-f* model in antiferromagnetic semiconductors

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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 $2 \times 2$ 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 present contribution we study how the conduction-electron state in an antiferromagnetic semiconductor varies with the temperature and/or with the antiferromagnetic ordering of the localized-spin system through the exchange interaction between the electron and the localized spins. In the previous paper (hereafter referred to as Ref. 1), one of the present authors (M. T.) studied the electron state by applying the effective-medium approach [2] for the *s-f* model [3, 4, 5] in an antiferromagnetic semiconductor [6]. Assuming the orthogonality of two eigenfunctions which were obtained for an electron moving in the effective medium, he calculated the density of states in an antiferromagnetic semiconductor with a weak exchange interaction. The method, however, cannot be applied to the case of a strong exchange interaction at finite temperatures. In particular, the above mentioned assumption of the orthogonality has to be considered with caution. The other author (W. N.) and coworkers [7, 8, 9] 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 $2 \times 2$ sublattice Bloch function representation.

In this study, 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 this purpose, we combine the two methods which were independently developed by the present authors. Using the Green function in the $2 \times 2$ sublattice Bloch function representation [7, 8, 9], we improve the effective-medium approach for the *s-f* model [1, 2] in order to study the conduction-electron states in anti-

ferromagnetic semiconductors. As shown in this paper, the present method considerably extends the applicable range of temperatures and exchange strengths. A brief report has been already presented previously [10].

The organization of this paper is as follows. In Sec. II, the improved effective-medium approach for the *s-f* model in an antiferromagnetic semiconductor is concisely formulated, avoiding duplicity with Ref. 1. In Sec. III, the numerical results are presented for three cases: two different types with classical localized spins and one with quantum spins. The two types are classified according to the distribution of electron transfer energy to the transfer between similar and/or different sublattice sites. For each case, the results of the density of states, the coherent potential (or self-energy), and the quasiparticle energy, are shown for typical exchange strengths and various temperatures, together with discussion regarding the effect of antiferromagnetic ordering of the localized spins on the conduction-electron state through the exchange interaction. In Sec. IV, concluding remarks are presented.

## 2 Basic Considerations

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 *s-f* exchange interaction. In this model, the total Hamiltonian, $H_t$, consists of $H_s$, $H_f$, and $H_{sf}$, which represent the translational energy of an $s$ electron, the Heisenberg-type exchange interaction between $f$ spins, and the *s-f* exchange interaction between an $s$ electron and $f$ spins, respectively. In this work, $H_f$ represents antiferromagnetic ordering between $f$ spins.

In the case of an antiferromagnetic semiconductor [6], spontaneous magnetization develops in opposite orientations for different sublattices below the Néel temperature ($T_N$). Here we assume that $f$ spins are situated regularly on two interpenetrating ferromagnetic sublattices, $A$ and $B$. We take the $+z$ direction as the orientation of spontaneous magnetization of the $f$ spin at the $A$ sublattice sites and we assume that no external field is applied. Thus, when the spontaneous magnetization of sublattice $A$ is $< S_z^A >_{\rm av}$ ($\equiv < S_z >_{\rm av}$), that of sublattice $B$ is $< S_z^B >_{\rm av}$ ($= - < S_z >_{\rm av}$), where $< >_{\rm av}$ represents a thermal average. 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], complex potentials, $\Sigma_p$ and $\Sigma_a$, are prepared in order to consider the effect of the fluctuation of antiferromagnetically ordered $f$ spins on the $s$ electron state; $\Sigma_p$ ($\Sigma_a$) is a short-range potential to which an $s$ electron is subjected when the orientation of its spin is parallel (antiparallel) to the orientation of the $f$ spin at that site in spontaneous magnetic ordering. Thus, the effective Hamiltonian for the $s$ electron moving in the effective-medium is described by

$$K = \sum_{m,n,\mu} \varepsilon_{mn} a^{\dagger}_{m\mu} a_{n\mu} + \sum_{m,\mu} \Sigma(m,\mu) a^{\dagger}_{m\mu} a_{m\mu} , \tag{2. 1}$$

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, $\Sigma_p$ ($\Sigma_a$) 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 Bloch representation, $K$ is represented by the $2 \times 2$ matrix [1]:

$$\begin{aligned} K &= \begin{pmatrix} < Ak,\uparrow |K| Ak,\uparrow > & < Ak,\uparrow |K| Bk,\uparrow > \\ < Bk,\uparrow |K| Ak,\uparrow > & < Bk,\uparrow |K| Bk,\uparrow > \end{pmatrix} , \\ &= \begin{pmatrix} \varepsilon_1(k) + \Sigma_p & \varepsilon_2(k) \\ \varepsilon_2(k) & \varepsilon_1(k) + \Sigma_a \end{pmatrix} \end{aligned} \tag{2. 2}$$

In Eq. (2. 2), $|Ak,\uparrow>$ ($|Bk,\uparrow>$) are the Bloch states related to the Wannier states on the $A(B)$ sublattice sites; Furthermore, $\varepsilon_1(k)[= \varepsilon^{AA}(k) = \varepsilon^{BB}(k)]$ 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.

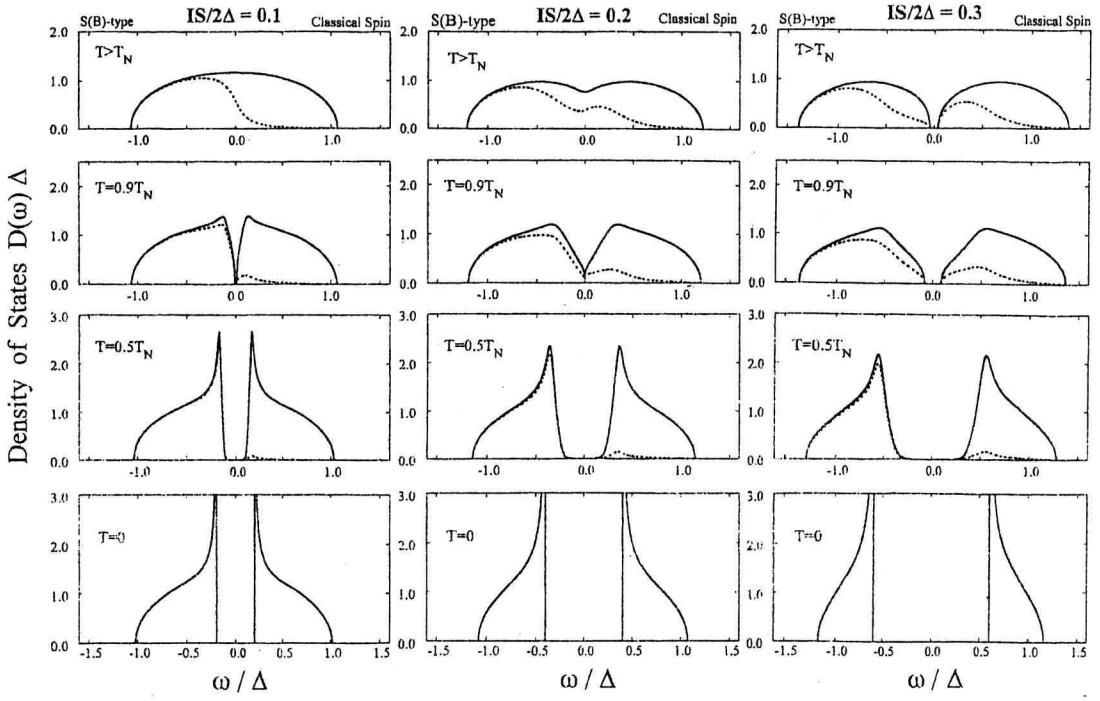


Figure 1: Density of states in an S(B)-type antiferromagnetic semiconductor with classical spins for $T \geq T_N$ and $T = 0.9T_N, 0.5T_N$, and 0; (a) $IS/2\Delta = 0.1$, (b) $IS/2\Delta = 0.2$, and (c) $IS/2\Delta = 0.3$. The solid line represents $D(\omega)\Delta$, the dotted line represents $D_p(\omega)\Delta$.

The matrix element of the reference propagator $(\omega - K)^{-1}$ is given by [7]

$$\frac{1}{\omega - K} = \frac{1}{D}\begin{pmatrix} \omega - \varepsilon_1(k) - \Sigma_a & \varepsilon_2(k) \\ \varepsilon_2(k) & \omega - \varepsilon_1(k) - \Sigma_p \end{pmatrix} , \quad (2.\ 3)$$

where

$$D = [\omega - (\varepsilon_1(k) + \Sigma_a)][\omega - (\varepsilon_1(k) + \Sigma_p)] - \varepsilon_2(k)^2 , \\ = (\omega - E_p)(\omega - E_a) , \quad (2.\ 4)$$

with

$$E_p = \frac{2\varepsilon_1(k) + \Sigma_p + \Sigma_a - \sqrt{4\varepsilon_2(k)^2 + (\Sigma_p - \Sigma_a)^2}}{2} , \quad (2.\ 5)$$

$$E_a = \frac{2\varepsilon_1(k) + \Sigma_p + \Sigma_a + \sqrt{4\varepsilon_2(k)^2 + (\Sigma_p - \Sigma_a)^2}}{2} . \quad (2.\ 6)$$

Note that $E_p$ and $E_a$ are generally complex, and are equal to the energy eigenvalues of $K$. The eigen states corresponding to two complex eigenvalues, $E_p$ and $E_a$, are hereafter called P-state and A-state, respectively; P(A)-state is mainly composed of Wannier states in which the orientation of the $s$ electron spin is parallel (antiparallel) to the orientation of the $f$ spin at each site.

In the effective-medium approach approximation [1], $K$ should be determined so that $(\omega - K)^{-1}$ is approximated to the thermal average of the propagator, $< (\omega - H)^{-1} >_{\rm av}$, where $H \equiv H_s + H_{sf}$. Within the single-site approximation, this leads to the condition that $\Sigma_p$ and $\Sigma_a$ are so self-consistently determined that the average scattering of the $s$ electron by a $f$ spin located in the effective medium described by $\Sigma_p$ and $\Sigma_a$ is zero [2]. For the application of the single-site approximation using the $t$ matrix formula, the diagonal matrix elements of $(\omega - K)^{-1}$ in the Wannier representation, or $F_\uparrow(\omega) =< Am \uparrow |(\omega - K)^{-1}|Am \uparrow >=< Bm \downarrow |(\omega - K)^{-1}|Bm \downarrow >$ and $F_\downarrow(\omega) =< Am \downarrow |(\omega - K)^{-1}|Am \downarrow >=< Bm \uparrow |(\omega - K)^{-1}|Bm \uparrow >$ (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 as $|\frac{IS}{\Delta}| > 0.2$ at antiferromagnetic temperatures ($T_N > T > 0$). The cause of the failure is ascribed to the assumption of orthogonality of the

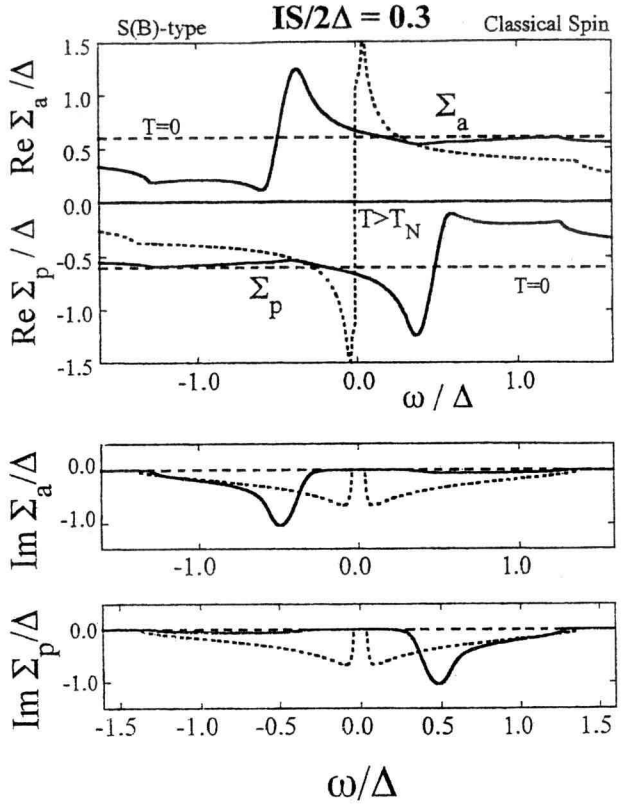


Figure 2: (a) $\mathrm{Re}\Sigma_a/\Delta$ (upper part) and $\mathrm{Re}\Sigma_p/\Delta$ (lower part), (b) $\mathrm{Im}\Sigma_a/\Delta$, and (c) $\mathrm{Im}\Sigma_p/\Delta$ in an S(B)-type antiferromagnetic semiconductor with classical spins with $IS/2\Delta = 0.3$ as a function of $\omega/\Delta$ for various temperatures: dashed line represents $T = 0$; solid line for $T = 0.5T_N$; dash-dotted line represents $T = 0.9T_N$; dotted line represents $T > T_N$ (or $\Sigma_{\mathrm{CPA}} = \Sigma_p = \Sigma_a$).

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. (2. 3). Consequently

$$F_\uparrow(\omega) = \frac{2}{N}\sum_{Ak}\frac{\omega - \varepsilon_1(k) - \Sigma_a}{(\omega - E_p)(\omega - E_a)}, \quad (2.\ 7)$$

$$= \frac{2}{N}\sum_{Ak}\left(\frac{\eta_A}{\omega - E_p} + \frac{\eta_B}{\omega - E_a}\right), \quad (2.\ 8)$$

and

$$F_\downarrow(\omega) = \frac{2}{N}\sum_{Ak}\left(\frac{\eta_B}{\omega - E_p} + \frac{\eta_A}{\omega - E_a}\right), \quad (2.\ 9)$$

with

$$\eta_A = \frac{\varepsilon_1(k) + \Sigma_a - E_p}{E_a - E_p}, \quad (2.\ 10)$$

$$\eta_B = \frac{\varepsilon_1(k) + \Sigma_a - E_a}{E_p - E_a}. \quad (2.\ 11)$$

Next, we introduce the semicircular band with a half bandwidth of $\Delta$,

$$\rho(\varepsilon) = \frac{2}{\pi\Delta}\sqrt{1 - \left(\frac{\varepsilon}{\Delta}\right)^2}, \quad (2.\ 12)$$

as an undisturbed (model) density of states (i.e., for $IS = 0$) [1]; In order to replace the summation over $k$ within the Brillouin zone by the integral of $\varepsilon$ using $\rho(\varepsilon)$, we need to determine the relationship between $\varepsilon$ and the Bloch energy [or $\varepsilon_1(k)$ and $\varepsilon_2(k)$]. It is difficult to specify a simple relationship because the Bloch energy is strongly related to the crystal structure (or tight-binding system). Note that the model density of states given by Eq. (2. 12) is not related to a specific tight-binding system. 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 $\varepsilon_1(k) \to 0$ and $\varepsilon_2(k) \to \varepsilon$. (ii) F-type: when the electron transfer between similar sublattice sites $\varepsilon_1(k)$ contributes to $\varepsilon$ as much as that between different sublattice sites $\varepsilon_2(k)$,

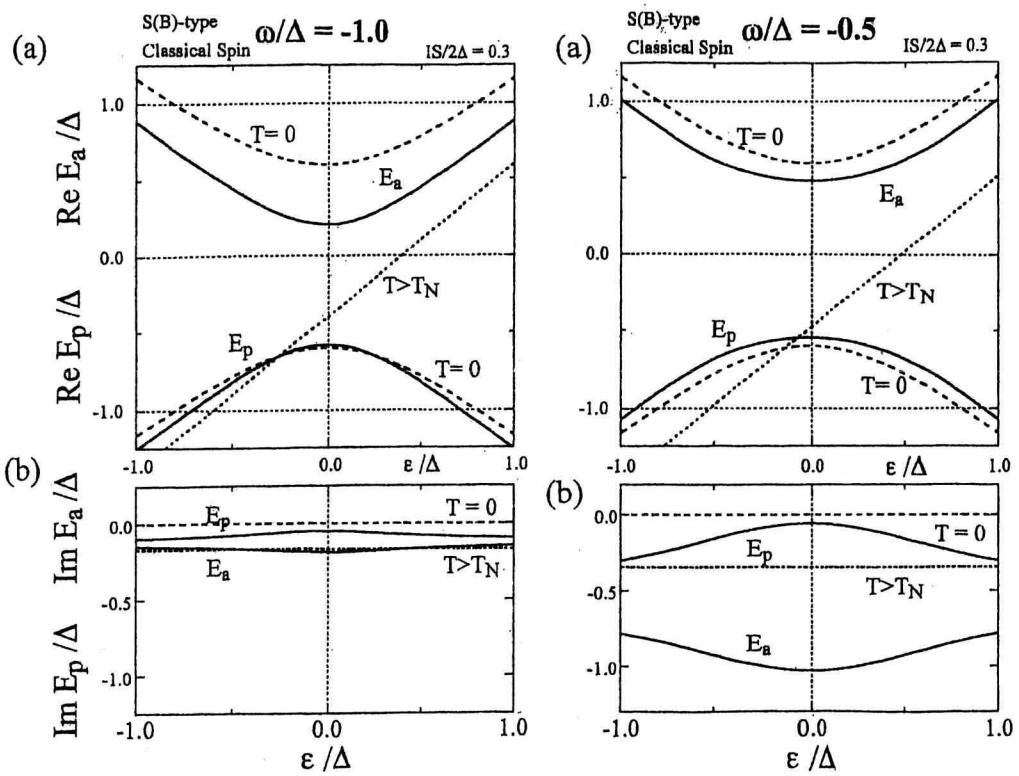


Figure 3: (a) $\mathrm{Re}E_a/\Delta$ and $\mathrm{Re}E_p/\Delta$, (b) $\mathrm{Im}E_a/\Delta$ and $\mathrm{Im}E_p/\Delta$, at $\omega/\Delta = -1.0$ (left figure) and $\omega/\Delta = -0.5$ (right figure), in an S(B)-type antiferromagnetic semiconductor with classical spins with $IS/2\Delta = 0.3$ as a function of $\varepsilon/\Delta$ for various temperatures: dashed line represents $T = 0$; solid line represents $T = 0.5T_N$; dotted line represents $T > T_N$ (or $E_a = E_p = \varepsilon + \Sigma_{\mathrm{CPA}}$).

we set $\varepsilon_1(k) \to \varepsilon/2$ and $\varepsilon_2(k) \to \varepsilon/2$. (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.)

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

$$F_\uparrow(\omega) = 2\int_{-\Delta}^{0} d\varepsilon\rho(\varepsilon)\frac{\eta_A}{\omega - E_p(\varepsilon)} + 2\int_{0}^{\Delta} d\varepsilon\rho(\varepsilon)\frac{\eta_B}{\omega - E_a(\varepsilon)}\,, \tag{2. 13}$$

$$F_\downarrow(\omega) = 2\int_{-\Delta}^{0} d\varepsilon\rho(\varepsilon)\frac{\eta_B}{\omega - E_p(\varepsilon)} + 2\int_{0}^{\Delta} d\varepsilon\rho(\varepsilon)\frac{\eta_A}{\omega - E_a(\varepsilon)}\,, \tag{2. 14}$$

(see also the discussion regarding Fig. 3). Note that $\eta_A + \eta_B = 1$. When we define $F_p(\omega)$ and $F_a(\omega)$ by

$$F_p(\omega) = \frac{2}{N}\sum_{Ak}\frac{1}{\omega - E_p} = 2\int_{-\Delta}^{0} d\varepsilon\rho(\varepsilon)\frac{1}{\omega - E_p(\varepsilon)}, \tag{2. 15}$$

$$F_a(\omega) = \frac{2}{N}\sum_{Ak}\frac{1}{\omega - E_a} = 2\int_{0}^{\Delta} d\varepsilon\rho(\varepsilon)\frac{1}{\omega - E_a(\varepsilon)}\,, \tag{2. 16}$$

then $F(\omega) \equiv F_\uparrow(\omega) + F_\downarrow(\omega) = F_p(\omega) + F_a(\omega)$. As can easily be seen by the definition, $F_\uparrow$ is related to the majority-spin ($\uparrow$) electron states in the $A$ sublattice, whereas $F_\downarrow$ is related to the minority-spin ($\downarrow$) electron states in the $A$ sublattice. In contrast, $F_p$ ($F_a$) is related to P(A)-states. The P(A)-state is mainly composed of Wannier states in which the orientation of the spin is parallel (antiparallel) to the orientation of the $f$ spin at each site. The total density of states is estimated by $D(\omega) = -\frac{1}{\pi}\mathrm{Im}F(\omega)$, while the density of states for

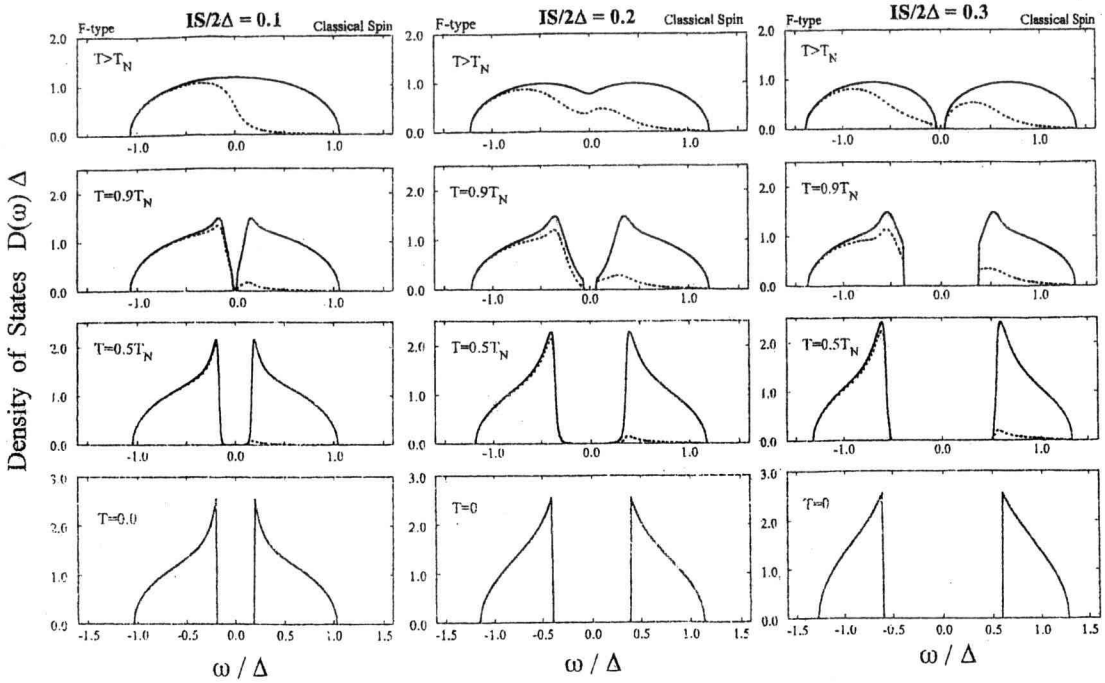


Figure 4: Same as Fig. 1, but for an F-type antiferromagnetic semiconductor with classical spins.

the P(A)-state is estimated by $D_p(\omega) = -\frac{1}{\pi}\mathrm{Im}F_p(\omega)$ $(D_a(\omega) = -\frac{1}{\pi}\mathrm{Im}F_a(\omega))$.

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 $\eta_A$ and $\eta_B$, which are defined by Eqs. (2. 10), and (2. 11), respectively. It should be reemphasized that in this work we do not adopt the assumption of the orthogonalization between the two eigenfunctions which belong to different complex eigenvalues, $E_p$ and $E_a$. This assumption was the cause of the unreasonable results obtained for the strong exchange interaction in the temperature region of $0 < T < T_N$ in the previous work. In the next section, we demonstrate how the present approach improves these unreasonable previous results.

## 3 Results and Discussion

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

In this subsection, we present the results for S(B)-type antiferromagnetic semiconductors with classical spins. 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. In the classical spin treatment, the operation of $1/S \to 0$ is taken while keeping $IS$ = constant. The values of $< S_z >_{\mathrm{av}} /S$, calculated by applying the molecular field approximation for classical spin, are 0.0, 0.39, 0.79, and 1.0 for $T \geq T_N$, $T = 0.9T_N, 0.5T_N$, and 0, respectively. Figure 1 presents the variation of the product of the density of states and the half-bandwidth $D(\omega)\Delta$ with temperature as a function of the reduced energy $\omega/\Delta$ 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 ($IS/2\Delta = 0.3$). The method reproduces the previous result [1] for both cases of $T \geq T_N$ and $T = 0$; The result for paramagnetic temperatures ($T \geq T_N$) agrees with that obtained using the coherent potential approximation (CPA) [11], while the result for the density of states for $T = 0$ is given by

$$D(\omega)\Delta = \frac{4|\omega|}{\pi\Delta}\left\{\frac{\Delta^2 + (IS)^2 - \omega^2}{\omega^2 - (IS)^2}\right\}^{1/2}, \quad (3.\ 1)$$

for $IS < |\omega| < \sqrt{\Delta^2 + (IS)^2}$ and 0 otherwise [1]. Although Eq. (3. 1) diverges at $\omega = \pm IS$, the total number of states is preserved. The present study reveals how the conduction-electron states in an antiferromagnetic semiconductor are modified with the

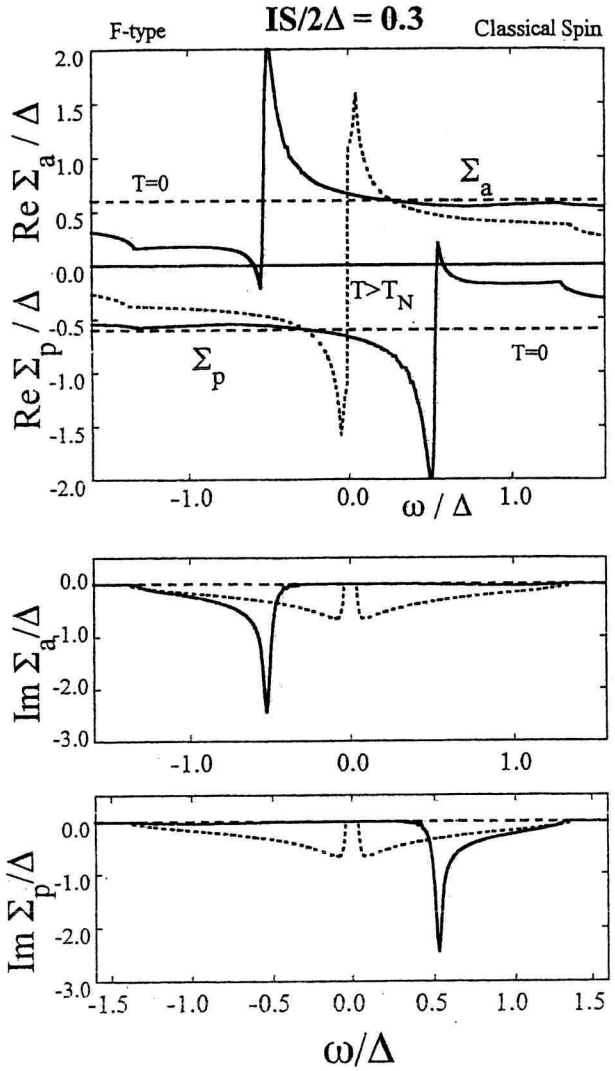


Figure 5: Same as Fig. 2, but for an F-type antiferromagnetic semiconductor with classical spins with $IS/2\Delta = 0.3$. (Note the difference in the scale of the vertical line.)

change in temperature or antiferromagnetic ordering of $f$ spins over a wide range of exchange strengths. 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" [7]. 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 product of the density of states of the P-state and the half-bandwidth $D_p(\omega)\Delta$ for discussion, $D_p(\omega) + D_a(\omega) = D(\omega)$. 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.

Since the result for a weak exchange strength ($IS/2\Delta = 0.1$) is almost similar to that reported in Ref. 1, we include a brief discussion here about the electron states with a strong exchange interaction ($IS/2\Delta = 0.3$). In order to demonstrate the effect of the magnetic ordering of $f$ spins on the conduction-electron state,

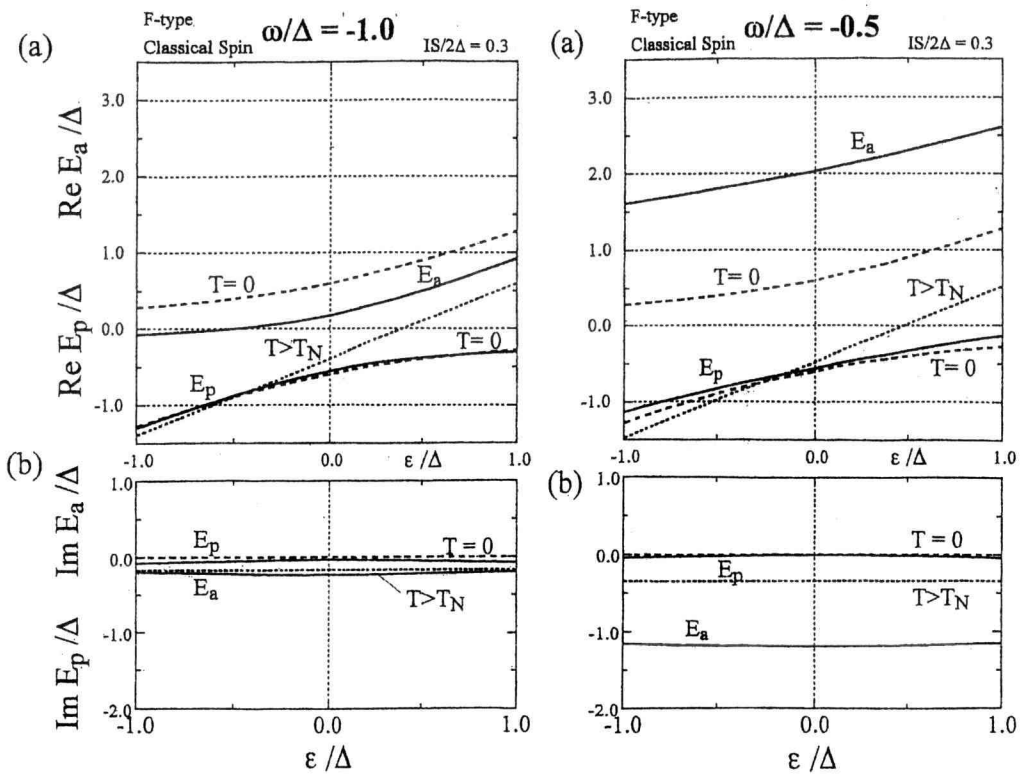


Figure 6: Same as Fig. 3, but for an F-type antiferromagnetic semiconductor with classical spins with $IS/2\Delta = 0.3$. (Note the difference in the scale of the vertical line.)

we present $\Sigma_p(\Sigma_a)$ as a function of $\omega$ in Fig. 2, and $E_p(E_a)$ as a function of $\varepsilon$ in Fig. 3. At $T = 0$, $\Sigma_p = -IS$ and $\Sigma_a = +IS$, so that $E_p[= -\sqrt{\varepsilon^2 + \Delta^2}]$ and $E_a[= \sqrt{\varepsilon^2 + \Delta^2}]$ are real. Thus, at $T = 0$, the P-state and A-state are energy eigenstates which are orthogonal to each other. On the other hand, at $T \geq T_N$, the present theory gives $\Sigma_p = \Sigma_a = \Sigma_{\rm CPA}$; $\mathrm{Re}\Sigma_{\rm CPA}(\omega) = -\mathrm{Re}\Sigma_{\rm CPA}(-\omega)$ and $\mathrm{Im}\Sigma_{\rm CPA}(\omega) = \mathrm{Im}\Sigma_{\rm CPA}(-\omega)$, and furthermore the quasiparticle energy $\omega = \varepsilon + \Sigma_{\rm CPA}$. Therefore, for all temperatures, we take $\omega = E_p(\varepsilon)$ for $\varepsilon < 0$ and $\omega = E_a(\varepsilon)$ for $\varepsilon > 0$ that $\omega = E_p(\varepsilon)$ [or $E_a(\varepsilon)$] agrees with the result of the CPA at $T \geq T_N$ (see Eq. () and Fig. 3). As the temperature decreases from $T_N$ to $T = 0$, the peak in $|\mathrm{Im}\Sigma_p|$ ($|\mathrm{Im}\Sigma_a|$) shifts to $\omega = -IS(\omega = +IS)$ (see Fig. 2), and is accompanied by the shift of the top edge of the lower-energy subband (the bottom edge of the higher-energy subband) (see Fig. 1(c)). The conduction electron with the spin which is antiparallel (parallel) to the orientation of the $f$ spin at that site is strongly scattered due to the fluctuation of the $f$ spin, particularly when it has an energy near the peak in $|\mathrm{Im}\Sigma_a|$ ($|\mathrm{Im}\Sigma_p|$).

Figure 3 represents $E_p(\varepsilon)(E_a(\varepsilon))$ for two cases of $\omega$ of the lower-energy subband: the left-hand side is $\omega/\Delta = -1.0$ (near the bottom edge) and the right-hand side is $\omega/\Delta = -0.5$ (near the top edge). For the S(B)-type antiferromagnetic semiconductor, $E_p(\varepsilon) = E_p(-\varepsilon)$, and $E_a(\varepsilon) = E_a(-\varepsilon)$. At $T_N > T > 0$, for $\omega \leq 0$, $|\mathrm{Im}E_a| \geq |\mathrm{Im}E_p|$ ; this suggests that the A-state is more strongly disturbed than the P-state due to the thermal fluctuation of $f$ spins, as previously described. (In contrast, $|\mathrm{Im}E_a| < |\mathrm{Im}E_p|$ for $\omega > 0$.) Comparing the two results of $\omega/\Delta = -1.0$ and $\omega/\Delta = -0.5$, it is verified that near the top of the lower-energy subband, the A-state (especially $\varepsilon \sim 0$) is strongly disturbed and is correlated with the P-state due to the thermal fluctuation of $f$ spins.

## 3.2 F-type antiferromagnetic semiconductors with classical spins

Figures 4-6 present the results for F-type antiferromagnetic semiconductors with classical spins. The difference in the results between the S(B)-type and the F-type arises from the distribution of $\varepsilon$ into $\varepsilon_1(k)$ and $\varepsilon_2(k)$; for S(B)-type $\varepsilon_1 = 0$ and $\varepsilon_2 = \varepsilon$, while for F-type $\varepsilon_1 = \varepsilon_2 = \varepsilon/2$. In Fig. 4, 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 for $T = 0$ is given by

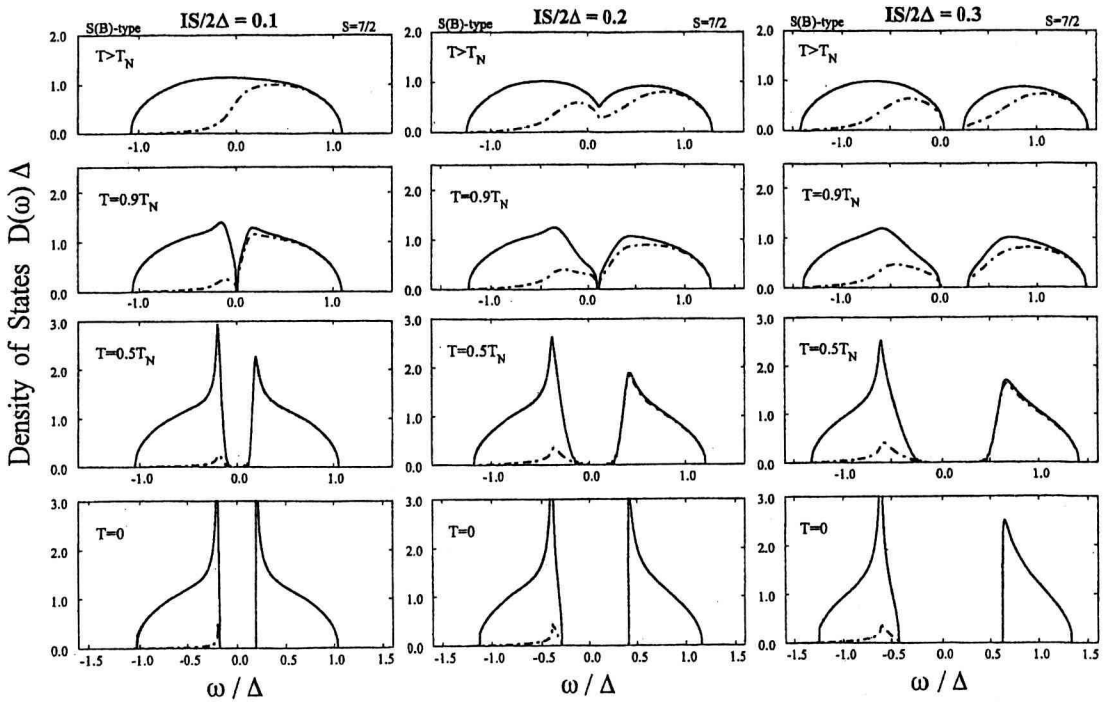


Figure 7: Same as Fig. 1, but for an S(B)-type antiferromagnetic semiconductor with $S = 7/2$. The solid line represents $D(\omega)\Delta$, the dotted line represents $D_a(\omega)\Delta$, rather than $D_p(\omega)\Delta$.

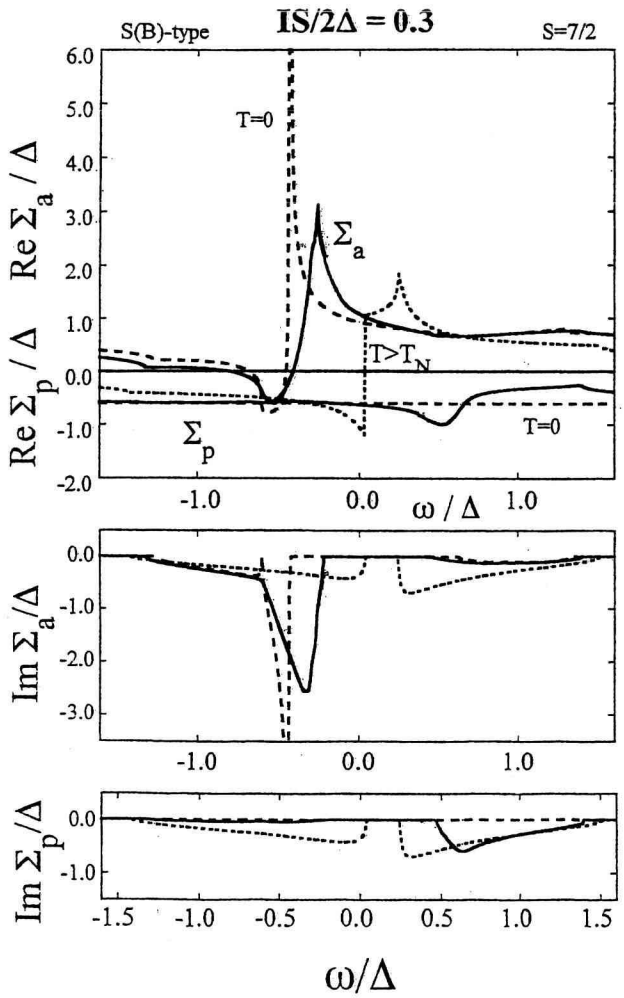


Figure 8: Same as Fig. 2, but for an S(B)-type antiferromagnetic semiconductor of $S = 7/2$ with $IS/2\Delta = 0.3$. (Note the difference in the scale of the vertical line.)

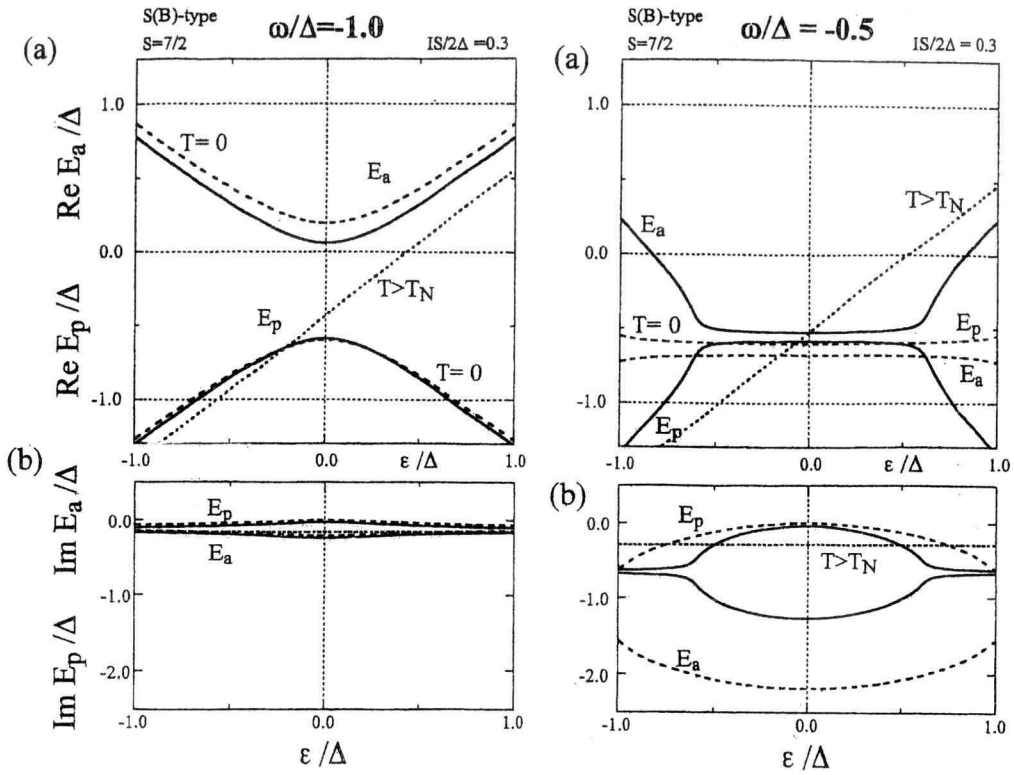


Figure 9: Same as Fig. 3, but for an S(B)-type antiferromagnetic semiconductor of $S = 7/2$ with $IS/2\Delta = 0.3$. (Note the difference in the scale of the vertical line.)

$$D(\omega)\Delta = \frac{4}{\pi}\left(\frac{\Delta}{\omega}\right)^2\left[\left(\frac{\omega}{\Delta}\right)^2+\left(\frac{IS}{\Delta}\right)^2\right]\left\{1-\left(\frac{\Delta}{\omega}\right)^2\left[\left(\frac{IS}{\Delta}\right)^2-\left(\frac{\omega}{\Delta}\right)^2\right]^2\right\}^{1/2}, \quad (3.\ 2)$$

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. (3. 2) in this paper.) Comparing Figs. 1 and 4, 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. The difference is that the S(B)-type has energies ($\omega = \pm IS$) at which the density of states diverge when $T = 0$, while the F-type has no such divergent point.

Since the result for the F-type with a weak exchange strength ($IS/2\Delta = 0.1$) is again similar to that reported in Ref. 1, we briefly discuss here the case of a strong exchange interaction ($IS/2\Delta = 0.3$). We present $\Sigma_p(\omega)$ and $\Sigma_a(\omega)$ in Fig. 5, and $E_p(\omega)$ and $E_a(\omega)$ in Fig. 6. At $T = 0$, $\Sigma_p = -IS$ and $\Sigma_a = +IS$, so that $E_p = [\varepsilon - \sqrt{\varepsilon^2 + \Delta^2}]/2$ and $E_a = [\varepsilon + \sqrt{\varepsilon^2 + \Delta^2}]/2$. On the other hand, at $T \geq T_N$, the present theory gives $\Sigma_p = \Sigma_a = \Sigma_{\rm CPA}$, and $E_p = E_a = \varepsilon + \Sigma_{\rm CPA}$. Comparing Fig. 5 with Fig. 2, at $T = 0.5T_N$, the peak in $|{\rm Im}\Sigma_a|$ ($|{\rm Im}\Sigma_p|$) is large and sharp, and furthermore, $|{\rm Re}\Sigma_a|$ ($|{\rm Re}\Sigma_p|$) varies rapidly near the energies of the peak. The energy of the peak approaches $\pm IS$ as $T \to 0$. The effective potential that an $s$ electron is subjected to in the F-type is larger than that in the S(B)-type in the antiferromagnetic temperature region ($T_N > T \geq 0$). The reason why the $s$ electron is strongly disturbed due to the thermal fluctuation of $f$ spins is because the electron can transfer both between similar sublattice sites and between different sublattice sites. Figure 6 shows that $|{\rm Im}E_a|$ at $\omega/\Delta = -0.5$ (see the right-hand side in Fig. 6) is rather larger than that at $\omega/\Delta = -1.0$. This also suggests that A-states (P-states) in a lower-energy subband (higher-energy subband) are strongly influenced by the thermally fluctuating $f$ spins accompanying the magnetization in the opposite orientation for different sublattices.

### 3.3 Effect of quantum spins

Thus far, we have discussed the conduction-electron state in an antiferromagnetic semiconductor, assuming a classical spin for the $f$ spin. Here, we investigate how the quantum effect of the $f$ spins modifies the $s$ electron interacting with antiferromagnetically ordered $f$ spins through the $s$-$f$ exchange interaction. As long as the $f$ spin is treated as a classical spin, we have $D(\omega) = D(-\omega)$. For a finite magnitude of $f$ spin, however, $D(\omega) \neq D(-\omega)$ in general. 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 $\Sigma_p$ and $\Sigma_a$ [see Eqs. (2), (2) and (2. 13) ]. 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 $\Sigma_a$ 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. (2. 8).

The results for an S(B)-type antiferromagnetic semiconductor with $S = \frac{7}{2}$ are presented in Figs. 7-9. The values of $< S_z >_{\mathrm{av}} /S$, calculated by applying the molecular field approximation for $S = \frac{7}{2}$, are 0.0, 0.44, 0.87, and 1.0 for $T \geq T_N$, $T = 0.9T_N, 0.5T_N$, and 0, respectively. The density of states shown in Fig. 7 is asymmetrical or $D(\omega) \neq D(-\omega)$, as a consequence of the quantum $f$ spin; The total number of states in the lower-energy subband is greater than that of the higher-energy subband. Even at $T = 0$, there is no divergent point in the density of states, unlike that of the S(B)-type with classical spin. At $T = 0$, the density of states for the A-state, $D_a(\omega)$, has a small peak near the energy of $\omega = -IS$ in the lower-energy subband. The incorporation rate of the A-state into the lower-energy subband depends on the temperature and/or the exchange strength.

Figure 8 shows the result for $\Sigma_p(\omega)$ and $\Sigma_a(\omega)$ for $IS/\Delta = 0.3$. Comparing Fig. 8 with Fig. 2, the effect of the quantum spin appears strikingly on $\Sigma_a$ at $\omega \leq 0$ with the decrease in $T$. At $T = 0$, $|\mathrm{Im}\Sigma_a|$ exhibits a sharp peak accompanied with a large change in $|\mathrm{Re}\Sigma_a|$, as a result of the spin-flip scattering of an $s$ electron due to the $s$-$f$ exchange interaction by the complete antiferromagnetic ordering of $f$ spins. The results for $E_p(\varepsilon)$ and $E_a(\varepsilon)$ are shown in Fig. 9 for $\omega/\Delta = -1.0$ (the left-hand side) and $\omega/\Delta = -0.5$ (the right-hand side). Comparing Fig. 9 with Fig. 3, both results for $\omega/\Delta = -1.0$ are similar, while the results for $\omega/\Delta = -0.5$ are very different. The large values of $|\mathrm{Im}E_a(\varepsilon)|$ and the strong modification in $|\mathrm{Re}E_a(\varepsilon)|$ at $\omega/\Delta = -0.5$ result from the fact that not only the thermal fluctuation of $f$ spins but also the quantum fluctuation enhances the exchange scattering of an electron in the A -state, particularly near the top of the lower-energy subband at antiferromagnetic temperatures ($T_N > T \geq 0$).

## 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 $2 \times 2$ sublattice Bloch function representation [7, 8, 9]. 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. The present study reveals how the conduction electron state is affected by the antiferromagnetic ordering of $f$ spins for a wide range of exchange strengths and temperatures.

In this paper, however, we did not present the numerical result for the F-type antiferromagnetic semiconductor with quantum $f$ spins because of the poorer convergence during the iteration process. Furthermore, throughout this study, calculation was performed only for the model density of states of semicircular 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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