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Abstract. The indirect exchange interaction between localized magnetic moments embedded in II–VI semiconductor hosts is theoretically studied. Based on realistic LCAO bands, the indirect exchange is calculated by the perturbation theory. In evaluating the second-order energy shift, a modified linear analytic tetrahedron method is used to perform the double Brillouin zone integration. From our results, two qualitative conclusions are reached. First, the indirect exchange is usually antiferromagnetic for the nearest few neighbours, becoming ferromagnetic as the distance between magnetic ions is increased. Second, the intrinsic cubic symmetry of the semiconductor host could induce strong directional dependence of the indirect exchange, and the sphericalization of the matrix element in the Brillouin zone might affect substantially the numerical accuracy of the calculated exchange coupling constant even when the band energy is essentially isotropic.

1. Introduction

Recently there has been considerable interest in the magnetic properties of semiconductors containing a few percent of magnetic ions [1–12]. For these diluted magnetic semiconductors (DMS) which crystallize in the structure of the non-magnetic semiconductor host (e.g. zinc-blende for $Cd_{1-x}Mn_xTe$), experimental results have shown evidence of an antiferromagnetic interaction between Mn^{2+} local moments. In the high-temperature limit, the behaviour of the magnetic susceptibility can be described rather well by the Curie–Weiss law with a negative paramagnetic Curie–Weiss temperature. In DMS, the magnetic interaction may be mediated by the spin polarization of valence band electrons due to their exchange interaction with separated local magnetic moments. The spin-polarized Bloch electrons will then cause an indirect interaction between two magnetic ions, the so-called indirect exchange interaction. The indirect exchange interaction is the complete analogue of the Ruderman–Kittel–Kasuya–Yosida (RKKY) interaction [13–15] in magnetic alloys. However, while intraband processes are involved in polarizing conduction electrons in the RKKY interaction, the polarization of valence band electrons in a semiconductor proceeds via interband electron–hole excitations.

The properties of the indirect exchange interaction have been studied in several model calculations [16–23]. However, most authors have assumed parabolic energy

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bands and a constant interband exchange matrix element. These assumptions are valid only in the immediate vicinity of band edges. As the polarization process involves interband transitions throughout the entire Brillouin zone (BZ), one may question the validity of the results which are based on the band edge structure alone. In addition, for direct gap semiconductors, the conduction and valence band edges are of different symmetry; while one is atomic s-like, the other is p-like. Hence the two band edge states are not coupled by the isotropic Coulomb interaction. The interband exchange matrix element exists only when the conduction band state contains both s and p components when away from the Γ point. Therefore a very important factor affecting the indirect exchange in DMS is the s–p mixing of bands, which is strong only in regions of the BZ distant from the Γ point.

In our previous works, the symmetry mixing of bands has been included and the band structures calculated via the $k \cdot p$ as well as semiempirical LCAO (linear combination of atomic orbitals) method have been used to study the indirect exchange interaction in a series of II–VI direct gap semiconductors, europium oxide and europium chalcogenides [24-27]. We show that the indirect exchange in DMS consists of two competing components, one ferromagnetic and one antiferromagnetic, mediated by electrons occupying different valence bands. While a pair of non-interacting bands makes an antiferromagnetic contribution, two bands which have local symmetry mixing with each other (e.g. s–p mixing) contribute a net ferromagnetic interaction. For interspin distance equal to the next nearest neighbour cation separation (R_0) and beyond, the antiferromagnetic part usually dominates the ferromagnetic one. Based on the above argument, phenomenological models have been proposed to explain the magnetic properties of some DMS such as $Pb_{1-x}Mn_xTe$ and $Hg_{1-x}Mn_xTe$ [28,29]. However, all of our previous models have employed isotropic band structures simulated only along the $\Gamma-X$ section in the BZ and the BZ is approximated by a sphere with radius $2\pi/R_0$. Under these assumptions, the symmetry of both the band states and the crystal structure is not treated consistently.

In determining the interband contribution to the indirect exchange, two band features are of importance: the energy separation between the initial and the final state, and the symmetry of their wavefunctions. The importance of the energy gap is obvious because it gives the electron–hole excitation energy. The second point needs some elaboration. A Bloch wavefunction has two kinds of symmetry: a translational symmetry characterized by its wave vector k and a local symmetry usually referred to as atomic s- or p-like. As the valence band electrons are polarized by a very localized interaction (i.e. their direct exchange with the local moment d electrons), the local symmetry of the initial and final states determines whether there is an interband exchange coupling between them. Owing to the translational symmetry, the Bloch electron changes its phase from one lattice point to another. Because of this phase change, different interband transitions interfere with each other. Hence it is the combined translational and local symmetries which determine the net contribution from a given valence–conduction band pair.

From the discussion above, it becomes obvious that one needs to know the details of the band structure before determining the nature of the indirect exchange. We have decided to use the semiempirical LCAO method [30] to simulate the band structure of some typical II–VI direct-gap semiconductors. This method is chosen because not only is the local symmetry of a state well represented by an atomic basis set, but also the crystal symmetry is reflected in the LCAO band energy and wavefunctions. By adopting a semiempirical procedure, we further ensure that the energy gaps and the

orbital mixing coefficients obtained are reliable.

With the non-magnetic band structure known, we treat the polarization of the valence band electron due to the Mn^{2+} local spin by the perturbation theory. In evaluating the second-order energy shift of the system, the double BZ integration of wavevectors k and k' for the valence and conduction bands is carried out by a modified linear analytic tetrahedron method [31–39]. In this method, the BZ is divided into a large number of tetrahedra, and the double integration over each pair of tetrahedra is approximated by the product of the integration of the rapidly oscillating phase and the average values of other slowly varying terms, i.e. the interband matrix element and the inverse of band energy difference [38, 39]. The integration of the phase can be calculated analytically and the result depends only on the phase values at the four vertices of the tetrahedron. The average of the inverse of band energy difference can also be integrated analytically once the band energy is linearly interpolated with respect to the energy values at the four vertices of the tetrahedron. With the sampling of finite energy bands near the energy gap region as the only limitation, the variations of both the band energy and band wavefunctions in the realistic BZ are treated explicitly.

2. Band structure

In this section we calculate the non-magnetic band structure of some typical II–VI semiconductors (i.e. CdTe, ZnTe and ZnSe, all with the Γ point band edge and the zinc-blende structure) by the LCAO method. We consider one conduction band generated from the cation ns ($n = 4, 5$ for Zn, Cd, respectively) orbital and three valence bands from the anion three np ($n = 4, 5$ for Se, Te, respectively) orbitals.

Starting from the atomic picture, one may say that bands are formed due to interatomic interactions. Through the nearest-neighbour interaction, a cation atomic orbital may mix with an anion orbital if they have considerable overlap. On the other hand, the next-nearest-neighbours always consist of the same kind of atoms and through their interaction, a cation (anion) orbital only mixes with other cation (anion) orbitals. In general the LCAO wavefunction of a state in the nth band may be expressed as a linear combination of various orbitals as follows.

$$| nk \rangle = \sum_{\mu} C_{\mu}(nk) \, | \mu k \rangle \qquad (2.1)$$

where the LCAO basis function $| \mu k \rangle$ is a Bloch sum of the corresponding atomic orbitals centred either at the cation (or anion) sites, i.e.

$$| \mu k \rangle = N^{-1/2} \sum_{i} e^{ik \cdot R_i} \, | \mu(R_i) \rangle \qquad (2.2)$$

and the μ summation runs over all orbital symmetries which are mixed into a given band.

To obtain quantitatively the energy $E(nk)$ of a band state and the mixing coefficients $C_{\mu}(nk)$, one has to solve the eigenvalue equation

$$\hat{H}(k) \, | nk \rangle = E(nk) \, | nk \rangle \, . \qquad (2.3)$$

The detailed forms of the matrix representation of the crystal Hamiltonian $\hat{H}$ with respect to the LCAO basis functions in (2.1) are worked out by Slater and Koster for

various crystal structures [30]. For reference, we quote the formula for these matrix elements below.

$$\langle \mu' k' \mid \hat{H} \mid \mu k \rangle = \delta_{kk'} \sum_j e^{i k \cdot (R_j + r_\lambda - r_{\lambda'})} E_{\mu' \mu} (lmn)_{\lambda' \lambda} \tag{2.4}$$

where λ denotes the atom in the unit cell (cation or anion in the present case) and $R_j + r_\lambda - r_{\lambda'} = R_0(l\hat{i} + m\hat{j} + n\hat{k})$. Neglecting energy integrals beyond the NNN (cation–cation or anion–anion) interaction, we give in table 1 the matrix representation of the crystal Hamiltonian for the zinc-blende structure and a general k in the BZ. As can be seen, there are eight energy integrals in the Hamiltonian matrix. We choose their values semiempirically to fit several measured energy gap values and also the p valence bandwidth. Our calculated energy band structure agrees with the non-local pseudopotential results [40,41] in their overall features. The fitted values of these energy integrals are given in table 2.

Table 1. LCAO crystal Hamiltonian matrix elements for the zinc-blende structure. The notations are the same as those of reference [30]. Other elements not shown can be obtained by cyclic permutation of $\{\xi, \eta, \zeta\}$ in accord with orbital symmetries $\{x, y, z\}$ of basis functions.

$(x/x) = E_{xx}(000)_{aa} + 4E_{xx}(\frac{1}{2}\frac{1}{2}0)_{aa} \cos \frac{\xi}{2}(\cos \frac{\eta}{2} + \cos \frac{\zeta}{2}) + 4E_{xx}(0\frac{1}{2}\frac{1}{2})_{aa} \cos \frac{\eta}{2} \cos \frac{\zeta}{2}$

$(x/y) = -4E_{xy}(\frac{1}{2}\frac{1}{2}0)_{aa} \sin \frac{\xi}{2} \sin \frac{\eta}{2} - 4iE_{xy}(0\frac{1}{2}\frac{1}{2})_{aa}(\cos \frac{\xi}{2} - \cos \frac{\eta}{2}) \sin \frac{\zeta}{2}$

$(x/s) = 4E_{xs}(\frac{1}{4}\frac{1}{4}\frac{1}{4})_{ac}(-\cos \frac{\xi}{4} \sin \frac{\eta}{4} \sin \frac{\zeta}{4} + i \sin \frac{\xi}{4} \cos \frac{\eta}{4} \cos \frac{\zeta}{4})$

$(s/s) = E_{ss}(000)_{cc} + 4E_{ss}(\frac{1}{2}\frac{1}{2}0)_{cc}(\cos \frac{\xi}{2} \cos \frac{\eta}{2} + \cos \frac{\eta}{2} \cos \frac{\zeta}{2} + \cos \frac{\zeta}{2} \cos \frac{\xi}{2})$

Table 2. Energy integrals (in eV) employed in the LCAO band calculation for CdTe, ZnTe, and ZnSe.

	CdTe	ZnTe	ZnSe
$E_{xx}(000)_{aa}$	−1.143	−1.447	−1.105
$E_{xx}(\frac{1}{2}\frac{1}{2}0)_{aa}$	0.062	0.087	0.018
$E_{xx}(0\frac{1}{2}\frac{1}{2})_{aa}$	0.162	0.188	0.240
$E_{xy}(\frac{1}{2}\frac{1}{2}0)_{aa}$	0.067	0.110	0.092
$E_{xy}(0\frac{1}{2}\frac{1}{2})_{aa}$	−0.115	−0.135	−0.227
$E_{xs}(\frac{1}{4}\frac{1}{4}\frac{1}{4})_{ac}$	1.178	1.171	1.343
$E_{ss}(000)_{cc}$	0.715	0.830	1.606
$E_{ss}(\frac{1}{2}\frac{1}{2}0)_{cc}$	0.073	0.131	0.096

3. Indirect exchange interaction

For a magnetic ion (e.g. Mn^{2+}) well-isolated in a non-magnetic semiconductor host, we may assume that the magnetic electrons are very localized. Since their spins tend to be parallel to each other by Hund's rule, a total spin S_i is now located at the

magnetic ion site R_i. The local spin S_i will magnetically polarize the valence band Bloch electrons through the direct exchange interaction between them, inducing the latter to make virtual interband transitions. The Bloch electrons polarized by S_i will then interact with another local spin S_j located at R_j, thus mediating an effective spin–spin interaction between S_i and S_j.

Let us assume that the exchange interaction between localized magnetic orbitals and Bloch electrons is independent of the magnetic quantum number. Then we may sum up the contribution of each individual magnetic orbital to obtain the exchange interaction of the entire magnetic ion with Bloch electrons, which now depends on the total spin S_i. The exchange interaction between the local spin S_i and Bloch electrons is assumed to take the form

$$\hat{H}_X = -\tfrac{1}{2} \sum_i J(r - R_i) S_i \cdot \sigma \tag{3.1}$$

where σ is the Pauli spin operator of the Bloch electron at position r, and $J(r - R_i)$ is the exchange integral centred at R_i. Because the trace of σ is equal to zero, the first-order energy shift produced by $\hat{H}_X$ vanishes. The second-order energy shift is

$$\Delta E^{(2)} = - \sum_{nk\sigma, n'k'\sigma'} \frac{\langle nk\sigma | \hat{H}_X | n'k'\sigma' \rangle \langle n'k'\sigma' | \hat{H}_X | nk\sigma \rangle}{E(n'k') - E(nk)} f_{nk}(1 - f_{n'k'}) \tag{3.2}$$

where $E(n'k')$ and $E(nk)$ are the energies of the conduction and valence band states $n'k'$ and nk respectively; $f_{n'k'}$ and f_{nk} are the corresponding Fermi distribution functions. The k and the k' summations are confined to the first BZ. For temperatures below 200 K, assuming that valence bands are completely filled and conduction bands completely empty the approximation for wide gap semiconductors is good. Thus the relevant Fermi factor $f_{nk}(1 - f_{n'k'})$ is set to 1.

When the explicit form of $\hat{H}_X$ is substituted in the above formula, $\Delta E^{(2)}$ can be rewritten as an effective S_i, S_j spin interaction:

$$\Delta E^{(2)} = \sum_{\substack{i,j \\ i > j}} \sum_{\alpha,\beta} I_{ij}^{\alpha\beta} S_i^\alpha S_j^\beta \tag{3.3}$$

with

$$I_{ij}^{\alpha\beta} = -\frac{1}{4} \sum_{nk\sigma, n'k'\sigma'} \frac{\langle nk\sigma | J(R_j)\sigma^\beta | n'k'\sigma' \rangle \langle n'k'\sigma' | J(R_i)\sigma^\alpha | nk\sigma \rangle}{E(n'k') - E(nk)} + (i \leftrightarrow j). \tag{3.4}$$

Since self-energy terms (i.e. those with $i = j$) do not concern the magnetic ordering of the material, only $i \neq j$ interacting terms being retained in (3.3).

Owing to the spin–orbit interaction acting on Bloch electrons, the indirect exchange in (3.3) should include various anisotropic contributions, such as the pseudodipolar interaction and the antisymmetric Dzialoshinski–Moriya (DM) interaction [42–44]. If the lack of inversion symmetry for the zinc-blende crystal is neglected, the DM interaction, averaged over the sample, is equal to zero and the resulting indirect exchange contains an isotropic term and a symmetric pseudodipolar term. Our previous calculation [29] shows that, with the spin–orbit interaction included, the antiferromagnetic contribution from the higher valence bands still dominates, but its strength

is reduced by about 20% due to additional orbital mixing between the conduction and the light hole bands by the spin–orbit interaction. The obtained indirect exchange is approximately isotropic to within an error of less than 2% at $R_{ij} = R_0$. The deviation from isotropic behaviour increases with increasing R_{ij} and is estimated to be about 20% at $R_{ij} = 5R_0$. If the effect of the spin–orbit interaction is neglected, the spin and space parts of the band state function are decoupled, i.e. $|nk\sigma\rangle = |nk\rangle \otimes |\sigma\rangle$, thus all terms non-diagonal in α, β vanish, and the energy shift reduces to the isotropic Heisenberg form:

$$\Delta E^{(2)} = \sum_{\substack{i,j \\ i>j}} I(R_{ij})S_i \cdot S_j \tag{3.5}$$

with the indirect exchange coupling constant $I_{ij}^{\alpha\alpha}$ rewritten as

$$I(R_{ij}) = -\frac{1}{2} \sum_{nk,n'k'} \frac{\left|M(n'k',nk)\right|^2 e^{i(k-k')\cdot R_{ij}}}{E(n'k') - E(nk)} + \text{CC}. \tag{3.6}$$

The oscillating factor $e^{i(k-k')\cdot R_{ij}}$ arising from the change of phase of Bloch electrons over two Mn^{2+} sites is displayed explicitly and the interband exchange matrix element M is independent of either of the two magnetic ion sites. Owing to this factor, different interband excitations interfere with each other, and the net indirect exchange can be obtained only when this interference is calculated explicitly throughout the entire BZ. The site-independent matrix element M evaluated with any Mn^{2+} lattice point as the origin is explicitly

$$M(n'k',nk) = \int dr_1 dr_2 \psi_{n'k'}^*(r_1)\phi_m^*(r_2)\frac{e^2}{r_{12}}\phi_m(r_1)\psi_{nk}(r_2) \tag{3.7}$$

where ϕ_m is the localized magnetic orbital of the magnetic quantum number m and ψ_{nk} denotes the non-magnetic Bloch wavefunction in the nk state. As the ground state of the Mn^{2+} ion is a spherically symmetric ^6S state, the integral M may be viewed qualitatively as the matrix element of a spherically symmetric local exchange operator connecting two interband Bloch states.

Using the LCAO wavefunction in (2.1), the interband matrix element M can be expanded as

$$M(n'k',nk) = N^{-1} \sum_{\mu,\nu} C_\mu^*(n'k')C_\nu(nk)J_{\mu\nu} \tag{3.8}$$

where we only retain in each Bloch sum $|\mu k\rangle$ one atomic orbital centred either at the magnetic ion site or at each of its four neighbouring sites, since the magnetic orbital is very localized and the contributions to the exchange integral from atomic orbitals at more distant neighbours are negligible. The $J_{\mu\nu}$ obtained are therefore of the order of atomic exchange. Since the exchange operator may be regarded as isotropic, only atomic orbitals having the same angular momentum and the same magnetic quantum number are connected by the local exchange. That is to say that among the s and the p orbitals only the diagonal exchange integrals $J_{\mu\mu}$ exist. By reason of symmetry all $J_{\mu\mu}$ connecting three p orbitals are equal to each other. Thus we only have to

Table 3. $M^{II}_{1-x}Mn_xX^{VI}$ local exchange parameters J_{ss} and J_{pp} (in eV) determined from experiments.

	$Hg_{1-x}Mn_xTe$	$Cd_{1-x}Mn_xTe$	$Zn_{1-x}Mn_xTe$	$Zn_{1-x}Mn_xSe$
J_{ss}	0.4	0.22	0.18	0.26
J_{pp}	−0.6	−0.88	−1.05	−1.31

consider two atomic exchange integrals J_{ss} and J_{pp}, denoting s–d and p–d exchange respectively, and we treat them as known parameters in this paper. Values of J_{ss} and J_{pp} determined from experiments [45–53] for some typical DMS are listed in table 3 for reference.

Considering all the above points, the interband exchange matrix element takes the general form

$$M(n'k', nk) = N^{-1} \sum_\mu C_\mu^*(n'k') C_\mu(nk) J_{\mu\mu} \tag{3.9}$$

and

$$\left| M(n'k', nk) \right|^2 = N^{-2} \sum_{\mu,\nu} M_{\mu\nu}^*(n'k') M_{\mu\nu}(nk) J_{\mu\mu} J_{\nu\nu} \tag{3.10}$$

where $M_{\mu\nu}(nk) = C_\mu^*(nk) C_\nu(nk)$ depends only on the band quantum number nk.

For computational convenience, $I(R_{ij})$ in (3.6) is rewritten as the sum of two real terms and the double summation of k, k' over the BZ is converted to the double integration via the following two equivalent versions of averaging over the BZ

$$N^{-1} \sum_k \longrightarrow \frac{1}{V_{BZ}} \int_{BZ} dk \tag{3.11}$$

where V_{BZ} is the volume of the first BZ and N, being the number of states inside the BZ, is also equal to the number of unit cells N inside the crystal in (2.2). The indirect exchange coupling constant is rewritten in its final form as:

$$I(R_{ij}) = -\frac{N^2}{V_{BZ}^2} \sum_{n,n'} \int \int_{BZ} dk dk' \frac{\cos(k' \cdot R_{ij}) \left| M(n'k', nk) \right|^2 \cos(k \cdot R_{ij})}{E(n'k') - E(nk)}$$
$$+ (\cos \rightarrow \sin). \tag{3.12}$$

4. Linear analytic tetrahedron method

In evaluating the double BZ integration, we use the linear analytic tetrahedron method (LATM). In this method, we divide the BZ into microcells, integrate over the microcell analytically, and sum over the contributions from each microcell numerically. Microcells of tetrahedron geometry are preferred since tetrahedra can make an exact division of the BZ and, as will be shown in the appendix, when the integrand exhibits some

functional form of a linear function, the contribution from one tetrahedron depends only on the values of the linear function at the vertices, not on the specific shape of the tetrahedron, thus rendering the results substantially simpler. In this problem, however, a double integration is required and the presence of the phase factor makes the situation more complicated. In the modified version of the LATM, the double integration over the BZ is rewritten as a double summation of the double integration over pairs of tetrahedron with index t and t',

$$
I(\boldsymbol{R}_{ij}) = -\frac{N^2}{V_{\mathrm{BZ}}^2} \sum_{nn',tt' \in \mathrm{BZ}} \int_t d\boldsymbol{k} \int_{t'} d\boldsymbol{k}' \frac{\cos(\boldsymbol{k}' \cdot \boldsymbol{R}_{ij})\big|M(n'\boldsymbol{k}',n\boldsymbol{k})\big|^2 \cos(\boldsymbol{k} \cdot \boldsymbol{R}_{ij})}{E(n'\boldsymbol{k}') - E(n\boldsymbol{k})}
$$
$$
+ (\cos \to \sin). \tag{4.1}
$$

The double integration over each t, t' tetrahedron pair is approximated by the product of the integration of the rapidly oscillating phase and the average values of other slowly varying terms, i.e. the interband matrix element and the inverse of band energy difference. The advantage of making such a separation is that the integration of the phase over the tetrahedron can be performed analytically. Since the matrix element and the inverse of band energy difference are always positive, this approximation is good even if R_{ij} is large as long as tetrahedra are small enough to account for the variation of the matrix element and the inverse of band energy difference throughout the BZ.

With the expansion of the matrix element (3.10) being substituted, the indirect exchange coupling constant is thus decomposed into components of various orbital symmetries

$$
I(\boldsymbol{R}_{ij}) = \sum_{\mu\nu,\xi} I_{\mu\nu}^{\xi}(\boldsymbol{R}_{ij}) \tag{4.2}
$$

with index ξ running over c(cos), s(sin) and μ, ν over s, x, y, z;

$$
I_{\mu\nu}^{\mathrm{c}}(\boldsymbol{R}_{ij}) \simeq -\frac{1}{V_{\mathrm{BZ}}^2} \sum_{nn',tt' \in \mathrm{BZ}} F(t') M_{\mu\nu}^*(n't') \Delta E^{-1}(n't',nt) M_{\mu\nu}(nt) F(t) J_{\mu\mu} J_{\nu\nu} \tag{4.3}
$$

$$
I_{\mu\nu}^{\mathrm{s}}(\boldsymbol{R}_{ij}) \simeq -\frac{1}{V_{\mathrm{BZ}}^2} \sum_{nn',tt' \in \mathrm{BZ}} G(t') M_{\mu\nu}^*(n't') \Delta E^{-1}(n't',nt) M_{\mu\nu}(nt) G(t) J_{\mu\mu} J_{\nu\nu} \tag{4.4}
$$

where $M_{\mu\nu}(nt)$ is the average of $M_{\mu\nu}(n\boldsymbol{k})$ over the tetrahedron t, $\Delta E^{-1}(n't',nt)$ is the average of $\big[E(n'\boldsymbol{k}') - E(n\boldsymbol{k})\big]^{-1}$ over the t, t' tetrahedron pair, and $F(t)$ and $G(t)$ are the integration of $\cos(\boldsymbol{k} \cdot \boldsymbol{R}_{ij})$ and $\sin(\boldsymbol{k} \cdot \boldsymbol{R}_{ij})$ over the tetrahedron t respectively.

The integration of $\cos(\boldsymbol{k} \cdot \boldsymbol{R}_{ij})$ over one tetrahedron is readily obtained via a linear transformation whose details are described in the appendix, and the result depends only on the volume of the tetrahedron and the values of $\boldsymbol{k} \cdot \boldsymbol{R}_{ij}$ at the four vertices of the tetrahedon, as expected:

$$
F(t) = -6v_0 \left(\frac{\sin\theta_1}{(\theta_1 - \theta_2)(\theta_1 - \theta_3)(\theta_1 - \theta_4)} + \frac{\sin\theta_2}{(\theta_2 - \theta_1)(\theta_2 - \theta_3)(\theta_2 - \theta_4)} \right.
$$
$$
\left. + \frac{\sin\theta_3}{(\theta_3 - \theta_1)(\theta_3 - \theta_2)(\theta_3 - \theta_4)} + \frac{\sin\theta_4}{(\theta_4 - \theta_1)(\theta_4 - \theta_2)(\theta_4 - \theta_3)} \right) \tag{4.5}
$$

where v_0 is the volume of the tetrahedron t, and $\theta_\gamma = \mathbf{k}_\gamma \cdot \mathbf{R}_{ij}$ is the phase value at the γth vertex of the tetrahedron t. When some of the θ_γs are equal, one should be careful in taking the limit. In particular, note the following cases:

(i) $\theta_1 = \theta_2$, $\theta_2 \neq \theta_3$, $\theta_3 \neq \theta_4$, $\theta_4 \neq \theta_2$

$$F(t) = 6v_0 \left(\frac{-\cos\theta_2}{(\theta_2 - \theta_3)(\theta_2 - \theta_4)} + \frac{2\theta_2 - \theta_3 - \theta_4}{(\theta_2 - \theta_3)^2(\theta_2 - \theta_4)^2} \sin\theta_2 \right.$$
$$\left. - \frac{\sin\theta_3}{(\theta_3 - \theta_2)^2(\theta_3 - \theta_4)} - \frac{\sin\theta_4}{(\theta_4 - \theta_2)^2(\theta_4 - \theta_3)} \right) \qquad (4.6)$$

(ii) $\theta_1 = \theta_2$, $\theta_3 = \theta_4$, $\theta_1 \neq \theta_3$

$$F(t) = 6v_0 \left(\frac{-(\cos\theta_2 + \cos\theta_4)}{(\theta_2 - \theta_4)^2} + \frac{2(\sin\theta_2 - \sin\theta_4)}{(\theta_2 - \theta_4)^3} \right) \qquad (4.7)$$

(iii) $\theta_1 = \theta_2 = \theta_3 \neq \theta_4$

$$F(t) = 3v_0 \left(\frac{\sin\theta_3}{\theta_3 - \theta_4} + \frac{2\cos\theta_3}{(\theta_3 - \theta_4)^2} - \frac{2(\sin\theta_3 - \sin\theta_4)}{(\theta_3 - \theta_4)^3} \right) \qquad (4.8)$$

(iv) $\theta_1 = \theta_2 = \theta_3 = \theta_4$

$$F(t) = v_0 \cos\theta_4 . \qquad (4.9)$$

The integration formulae of $\sin(\mathbf{k} \cdot \mathbf{R}_{ij})$ can be obtained in similar ways or by converting 'cos' into 'sin', 'sin' into 'cos' and changing the sign of the terms with inverse odd power of θ in the corresponding $\cos(\mathbf{k} \cdot \mathbf{R}_{ij})$ integration formula.

The average of the inverse of band energy difference over the tetrahedron pair t, t' is by definition

$$\Delta E^{-1}(n't', nt) = v_0'^{-1} v_0^{-1} \int_{t'} \mathrm{d}k' \int_t \mathrm{d}k \frac{1}{E(n'k') - E(nk)} \qquad (4.10)$$

and the integration can be carried out with the band energies being linearly interpolated in the tetrahedron t and t'. Since for II–VI semiconductors under investigation the dispersion of the conduction band is much smaller, it is sufficient to approximate the second integration by the average of the first integration at the four vertices of the tetrahedron t'.

As for the average of the matrix element over one tetrahedron, we directly use the value at the centre of the tetrahedron, rather than the average of values at the four vertices in order to avoid highly symmetrical points in the BZ, for the eigenenergies at these points are degenerate and the corresponding eigenfunctions are thus not uniquely defined, which may cause difficulties in the numerical scheme. If the density of mesh is fine enough, the variation of the matrix element inside the tetrahedron should be nearly linear and its average is thus well approximated by its value at the centre of the tetrahedron.

Since $\Delta E^{-1}(n't', nt)$ with t' and t taken from any of $*t'$ and $*t$ respectively are all equal, we may first sum $M_{\mu\nu}^*(n't')F(t')$ over $*t'$ and sum $M_{\mu\nu}(nt)F(t)$ over $*t$, thus contracting the double summation of t, t' into the irreducible part of the BZ:

$$I_{\mu\nu}^c(\boldsymbol{R}_{ij}) \simeq -\frac{1}{V_{BZ}^2} \sum_{\substack{n, n' \\ t, t' \in \text{IrredBZ}}} \left[\sum_{t' \in *t'} M_{\mu\nu}^*(n't')F(t') \right] \Delta E^{-1}(n't', nt) \left[\sum_{t \in *t} M_{\mu\nu}(nt)F(t) \right]$$

(4.11)

where $*t$ indicates the set of tetrahedra derived from the tetrahedron t by applying on it the symmetry operations of the point group of the crystal.

Since LCAO basis orbitals have definite transformation properties under the point group operations of the crystal, the various orbital symmetry components in (4.2) of the indirect exchange coupling constant should also exhibit related crystal symmetry. For example, if $\boldsymbol{R}_{ij} = (R_x, R_y, R_z)$ is changed to its rotated point, say (R_z, R_x, R_y), then the I_{ss} component remains invariant while $\{I_{sx}, I_{sy}, I_{sz}\}$, $\{I_{xx}, I_{yy}, I_{zz}\}$, and $\{I_{yz}, I_{xz}, I_{xy}\}$ components are changed to $\{I_{sz}, I_{sx}, I_{sy}\}$, $\{I_{zz}, I_{xx}, I_{yy}\}$, and $\{I_{xy}, I_{yz}, I_{xz}\}$ components respectively. Similarity holds if $\boldsymbol{R}_{ij}$ is changed to its mirror-reflected point, e.g. (R_y, R_x, R_z). In summary, I_{ss} transforms like 1, and $\{I_{sx}, I_{sy}, I_{sz}\}$, $\{I_{xx}, I_{yy}, I_{zz}\}$, and $\{I_{yz}, I_{xz}, I_{xy}\}$ transform like $\{x, y, z\}$. This implies that $I(\boldsymbol{R}_{ij})$ for all structurally equivalent $\boldsymbol{R}_{ij}$ are equal to each other. All the calculated numerical data of the components of the indirect exchange coupling constant confirm these transformation properties.

The double BZ integration program is tested in two ways via the following well known relation:

$$\iint_{BZ} d\boldsymbol{k} d\boldsymbol{k}' \, e^{i(\boldsymbol{k}-\boldsymbol{k}')\cdot\boldsymbol{R}_{ij}} = V_{BZ}^2 \delta_{ij} .$$

(4.12)

First, the integration of (4.12) is identically equal to zero for any lattice vector $\boldsymbol{R}_{ij}$ except $\boldsymbol{R}_{ij} = 0$. Second, if $\boldsymbol{R}_{ij}$ is replaced by some non-lattice vector $\boldsymbol{R}$, the integration is generally not equal to zero and should be independent of the total number of tetrahedra established in the BZ since the integration formulae of the phase (4.5)–(4.9) are exact. Calculated $I(\boldsymbol{R}_{ij})$ for $Cd_{1-x}Mn_xTe$, $Zn_{1-x}Mn_xTe$, and $Zn_{1-x}Mn_xSe$ up to $R_{ij} = 3R_0$ using a mesh of 18000 tetrahedra established in the BZ are listed in table 4.

5. Discussions

Comparing our present results with those obtained previously, we see that even some of the qualitative features are changed. The calculated indirect exchange coupling constant shows that the indirect exchange is usually antiferromagnetic for the nearest few neighbours, but eventually turns to ferromagnetic as the distance between magnetic ions is increased. Furthermore, there is a strong directional dependence in the obtained indirect exchange coupling constant, leading to the result that the magnitude of the indirect exchange coupling constant for the second, third, and fourth neighbours varies in the reverse order of the separation distance of magnetic ions. This is because the second nearest neighbour, which lies in a highly symmetrical direction of the host crystal, would force the cancellation of all of the orbital symmetry cross terms except one, say I_{sx}^s if $\boldsymbol{R}_{ij}$ is along [100], in the components of the indirect exchange coupling

Table 4. Calculated $M^{II}_{1-x}Mn_x X^{VI}$ indirect exchange coupling constants $I(R_{ij})$ (in K) for the nth nearest neighbours.

n	R_{ij}/R_0	$Cd_{1-x}Mn_x Te$	$Zn_{1-x}Mn_x Te$	$Zn_{1-x}Mn_x Se$
1	$(\frac{1}{2},\frac{1}{2},0)$	11.1	17.1	18.7
2	$(1,0,0)$	0.0621	−0.0928	−0.208
3	$(1,\frac{1}{2},\frac{1}{2})$	0.270	0.240	0.226
4	$(1,1,0)$	0.723	0.820	1.10
5	$(\frac{3}{2},\frac{1}{2},0)$	−0.0445	−0.0486	−0.0819
6	$(1,1,1)$	−0.140	−0.129	−0.207
7	$(\frac{3}{2},1,\frac{1}{2})$	−0.0279	−0.0305	−0.0550
8	$(2,0,0)$	−0.0211	−0.0250	−0.0412
9	$(\frac{3}{2},\frac{3}{2},0)$	−0.0108	−0.0164	−0.0277
10	$(2,\frac{1}{2},\frac{1}{2})$	0.0338	0.0341	0.0448
11	$(2,1,0)$	−0.00110	−0.00541	−0.0102
12	$(\frac{3}{2},\frac{3}{2},1)$	−0.0363	−0.0382	−0.0631
13	$(2,1,1)$	−0.00453	−0.00732	−0.0130
14	$(\frac{5}{2},\frac{1}{2},0)$	−0.0187	−0.0175	−0.0278
15	$(2,\frac{3}{2},\frac{1}{2})$	0.000404	−0.00184	−0.00402
16	$(\frac{5}{2},1,\frac{1}{2})$	−0.00442	−0.00437	−0.00705
17	$(2,2,0)$	0.00483	0.00423	0.00612
18	$(\frac{5}{2},\frac{3}{2},0)$	−0.000506	−0.000759	−0.00131
19	$(2,\frac{3}{2},\frac{3}{2})$	−0.0289	−0.0267	−0.0425
20	$(3,0,0)$	−0.0136	−0.0140	−0.0225

constant. This can be readily shown by summing $M_{\mu\nu}(nt)F(t)$ and $M_{\mu\nu}(nt)G(t)$ over $*t$ explicitly. Note that the same argument still remains true in the central region of the BZ where the band energy is essentially isotropic. We thus conclude that it is the intrinsic cubic symmetry of the band wavefunction, not the slightly anisotropic band energy that induces the strong directional dependence, in the indirect exchange between magnetic ions in DMS.

Now, we compare our theoretical calculation with experimental results. At high temperatures, the DC magnetic susceptibility χ for DMS can be approximated by the Curie–Weiss law

$$\chi = \frac{C}{(T-\Theta)} \tag{5.1}$$

where C is the Curie constant, and Θ, being the paramagnetic Curie–Weiss temperature, can be expressed in terms of the exchange coupling constant $I(R_{ij})$ as follows:

$$\Theta = -\frac{S(S+1)}{3N_M} \frac{\overline{\sum_{i \neq j} I(R_{ij})}}{k_B} \tag{5.2}$$

in which the summation over i and j runs over the actual positions of magnetic ions, N_M is the total number of magnetic ions, and the overbar denotes configuration average. A quantitative analysis of the magnetic properties of DMS requires detailed information about the distribution of magnetic ions throughout the host crystal. However,

for $Cd_{1-x}Mn_xTe$, $Zn_{1-x}Mn_xTe$, and $Zn_{1-x}Mn_xSe$, experimental results [10,11] show that $\Theta(x)$ can be well approximated by $\Theta(x) = \Theta_0 x$, which implies that a completely random distribution of Mn^{2+} ions in the host crystal is a reasonable assumption. Under this assumption, we get

$$\Theta_0 = -\frac{S(S+1)}{3} \frac{\sum_{j \neq i} I(R_{ij})}{k_B} \tag{5.3}$$

and summation over j now runs over all cation sites which forms an FCC lattice. Though the lattice sum of $I(R_{ij})$ can be directly obtained from the $q = 0$ component of the Fourier expansion of $I(R_{ij})$, we would like to point out that the dilution of magnetic impurities in various polar semiconductors is not always in a random sense as those mentioned above. For example, experimental investigations of the magnetic properties of $Pb_{1-x}Mn_xTe$ indicate that the formation of magnetic ion clusters in which the clusters consisting of three Mn^{2+} ions predominate in the composition range $x < 1\%$ seems to be a better assumption [3], in which case calculating $I(R_{ij})$ in real space is necessary. Since the indirect exchange between two magnetic ions separated by any lattice vector can be calculated, the lattice sum in (5.3) can be carried out explicitly. With the total spin of the Mn^{2+} ion $S \simeq \frac{5}{2}$, the theoretical values of Θ_0 for $Cd_{1-x}Mn_xTe$, $Zn_{1-x}Mn_xTe$, and $Zn_{1-x}Mn_xTe$ are -415 K, -623 K, and -673 K respectively, and are compared with those obtained from experimental results, namely -470 ± 34 K, -831 ± 63 K, and -956 ± 50 K respectively [11,12].

Larson and co-workers, using elaborated fourth-order perturbation theory, establish the dominance of superexchange in the short-range region of the magnetic interactions in DMS [54–56]. However, the indirect exchange (Bloembergen–Rowland interactions) might not be neglected. Besides, in the BZ integration they use the matrix element along Γ–X and then make the isotropic approximation. For R_{ij} along [100], this would result in the inclusion of orbital symmetry cross terms which should mutually cancel out altogether (with the exception of one) based on purely symmetrical arguments. (More explicitly, the relevant matrix element $|\tilde{V}_{pd}(nk)|^2$, in our notation, is proportional to $\left| \sum_{\mu=x,y,z} C_\mu(nk) \right|^2$. For R_{ij} along [100], terms containing $C_\mu^*(nk)C_\nu(nk)\cos(k \cdot R_{ij})$ or $C_\mu^*(nk)C_\nu(nk)\sin(k \cdot R_{ij})$ with $\mu \neq \nu$ are identically equal to zero except $C_y^*(nk)C_z(nk)\sin(k \cdot R_{ij})$ and its complex conjugate after performing summation over $*k$, as a direct result of the transformation property of $C_\mu(nk)$.) Since orbital symmetry cross terms are of the same order of magnitude as diagonal terms, making isotropic approximation might affect substantially the numerical accuracy of the calculated exchange coupling constant. For R_{ij} along other directions, this might also have large effect since the cubic symmetry of the crystal is still not correctly reflected.

Recently, there have been some experiments [12] performed to test whether the underlying mechanism of the magnetic interaction in DMS depends on the energy gap of the host crystal. It was shown that the measured Curie–Weiss temperatures for $Hg_{0.95}Mn_{0.05}Te$ and $Hg_{0.87}Cd_{0.08}Mn_{0.05}Te$ are practically coincident, despite the drastic difference between their energy gaps: -0.13 and 0.02 eV for each of the two alloys. Since the indirect exchange is mediated by the virtual interband electron–hole excitations, we might intuitively expect that this mechanism should be sensitive to the change in the magnitude of the energy gap, especially near the zero-gap region. We suggest, however, that with our indirect exchange mechanism the same qualitative

conclusion can be reached after detailed analysis. As stressed at the beginning of this paper, the virtual transition across the energy gap is forbidden due to the contradiction of the symmetry of band wavefunctions. The matrix element thus vanishes at Γ and remains small in the neighbourhood of Γ. In addition, the density of states is also zero at Γ and remains small near Γ. These make the contribution to the indirect exchange mainly from virtual transitions in portions of the BZ away from Γ where the orbital symmetry mixing is strong and the excitation energy is not so small. The sensitivity of energy gap dependence is thus reduced. Furthermore, since the local exchange parameter squared J_{pp}^2 in $Cd_{1-x}Mn_xTe$ is about three times larger than that in $Hg_{1-x}Mn_xTe$, the adulteration of $Cd_{1-x}Mn_xTe$ in $Hg_{1-x}Mn_xTe$ would make the effective J_{pp}^2 become larger. These two effects mutually compensate, with the result that the indirect exchange does not depend on the forbidden energy gap appreciably. Similar arguments can be applied to the experimental results of other DMS samples provided. The concentration-normalized Curie–Weiss temperatures Θ_0 for $Cd_{1-x}Mn_xTe$, $Zn_{1-x}Mn_xTe$, and $Zn_{1-x}Mn_xTe$ investigated above also do not exhibit the apparent energy gap correlation.

Acknowledgments

Appendix

In this section, we show that when the integrand exhibits some functional form of a linear function $f(k)$ (e.g. $1/f(k)$ or $\cos[f(k)]$), the result of the integration over a tetrahedron depends only on the values of $f(k)$ at the four vertices of the tetrahedron, not on the specific shape of the tetrahedron.

Consider $1/f(k)$, taking the integration of the inverse of band energy difference as an example. First, we perform a linear transformation to change integration variables from k to $\{x, y, z\}$ via

$$k = (k_1 - k_4)x + (k_2 - k_4)y + (k_3 - k_4)z + k_4 \tag{A1}$$

with k_i being the coordinate of the ith vertex of the tetrahedron. Under this transformation, the integration domain becomes the tetrahedron with (000), (100), (010) and (001) as its four vertices. When the band energy $E(k)$ is linearly interpolated with respect to the four band energies at the vertices of the tetrahedron, $E(k)$ can be expanded to obtain its dependence on the new integration variables

$$E(k) = (E_1 - E_4)x + (E_2 - E_4)y + (E_3 - E_4)z + E_4$$

with $E_i = E(k_i)$. Next, we set $V_i = E(k_j') - E_i$. The integration of the inverse of the linearized band energy difference is thus straightforward:

$$\int_t dk \frac{1}{E(k_j') - E(k)} = 6v_0 \int_0^1 dz \int_0^{1-z} dy \int_0^{1-z-y} dx$$

$$\times \frac{1}{(V_1 - V_4)x + (V_2 - V_4)y + (V_3 - V_4)z + V_4}$$

where $6v_0$, being six times the volume of the tetrahedron, is the Jacobian of the transformation of variables.

The integration of $\cos[f(k)]$ with $f(k) = k \cdot R$ can be similarly carried out. We rewrite k as in (A1), and thus $k \cdot R = (\theta_1 - \theta_4)x + (\theta_2 - \theta_4)y + (\theta_3 - \theta_4)z + \theta_4$ with $\theta_i = k_i \cdot R$. The integration of $\cos(k \cdot R)$ is also straightforward:

$$\int_t dk \cos(k \cdot R) = 6v_0 \int_0^1 dz \int_0^{1-z} dy \int_0^{1-z-y} dx$$

$$\times \cos[(\theta_1 - \theta_4)x + (\theta_2 - \theta_4)y + (\theta_3 - \theta_4)z + \theta_4].$$

When some θ_is become degenerate (e.g. $\theta_1 = \theta_4$), we obtain the corresponding formula by integrating the function $\cos[(\theta_2 - \theta_4)y + (\theta_3 - \theta_4)z + \theta_4]$, rather than taking the limit directly from the integration formula for the non-degenerate case.

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