

Improved Effective-Medium Approach to the s - f Model in Antiferromagnetic Semiconductors

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Abstract

Improving the effective-medium approach for the s - f model in antiferromagnetic semiconductors, we calculate the density of states using the corrected Green function in the 2×2 sublattice Bloch function representation. The present results with classical spin at $T = 0$ and $T \geq T_N$ agree with that obtained by Takahashi (1997). The present approach is expected to be applicable for a wide range of exchange interaction strength and temperature; Further, the quantum effect in the band of antiferromagnetic semiconductors is discussed.

1 Introduction

In the case of antiferromagnetic semiconductors, the spontaneous magnetization develops in the opposite orientations for different sublattices below the Néel temperature (T_N). Here we assume that magnetic moments (hereafter referred to as f spins) are situated regularly on two interpenetrating ferromagnetic sublattice A and B . We take the $+z$ direction as the orientation of spontaneous magnetization of the f spin at the sites of A sublattice and we assume that no external field is applied. 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 $\langle S_z^B \rangle_{av}$ ($= -\langle S_z \rangle_{av}$), where $\langle \rangle_{av}$ represents a thermal average.

When a single electron (hereafter referred to as an s electron) is injected into an otherwise empty conduction band, it moves in the crystal while interacting with f spins through the s - f exchange interaction. This situation can be described well by the s - f exchange model. [1, 2, 3] In this model, the total Hamiltonian H_t consists of H_s , H_f , and H_{sf} ; H_s stands for the translational energy of an s electron, H_f for the Heisenberg exchange interaction between f spins, and H_{sf} for the s - f exchange interaction between an s electron and f spins. In this work, H_f represents antiferromagnetic ordering between f spins. The situation and notation used in this work are the same as that used in the previous study by Takahashi. [4]

When spontaneous magnetization arises, the effective potential due to s - f exchange interaction to which an s electron is subjected at each site differs according to the orientation (i.e., \uparrow or \downarrow) of the electron spin and to sublattice species (i.e., A and B) of the site. In the mean-field approach (the "Zener model"), the effective potentials to which s electrons with up spin are subjected are assumed to be $-I \langle S_z \rangle_{av}$ for A sublattice sites and $+I \langle S_z \rangle_{av}$ for B sublattice sites; no spin flip process is taken into account. The energy of a conduction electron with up spin is

$$\varepsilon(k, \uparrow) = \varepsilon_1(k) \pm \sqrt{|\varepsilon_2(k)|^2 + (I \langle S_z \rangle_{av})^2}, \quad (1)$$

where $\varepsilon_1(k) [= \varepsilon^{AA}(k) = \varepsilon^{BB}(k)]$ 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. Each of the energy levels $\varepsilon(k, \uparrow)$ and $\varepsilon(k, \downarrow)$ is spin degenerate, at least as long as no external field is applied. Because the mean-field approach gives the energy $\varepsilon(k, \uparrow) = \varepsilon_1(k, \uparrow) \pm \varepsilon_2(k, \uparrow)$ at $T > T_N$ and $\varepsilon(k, \uparrow) = \varepsilon_1(k, \uparrow) \pm \sqrt{|\varepsilon_2(k, \uparrow)|^2 + (IS)^2}$ at $T = 0$, the mean-field theory cannot explain a magnetic blueshift observed in antiferromagnetic semiconductors. This discrepancy was first pointed out by von der Linden and Nolting [5]; they insisted that a drastic shift of lower conduction band edge compared to the free band position (or paramagnetic preshift) occurs at $T > T_N$, and presented the many body approach to take into account dynamic spin flip processes.

In the previous work, [4] introducing the effective-medium for a (test) electron in an antimagnetic semiconductor, Takahashi estimated the energy eigenvalues for the reference Hamiltonian by using the condition similar to the coherent potential approximation (CPA) for the self-energy. Further, assuming the orthogonality of the eigenfunctions of the reference Hamiltonian, Takahashi studied the temperature dependence of the density of states, and the calculated the energy of the band at $T \geq T_N$ and $T =$ as a function of exchange strength to explain magnetic redshift and/or blue shift of the optical absorption edge observed in Eu-chalcogenides consistently. However, the method developed by Takahashi is not applicable for the case of a strong exchange interaction at the temperature of $0 < T < T_N$. Assuming the orthogonality between the eigen functions of reference Hamiltonian may cause this difficulty; when the reference Hamiltonian is not Hermitian, the assumption is not suitable.

The aim of the study is to devise an improved theory for the s - f model in antiferromagnetic semiconductors that is applicable to wide range of exchange interaction strength and temperature. For the purpose, improving the effective-medium approach we present a new method to calculate the reference Green function directly without using the false assumption of orthogonality.

2 Basic Consideration

Since the situation we treat is equivalent to the previous study,[4] here we mention briefly an effective medium approach. Complex potentials Σ_p (Σ_a) is prepared as a short-range potential to which an s electron is subjected when the orientation of its spin is parallel (antiparallel) to the orientation of spontaneous magnetic moment at that site. The (unperturbed) reference Hamiltonian K for the electron is

$$K = \sum_{m,n,\mu} \varepsilon_{mn} a_{m\mu}^\dagger a_{n\mu} + \sum_{m,\mu} \Sigma(m, \mu) a_{m\mu}^\dagger a_{m\mu}, \quad (2)$$

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). Since K includes no spin-flip term, the orientation of the spin of an electron moving in the effective medium remains unchanged. Furthermore, the formula is symmetric for both \uparrow and \downarrow spins as long as no magnetic field is applied.

The Bloch electron states with a wave vector k , $|Ak, \uparrow\rangle$ and $|Bk, \uparrow\rangle$, are related to the Wannier states on the $Am(Bm)$ site of the A(B) sublattice $|Am(Bm), \uparrow\rangle$ as

$$|Ak(Bk), \uparrow\rangle = \sqrt{\frac{2}{N}} \sum_{Am(Bm)} e^{ik \cdot m} |Am(Bm), \uparrow\rangle. \quad (3)$$

Note that the number of each sublattice is $N/2$, and so these functions satisfy the orthonormalities each other.

In the Bloch representation, K is given by the 2×2 matrix;

$$\begin{aligned} K &= \begin{pmatrix} \langle Ak, \uparrow | K | Ak, \uparrow \rangle & \langle Ak, \uparrow | K | Bk, \uparrow \rangle \\ \langle Bk, \uparrow | K | Ak, \uparrow \rangle & \langle Bk, \uparrow | K | Bk, \uparrow \rangle \end{pmatrix}, \\ &= \begin{pmatrix} \varepsilon_1(k) + \Sigma_p & \varepsilon_2(k) \\ \varepsilon_2(k) & \varepsilon_1(k) + \Sigma_a \end{pmatrix}. \end{aligned} \quad (4)$$

Thus, the matrix element of unperturbed propagator P is given by

$$P \equiv (\omega 1 - K)^{-1}, \quad (5)$$

$$= \frac{1}{D} \begin{pmatrix} \omega - (\varepsilon_1(k) + \Sigma_a) & \varepsilon_2(k) \\ \varepsilon_2(k) & \omega - (\varepsilon_1(k) + \Sigma_p) \end{pmatrix}, \quad (6)$$

where

$$D = [\omega - (\varepsilon_1(k) + \Sigma_a)][\omega - (\varepsilon_1(k) + \Sigma_p)] - \varepsilon_2(k)^2, \quad (7)$$

$$= (\omega - E_p)(\omega - E_a), \quad (8)$$

with

$$E_p = \frac{2\varepsilon_1(k) + \Sigma_p + \Sigma_a - \sqrt{4\varepsilon_2(k)^2 + (\Sigma_p - \Sigma_a)^2}}{2}, \quad (9)$$

$$E_a = \frac{2\varepsilon_1(k) + \Sigma_p + \Sigma_a + \sqrt{4\varepsilon_2(k)^2 + (\Sigma_p - \Sigma_a)^2}}{2}. \quad (10)$$

Note that E_p and E_a are generally complex, and equal to the energy eigenvalues of K .

We need the diagonal matrix elements of P in the Wannier representation, or $F_\uparrow(\omega) \equiv \langle Am \uparrow | P | Am \uparrow \rangle = \langle Bm \downarrow | P | Bm \downarrow \rangle$ and $F_\downarrow(\omega) \equiv \langle Am \downarrow | P | Am \downarrow \rangle = \langle Bm \uparrow | P | Bm \uparrow \rangle$ (independent of m). In the previous work, [4] Takahashi first calculated the energy eigenvalues of E_p and E_a and two eigenfunctions by solving the secular equation; The eigenfunction which belongs to E_p (E_a) is mainly composed of the Wannier states in which the orientation of the spin is parallel (antiparallel) to the orientation of the spontaneous magnetic moment at each site. Then, assuming the orthogonalization of two eigenfunctions, Takahashi calculated $F_\uparrow(\omega)$ and $F_\downarrow(\omega)$. However, the method previously presented by Takahashi is not suitable, because two eigenfunctions are not orthogonal each other when K is not Hermitian. In result, Takahashi failed to calculate the density of states for the case of strong exchange interaction as $|\frac{IS}{\Delta}| > 0.2$ at finite temperatures.

In this work, we calculate $F_\uparrow(\omega)$ and $F_\downarrow(\omega)$ directly using the matrix element of P shown in Eq. (6);

$$F_\uparrow(\omega) \equiv \langle Am \uparrow | P | Am \uparrow \rangle (= \langle Bm \downarrow | P | Bm \downarrow \rangle), \quad (11)$$

$$= \sum_{Ak} \langle Am \uparrow | Ak \uparrow \rangle \langle Ak \uparrow | P | Ak \uparrow \rangle \langle Ak \uparrow | Am \uparrow \rangle, \quad (12)$$

$$= \frac{2}{N} \sum_{Ak} \frac{\omega - (\varepsilon_1(k) + \Sigma_a)}{(\omega - E_p)(\omega - E_a)}, \quad (13)$$

$$= \frac{2}{N} \sum_{Ak} \left(\frac{\eta_A}{\omega - E_p} + \frac{\eta_B}{\omega - E_a} \right), \quad (14)$$

with

$$\eta_A = \frac{\varepsilon_1(k) + \Sigma_a - E_p}{E_a - E_p}, \quad (15)$$

$$\eta_B = \frac{\varepsilon_1(k) + \Sigma_a - E_a}{E_p - E_a}, \quad (16)$$

and

$$F_{\downarrow}(\omega) \equiv \langle Am \downarrow | P | Am \downarrow \rangle (= \langle Bm \uparrow | P | Bm \uparrow \rangle) \quad (17)$$

$$= \frac{2}{N} \sum_{Ak} \left(\frac{\eta_B}{\omega - E_p} + \frac{\eta_A}{\omega - E_a} \right). \quad (18)$$

Note that $\eta_A + \eta_B = 1$. When we define $F_p(\omega)$ and $F_a(\omega)$ by

$$F_p(\omega) = \frac{2}{N} \sum_{Ak} \frac{1}{\omega - E_p}, \quad (19)$$

$$F_a(\omega) = \frac{2}{N} \sum_{Ak} \frac{1}{\omega - E_a}, \quad (20)$$

then

$$F_{\uparrow}(\omega) + F_{\downarrow}(\omega) = F_p(\omega) + F_a(\omega) \quad (21)$$

Next, we introduce the semicircular band with a half bandwidth of Δ ,

$$\rho(\varepsilon) = \frac{2}{\pi\Delta} \sqrt{1 - \left(\frac{\varepsilon}{\Delta}\right)^2} \quad (22)$$

as an undisturbed (model) density of states (i.e., for $IS = 0$); In order to replace the summation over k within the Brillouin zone by the integral of ε using $\rho(\varepsilon)$, we need the relation between ε and the Bloch energy [or $\varepsilon_1(k)$ and $\varepsilon_2(k)$]. It is not so easy to specify a simple relation 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. (22) is not related to a specific tight-binding system. In this work we proceed to calculate for two cases assumed following. (i) 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) When the electron transfer between similar sublattice site $\varepsilon_1(k)$ contributes to ε as much as that between different sublattice site $\varepsilon_2(k)$, we set $\varepsilon_1(k) \rightarrow \varepsilon/2$ and $\varepsilon_2(k) \rightarrow \varepsilon/2$. (In the previous paper [4] Takahashi called the above assortment sc (bcc) structure and/or fcc structure, but it may cause a misunderstanding.)

Further, we calculate $F_{\uparrow}(\omega)$ and $F_{\downarrow}(\omega)$ by

$$F_{\uparrow}(\omega) = 2 \int_{-\Delta}^0 d\varepsilon \rho(\varepsilon) \frac{\eta_A}{\omega - E_p(\varepsilon)} + 2 \int_0^{\Delta} d\varepsilon \rho(\varepsilon) \frac{\eta_B}{\omega - E_a(\varepsilon)}, \quad (23)$$

$$F_{\downarrow}(\omega) = 2 \int_{-\Delta}^0 d\varepsilon \rho(\varepsilon) \frac{\eta_B}{\omega - E_p(\varepsilon)} + 2 \int_0^{\Delta} d\varepsilon \rho(\varepsilon) \frac{\eta_A}{\omega - E_a(\varepsilon)}. \quad (24)$$

Using the single-site approximation using the t matrix formula, [3] together with $F_{\uparrow}(\omega)$ and $F_{\downarrow}(\omega)$ defined above, we can calculate the density of states in antiferromagnetic semiconductors.

In the above expressions, the difference of the present approach with the previous one by Takahashi is just replacing $|c_A|^2$ and $|c_B|^2$ [defined by Eqs. (2.21) and (2.22) in the previous paper [4]] by η_A and η_B defined by Eqs. (15) and (16), respectively. We should emphasize that in this work we do not use the assumption of the orthogonalization between two eigenfunctions which belongs to energy eigenvalues E_p and E_a ; the assumption caused unreasonable result for strong exchange interaction at the temperature region as $0 < T < T_N$ in the previous work. The present approach improves the unreasonable previous result considerably, as shown in following sections.

3 Result and Discussion

First, the present result at paramagnetic temperature ($T \geq T_N$) agrees with that obtained using the CPA.[6]

Next, the present approach with classical spin at $T = 0$ reproduces the previous result; [4] this is because thermal and quantum fluctuation of f is absent in this situation. Thus, we have the following density of states with classical spins at $T = 0$ for two cases discussed before:

(i) When we set $\varepsilon_1(k) \rightarrow 0$ and $\varepsilon_2(k) \rightarrow \varepsilon$ because the nearest neighbors of each atom are from the other sublattice;

$$D(\omega)\Delta = \frac{4|\omega|}{\pi\Delta} \left\{ \frac{\Delta^2 + (IS)^2 - \omega^2}{\omega^2 - (IS)^2} \right\}^{\frac{1}{2}}. \quad (25)$$

for $IS < |\omega| < \sqrt{\Delta^2 + (IS)^2}$ and 0 otherwise.

(ii) When we set $\varepsilon_1(k) \rightarrow \varepsilon/2$ and $\varepsilon_2(k) \rightarrow \varepsilon/2$ because the electron transfer between similar sublattice site $\varepsilon_1(k)$ contributes to ε as much as that between different sublattice site $\varepsilon_2(k)$;

$$D(\omega)\Delta = \frac{4}{\pi} \left(\frac{\Delta}{\omega} \right)^2 \left[\left(\frac{\omega}{\Delta} \right)^2 + \left(\frac{IS}{\Delta} \right)^2 \right] \left\{ 1 - \left(\frac{\Delta}{\omega} \right)^2 \left[\left(\frac{IS}{\Delta} \right)^2 - \left(\frac{\omega}{\Delta} \right)^2 \right] \right\}^{1/2}. \quad (26)$$

for $IS < |\omega| < [\Delta + \sqrt{\Delta^2 + 4(IS)^2}]/2$ and 0 otherwise.

As long as we treated f spin as classical spin, we have $D(\omega) = D(-\omega)$. However, for a finite magnitude of f spin, $D(\omega) \neq D(-\omega)$ in general. When $T = 0$, we have the coherent potentials $\Sigma_p = -IS$, and $\Sigma_a = IS(1 + IF_\uparrow)/(1 - IF_\uparrow)$ with $F_\uparrow = 2[\omega - IS - \{(\omega - IS)^2 - \Delta^2\}^{1/2}]/\Delta^2$.

For further consideration, we need numerical calculation. The calculation is now in progress.

References

- [1] P. Wachter, in *Handbook on the Physics and Chemistry of Rare Earths*, edited by K. A. Gschneider, Jr. and L. Eyring (North-Holland, Amsterdam, 1979), p. 507.
- [2] W. Nolting, S. Mathi Jaya, and S. Rex, *Phys. Rev. B* **54**, 14455 (1996).
- [3] M. Takahashi and K. Mitsui, *Phys. Rev. B* **54**, 11298 (1996).
- [4] M. Takahashi, *Phys. Rev. B* **55**, 6950 (1997).
- [5] W. von der Linden and W. Nolting, *Z. Phys. B* **48**, 191 (1982).
- [6] A. Rangette, A. Yanase, and J. Kübler, *Solid State Commun.* **12**, 171 (1973).