Exchange-induced band splitting in diluted magnetic semiconductors under a weak magnetic field

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Abstract

The extended electron (hole) state in diluted magnetic semiconductors (DMS) like as $A^{II}_{1-x}Mn_xC^{VI}$ alloys is studied theoretically. Appling the dynamical coherent potential approximation (DCPA) to the model we proposed previously, we formulate the expression for the band edge energy of DMS with under a weak magnetic field. The results are compared with the abrormal x dependence in *p-d* exchange integral $N_0\beta$ that is observed in $Zn_{1-x}Mn_xTe$ and $Cd_{1-x}Mn_xTe$.

Key Word: diluted magnetic semiconductor (DMS), *sp-d* exchange interaction, coherent potential approximation (CPA)

1 Introduction

In the previous publications, applying the single site approximation [1] to the new model which was proposed for diluted magnetic semiconductors (DMS) such type alloys as $A^{II}_{1-x}Mn_xC^{VI}$ [2], we explained consistently the bowing effect [3] and anomalous x dependence of apparent exchange integral $N_0\beta$ [4] experimentally observed in $Cd_{1-x}Mn_xS$. In this work, extending the previous method we intend to explain an anomalous x dependence of the *p-d* exchange integral $N_0\beta$, experimentally observed in $Zn_{1-x}Mn_xTe$ [5] and $Cd_{1-x}Mn_xTe$ [6, 7].

First we summarize the experimental data briefly. Usually the values of the exchange integral in DMSs are estimated based on the virtual crystal approximation (VCA). In standard VCA, the energy splitting between σ^+ and σ^- transition of A exciton in DMS is given as

$$\Delta E = N_0(\alpha - \beta)x < S_z >, \qquad (1)$$

where $N_0\alpha$ and $N_0\beta$ are the exchange constants for conduction electrons and valence electrons, respectively, and $< S_z >$ is the thermally averaged value of the d spin operator S_z on Mn^{2+} ions.

In the cases of $Zn_{1-x}Mn_xTe$ [5], the curves of the splitting ΔE as a function of $|x < S_z > |$ are found to be roughly linear, but the slope is drastically reduced at high x values. In Table 1, the experimental observed results of $N_0(\alpha-\beta)$ and $N_0\beta$ in $Zn_{1-x}Mn_xTe$ are presented for various values of x; the values of $N_0\beta$ are estimated assuming $N_0\alpha = 0.18$ eV. Further, the x dependence of $N_0\beta$ is depicted in Fig. 1. In the cases of $Cd_{1-x}Mn_xTe$ [6], the x dependence of the exchange integral is more complicated as shown in Table 2 and Fig. 2.

The above-mentioned observation cannot be explained by the standard VCA, because the VCA predicts that the slope of ΔE vs. $|x < S_z > |$ is independent of x. This may be explained by taking the multiple scattering into consideration. It should be emphasized that the exchange integrals are estimated based on the experimental observation under

Table 1: $Zn_{1-x}Mn_xTe$

(Lascaray *et. al.* PRB 35, 675, 1987)

x		0.25	0.45	0.55	0.60	0.71
$N_0(\alpha-\beta)$	(eV)	1.13	0.94	0.64	0.54	0.39
$N_0\beta$	(eV)	-0.95	-0.76	-0.46	-0.36	-0.21

($N_0\alpha = 0.18$ eV)

a weak magnetic field (or with a weak magnetization). In the next section, we formulate the single site approximation approach for a DMS with a weak magnetization $< S_z >$.

2 Basic Consideration

Applying the single site approximation to our model leads to the condition for the complex effective potentials (coherent potentials) $\Sigma_\uparrow$ and $\Sigma_\downarrow$:

$$(1-x)t^A_{\uparrow\uparrow} + x < t^M_{\uparrow\uparrow} > \;=\; 0. \qquad (2)$$

Here, $(1-x)$ and x are the mole fraction of A (i.e., Cd or Zn) and Mn atoms respectively. The t matrix for an A atom with chemical potential E_A embedded in the effective medium is given by

$$t^A_{\uparrow\uparrow} \;=\; \frac{E_A - \Sigma_\uparrow}{1-(E_A-\Sigma_\uparrow)F_\uparrow}. \qquad (3)$$

The t matrix for an Mn atom with chemical potential E_M and localized d spin operator $S \equiv (S_x, S_y, S_z)$ embedded in the effective medium is given by [1]

$$t^M_{\uparrow\uparrow} \;=\; \frac{V_\uparrow + F_\downarrow(W_\uparrow - V_\uparrow U_\downarrow)}{1 - F_\downarrow U_\downarrow - F_\uparrow[V_\uparrow + F_\downarrow(W_\uparrow - V_\uparrow U_\downarrow)]} \qquad (4)$$

where in the classical spin limit

$$U_\uparrow \;\approx\; V_\uparrow = -IS_z - \Sigma_\uparrow + E_M\ , \qquad (5)$$

$$U_\downarrow \;\approx\; V_\downarrow = +IS_z - \Sigma_\downarrow + E_M\ , \qquad (6)$$

$$W_\uparrow \;=\; I^2 S_- S_+ \approx I^2[S(S+1) - S_z^2] \qquad (7)$$

$$W_\uparrow - V_\uparrow U_\downarrow \;\approx\; (IS)^2 + (IS_z)(\Sigma_\uparrow - \Sigma_\downarrow) - (\Sigma_\uparrow - E_M)(\Sigma_\downarrow - E_M)\ . \qquad (8)$$

Since we treat the case of a weak magnetization in this work, we assume further approximations in the expression of t matrix for simplification:

$$F \;=\; F_\uparrow = F_\downarrow\ , \qquad (9)$$

$$\Sigma \;=\; \Sigma_\uparrow = \Sigma_\downarrow\ , \qquad (10)$$

thus,

$$W_\uparrow - V_\uparrow U_\downarrow \;\approx (IS)^2 - (\Sigma - E_M)^2 \qquad (11)$$

Accordingly, Eq. (2) leads to

$$(1-x)\frac{E_A - \Sigma}{1-(E_A-\Sigma)F} + x\frac{-I < S_z > -\Sigma + E_M + F[(IS)^2 - (E_M-\Sigma)^2]}{1 - 2F(E_M-\Sigma) - F^2[(IS)^2 - (E_M-\Sigma)^2]} = 0. \qquad (12)$$

That is,

Subtracting Eq.(??)-Eq.(??) leads to

$$(\Sigma_p - \Sigma_a) = \frac{2xI < S_z >}{\left(1+\frac{2E_M}{\Delta}\right)^2 - (\frac{2IS}{\Delta})^2 + \frac{2E_M}{\Delta}x} \qquad (13)$$

Eq. (13) is the equation we are asking.

3 Results and Discussion

Eq. (13)shows that exchange splitting $\Delta E = (\Sigma_p - \Sigma_a)$ is proportional to $2xI < S_z >$, but the coefficient is not constant but the function of x. The result may explain the experimental observation that the slope of $(\Sigma_p - \Sigma_a)$ vs. $x < S_z >$ is drastically reduced at high x values.

However, we don't think the present result also explains the increase of the slope at low x values. The caution may be ascribed to the behavior of $N_0\alpha$ rather than $N_0\beta$. Furthermore, the roll of offset energy E_M is not clear; $E_M = 0.53$eV for $Zn_{1-x}Mn_xTe$ and $E_M = 0.44$eV for $Cd_{1-x}Mn_xTe$. the difference in E_M may explain the deference between $Zn_{1-x}Mn_xTe$ and $Cd_{1-x}Mn_xTe$. These are the coming theme to be investigated.

References

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Table 2: $Cd_{1-x}Mn_xTe$

(Lascaray *et. al.* PRB 38, 7602, 1988)

x		0.09	0.14	0.25	0.39	0.67	0.73
$N_0(\alpha-\beta)$	(eV)	1.07	1.13	1.22	1.32	0.67	0.46
$N_0\beta$	(eV)	-0.85	-0.91	-1.00	-1.10	-0.45	-0.24

($N_0\alpha = 0.22$ eV)

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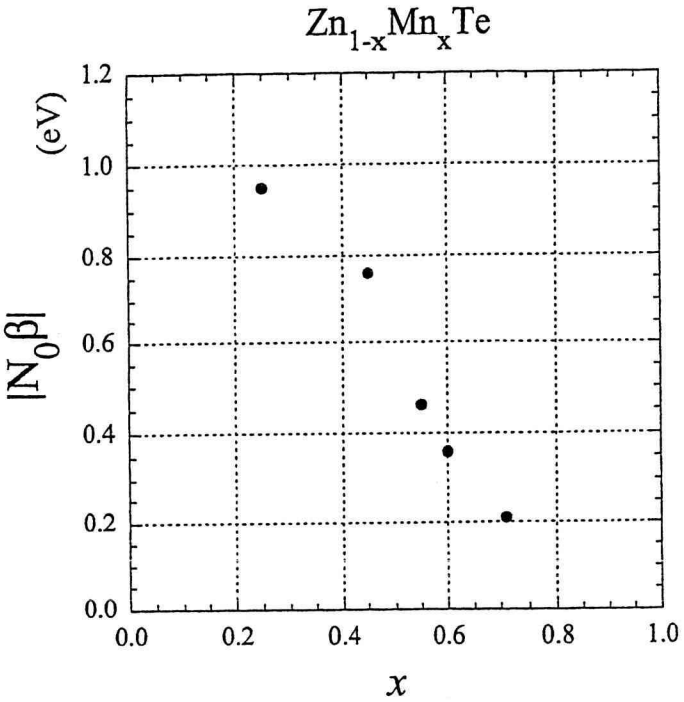

Figure 1: $N_0\beta$ in $Zn_{1-x}Mn_xTe$ as a function of Mn mole concentration x

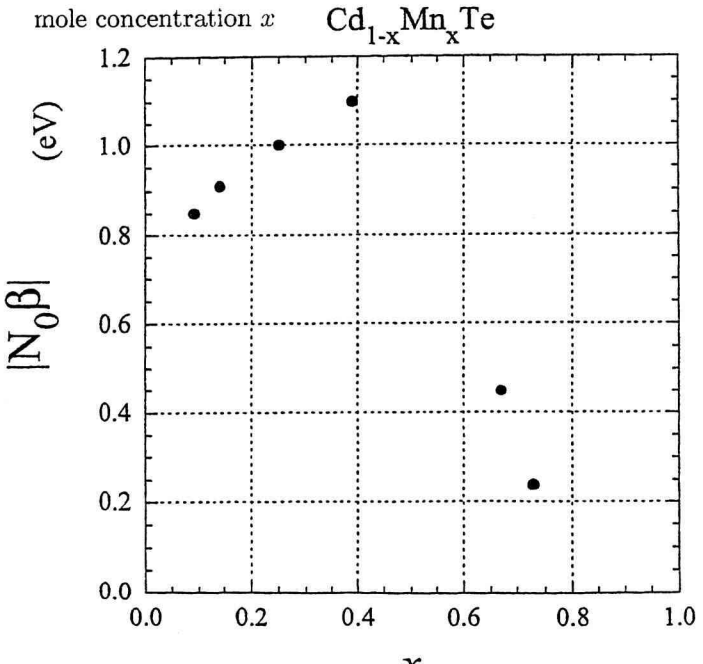

Figure 2: $N_0\beta$ in $Cd_{1-x}Mn_xTe$ as a function of Mn mole concentration x