Indirect exchange interaction in the zero-gap semiconductor $\text{Hg}_{1-x}\text{Mn}_x\text{Te}$

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A phenomenological model is presented to explain the variation of the Curie-Weiss temperature of $\text{Hg}_{1-x}\text{Mn}_x\text{Te}$ with Mn concentration x . The band structure of HgTe is first calculated by the four-band $\mathbf{k}\cdot\mathbf{p}$ method with spin-orbit interaction included, and then used in a perturbative calculation of the indirect exchange interaction between Mn ions. For the case with interspin distances larger than the lattice constant, the indirect exchange is antiferromagnetic. With the assumption that the formation of nearest-neighbor Mn pairs may be neglected, or that the nearest-neighbor exchange couplings are locked in, the almost linear variation of the Curie-Weiss temperature with x can be explained for the case of low manganese concentration.

I. INTRODUCTION

Recently there has been some interest in the magnetic properties of semiconductors containing a few percent of magnetic ions.¹⁻⁷ For the zero-gap semiconductor $\text{Hg}_{1-x}\text{Mn}_x\text{Te}$, various experiments^{3,4,8} have shown evidence of an antiferromagnetic interaction between the Mn^{2+} localized moments. At high temperature the magnetic susceptibility can be described rather well by the Curie-Weiss law with a negative paramagnetic Curie-Weiss temperature which varies almost linearly with the Mn concentration x over a rather wide range of concentration ($0.1\% < x < 30\%$). For a dilute magnetic semiconductor, the superexchange mechanism,⁹ which is usually dominant in magnetic insulators, is now less important as the magnetic wave functions become very well localized and the transfer integral between two magnetic sites approaches zero. However, the exchange polarization effect, which is usually negligible in magnetic insulators, will be enhanced in a semiconductor because of the small energy gap. It is believed that in dilute magnetic semiconductors, the magnetic interaction may be mediated by the spin-dependent spatial polarization of the valence-band electrons due to their exchange interactions with the separated localized magnetic moments. The polarized Bloch electrons will then mediate a spin interaction between two magnetic ions, the so-called indirect exchange interaction. The polarization process in a semiconductor involves interband electron-hole excitations which depend on the band structure of the host semiconductor. The indirect exchange interaction is the complete analog of the Ruderman-Kittel-Kasuya-Yosida (RKKY) interaction¹⁰ in metallic magnetic alloys. In semiconductors the RKKY interaction itself is usually not important except for degenerate samples with a high concentration of free electrons.

The properties of the indirect exchange interaction have been studied in several model calculations.¹¹⁻¹⁷ However, most authors have assumed parabolic energy bands and a constant interband-exchange matrix element. These assumptions are valid only in the immediate vicinity of the band edges. For direct-gap semiconductors with

s - and p -band edges located at the center of the Brillouin zone (Γ point), the conduction- and valence-band edges are of different symmetry. 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 contains both s and p components outside the Γ point. Therefore a very important factor affecting the indirect exchange interaction in semiconductors is the s - p mixing of the band states, which is strong only in regions of the Brillouin zone distant from the Γ point. Based on the band structure calculated by the isotropic $\mathbf{k}\cdot\mathbf{p}$ method,¹⁸ our previous work^{19,20} shows that the indirect exchange interaction in magnetic semiconductors consists of two competing components, one ferromagnetic and one antiferromagnetic, mediated by electrons occupying different valence bands. While a pair of noninteracting bands makes an antiferromagnetic contribution at large interspin distances, two bands which have local symmetry mixing with each other (e.g., s - p mixing) will contribute a net ferromagnetic interaction. For interspin distances equal to the lattice constant (i.e., next-nearest-neighbor cation separation) and beyond, the antiferromagnetic part usually dominates the ferromagnetic component in narrow-gap semiconductors.

The magnetic properties of $\text{Hg}_{1-x}\text{Mn}_x\text{Te}$ have been studied^{13,21,22} with the indirect exchange interaction as the dominant magnetic mechanism. With parabolic bands and band-edge Bloch functions, Bastard and Lewiner¹³ get a Curie-Weiss temperature of 6.9 K for $x=1\%$ in agreement with experiment. However, if the spin-orbit interaction is taken into account by using band-edge Bloch functions corresponding to an infinite spin-orbit splitting energy,²¹ the indirect exchange calculated with the same parabolic bands is still antiferromagnetic but smaller by more than 1 order of magnitude than that of experimental result. By using linear bands and band-edge Bloch functions corresponding to an infinite spin-orbit splitting energy,²² the calculated Curie-Weiss temperature is about half of the experimental result for $x=5\%$. These previous studies show that a more realistic band structure and Bloch wave functions with a finite spin-orbit splitting energy are important factors in pro-

viding an explanation for the magnetic properties of $\text{Hg}_{1-x}\text{Mn}_x\text{Te}$ by the indirect exchange mechanism.

From the above discussion, it becomes obvious that one needs to know the band structure before determining the nature of the indirect exchange. We have decided to use the $\mathbf{k}\cdot\mathbf{p}$ method¹⁸ to calculate the band structure of HgTe . Although, strictly speaking, this method is only valid in the vicinity of the Γ point, it does give a fairly good account of the s - p mixing of bands and the effect of spin-orbit interaction in a large portion of the Brillouin zone. For the zero-gap semiconductor HgTe , it is a good approximation to first ignore all $\mathbf{k}\cdot\mathbf{p}$ interactions except the kP interaction, P being the momentum matrix element between s - and p -band-edge states at the Γ point, and then treat the kP and spin-orbit interactions exactly. This method is chosen because the local symmetry of the band states is well represented by atomic-orbit-like basis functions, e.g., by $|S\rangle$, $|X\rangle$, $|Y\rangle$, and $|Z\rangle$, and then the values of the exchange matrix element between the basis functions can be determined from experimental results. By adopting the $\mathbf{k}\cdot\mathbf{p}$ method we further ensure that the energy gap, the spin-orbit splitting energy, and the mixing coefficients of band states obtained are reliable.

With the band structure known, we treat the spin polarization of the valence-band electrons due to the Mn^{2+} local moment by perturbation theory. Numerical calculation indicates that there is a long-range antiferromagnetic exchange interaction between Mn^{2+} ions separated by distances larger than the lattice constant. With the assumption that the formation of nearest-neighbor Mn pairs may be neglected or that the nearest-neighbor exchange couplings are locked in, the almost linear variation of the measured Curie-Weiss temperature with Mn concentration x in the dilute impurity case can be explained by the indirect exchange mechanism.

This paper is organized as follows: Section II describes the band structure, and Sec. III the indirect exchange calculation. Finally, Sec. IV is devoted to a comparison with experimental results.

II. ENERGY BAND

The $\text{Hg}_{1-x}\text{Mn}_x\text{Te}$ compounds are random ternary alloys which crystallize in the zinc-blende structure. Experimental results²³ show that the Mn centers will not greatly change the Bloch wave functions in their vicinities. At the Γ point, both the conduction and the heavy-hole valence bands of HgTe have Γ_8 symmetry (p symmetry, $|\frac{3}{2}, \pm\frac{1}{2}\rangle$ and $|\frac{3}{2}, \pm\frac{3}{2}\rangle$ states, respectively), the light-hole band has Γ_6 symmetry (s symmetry, $|\frac{1}{2}, \pm\frac{1}{2}\rangle$ state) and lies at $|E_g|$ below the degenerate Γ_8 band, E_g being the s - p energy gap, i.e., $E_g = E(\Gamma_6) - E(\Gamma_8)$. There is a lower split-off band with Γ_7 symmetry (p symmetry, $|\frac{1}{2}, \pm\frac{1}{2}\rangle$ state) lying at Δ , the spin-orbit splitting energy, below the Γ_8 bands. The introduction of Mn to the HgTe matrix will increase E_g continuously with x , and $\text{Hg}_{1-x}\text{Mn}_x\text{Te}$ will become a true zero-gap semiconductor, with $E_g \simeq 0$, i.e., Γ_8 and Γ_6 bands degenerate, for $x \simeq 7.5\%$. As x increases further, the zero-gap $\text{Hg}_{1-x}\text{Mn}_x\text{Te}$ will undergo a configuration transition to semiconducting $\text{Hg}_{1-x}\text{Mn}_x\text{Te}$, with $E_g > 0$ for $x > 7.5\%$.

In the semiconducting configuration, the structure of the Γ_8 and Γ_6 bands is inverted; i.e., the Γ_6 conduction band lies at E_g above the degenerate Γ_8 valence bands. For band states with $k \neq 0$, there is a mixing of the symmetry among the Γ_6 , Γ_8 , and Γ_7 bands. These effects can be treated by the small-gap approximation of the $\mathbf{k}\cdot\mathbf{p}$ method. Following Kane,¹⁸ we first rotate the coordinate system such that the z' axis orients along the wave vector $\mathbf{k}$.

We construct a new set of p -like basis functions $|X'\rangle$, $|Y'\rangle$, and $|Z'\rangle$ which transform as the primed coordinates x', y', z' . Among these basis states, only the $|Z'\rangle_{\downarrow}$ state is coupled to the $|S\rangle_{\downarrow}$ state by the kP interaction, P being the momentum matrix element between $|S\rangle$ and $|Z\rangle$ states, and the $|(X' - iY')/\sqrt{2}\rangle_{\uparrow}$ state is coupled to the $|Z'\rangle_{\downarrow}$ state by a constant spin-orbit interaction term $\sqrt{2}\Delta/3$. $|\uparrow\rangle$ and $|\downarrow\rangle$ denote the bare-electron spin eigenfunctions of spin-up and spin-down states, respectively. Similar couplings exist for the corresponding Kramers degenerate states of these basis functions. In the zero-gap configuration, the exchange-induced interband excitations between p -like states in the vicinity of the degenerate band edges are allowed. But, as the conduction band mixes in s -like states, interband exchange couplings start to change their character. Because of the kP and spin-orbit interactions, four bands are generated which separate in energy. These are the conduction band (labeled c), the heavy-hole band (labeled v_1), the light-hole band (labeled v_2), and the lowest split-off band (labeled v_3).

The cell-periodic part of the Bloch wave function is denoted by $u_{n\mathbf{k}\sigma}$ with n being the band index, and the pseudospin index $\sigma = \pm 1$ labels the Kramers degeneracy of the bands, although in the zinc-blende structure the Kramers doublets will split by very small amounts. In the small-gap approximation, $u_{n\mathbf{k}\sigma}$ is given by

$$u_{n\mathbf{k}+} = a_n(\mathbf{k}) |iS\rangle_{\downarrow} + b_n(\mathbf{k}) |R'_{-}\rangle_{\uparrow} + c_n(\mathbf{k}) |Z'\rangle_{\downarrow} \quad (1)$$

and

$$u_{n\mathbf{k}-} = a_n(\mathbf{k}) |iS\rangle_{\uparrow} + b_n(\mathbf{k}) |-R'_{+}\rangle_{\downarrow} + c_n(\mathbf{k}) |Z'\rangle_{\downarrow}$$

for $n = c, v_2, v_3$, respectively. For the flat heavy-hole band ($n = v_1$) we have

$$u_{n\mathbf{k}+} = |R'_{+}\rangle_{\uparrow}$$

and

$$u_{n\mathbf{k}-} = |-R'_{-}\rangle_{\downarrow},$$

where $R'_{\pm} = (X' \pm iY')/\sqrt{2}$. In the $\mathbf{k}\cdot\mathbf{p}$ method, $|S\rangle$, $|X\rangle$, $|Y\rangle$, and $|Z\rangle$ are periodic functions which transform like s and p functions under the operation of tetrahedral group at the Γ point. The real mixing coefficients $a_n(\mathbf{k})$, $b_n(\mathbf{k})$, $c_n(\mathbf{k})$, and the band energy $\epsilon_n(\mathbf{k})$ can be obtained from the eigenvalue equation of the 3×3 Hamiltonian matrix

$$\begin{pmatrix} E_g & 0 & Pk \\ 0 & -2\Delta/3 & \sqrt{2}\Delta/3 \\ Pk & \sqrt{2}\Delta/3 & -\Delta/3 \end{pmatrix}, \quad (3)$$

where $P = (-i\hbar/m)\langle S | p_z | Z \rangle$ is the real momentum matrix element which is assumed to be independent of the coordinate transformation. To the energy eigenvalues for the conduction and split-off valence bands we add the free-electron kinetic energy $\hbar^2 k^2/2m$ generated by the plane-wave part of the Bloch functions. The heavy-hole (v_1) valence band is assumed to be flat, although inclusion of higher band interactions will result in a very small negative curvature for this band.

Since the direction of the wave vector $\mathbf{k}$ is used as the axis of quantization for the basis functions, the band energies $\epsilon_n(\mathbf{k})$ and the mixing coefficients depend only on the magnitude of the $\mathbf{k}$ vector. We have made this isotropic band approximation by assuming that the basis orbitals are always quantized along the $\mathbf{k}$ direction. For HgTe, which possesses a high degree of symmetry (cubic symmetry), this is not a bad approximation. We have also extended the four-band $\mathbf{k}\cdot\mathbf{p}$ formalism which, strictly speaking, is only valid in the vicinity of the Γ point, to the entire Brillouin zone. This approximation is particularly bad for the conduction band in the region where it intersects other higher-energy bands. However, apart from this region and the vicinity of the zone boundary, the $\mathbf{k}\cdot\mathbf{p}$ energy bands do resemble, even quantitatively in the symmetry directions, the energy bands obtained by a more elaborate scheme (e.g., the pseudopotential method²⁴) after the inclusion of higher band interactions.

III. INDIRECT EXCHANGE INTERACTION

A localized spin $\mathbf{S}_i$ associated with a magnetic ion embedded in a nonmagnetic semiconductor lattice will magnetically polarize the band electrons of the host through the direct exchange interaction between the magnetic electrons and the Bloch electrons, inducing the latter to make virtual interband transitions. The Bloch electrons polarized by $\mathbf{S}_i$ will then interact with another spin $\mathbf{S}_j$ localized at a different lattice site, and thus mediate an effective interaction between $\mathbf{S}_i$ and $\mathbf{S}_j$. The exchange in-

teraction between the localized spin $\mathbf{S}_i$ and the Bloch electron is assumed to take the form

$$H_{ex} = \sum_{\mathbf{R}_i} J(\mathbf{r} - \mathbf{R}_i) \mathbf{S}_i \cdot \mathbf{s}, \quad (4)$$

where the $\mathbf{S}_i$ are the localized spins located at $\mathbf{R}_i$, and $\mathbf{s}$ is the Bloch electron spin. $J(\mathbf{r} - \mathbf{R}_i)$ is the exchange coupling constant centered at $\mathbf{R}_i$. When there is more than one magnetic electron localized at one magnetic ion site as is usually the case, we assume that the exchange coupling constant J is independent of the magnetic quantum number characterizing them. Because the trace of $\mathbf{s}$ is equal to zero, the first-order energy shift produced by H_{ex} vanishes. The second-order energy shift is

$$\Delta E = - \sum_{n', \mathbf{k}', \sigma'} \sum_{n, \mathbf{k}, \sigma} \frac{f(\epsilon_n(\mathbf{k}))[1 - f(\epsilon_{n'}(\mathbf{k}'))]}{\epsilon_{n'}(\mathbf{k}') - \epsilon_n(\mathbf{k})} \times |\langle \Psi_{n' \mathbf{k}' \sigma'} \phi_f | H_{ex} | \Psi_{n \mathbf{k} \sigma} \phi_i \rangle|^2, \quad (5)$$

where $\epsilon_{n'}(\mathbf{k}')$ and $\epsilon_n(\mathbf{k})$ are the band energies of the n th conduction band and the n th valence band, respectively, and $\Psi_{n' \mathbf{k}' \sigma'}$ and $\Psi_{n \mathbf{k} \sigma}$ are their corresponding Bloch wave functions. ϕ is the wave function of the magnetic electrons. The summations of $\mathbf{k}$ and $\mathbf{k}'$ are over the first Brillouin zone. The Bloch wave function can be written as

$$\Psi_{n \mathbf{k} \sigma} = \frac{1}{\Omega} u_{n \mathbf{k} \sigma} e^{i \mathbf{k} \cdot \mathbf{r}}, \quad (6)$$

where Ω is the volume of the crystal.

If we assume that the valence bands are completely filled and the conduction band completely empty, assumptions which are approximately valid for temperatures in the range from 4 to 200 K and for all $\mathbf{k}$, then the second-order energy shift ΔE can be written as an effective spin-spin Hamiltonian form

$$\Delta E = - \sum_{i,j} \sum_{\alpha, \beta} I^{\alpha\beta}(\mathbf{R}_{ij}) S_i^\alpha S_j^\beta, \quad \alpha, \beta = x, y, z \quad (7)$$

with

$$I^{\alpha\beta}(\mathbf{R}_{ij}) = \frac{1}{\Omega^2} \sum_{n', \mathbf{k}', \sigma'} \sum_{n, \mathbf{k}, \sigma} \frac{e^{i(\mathbf{k}' - \mathbf{k}) \cdot \mathbf{R}_{ij}}}{\epsilon_{n'}(\mathbf{k}') - \epsilon_n(\mathbf{k})} \sum_{\sigma, \sigma'} (\langle u_{n \mathbf{k} \sigma} | J S^\alpha | u_{n' \mathbf{k}' \sigma'} \rangle \langle u_{n' \mathbf{k}' \sigma'} | J S^\beta | u_{n \mathbf{k} \sigma} \rangle + \langle u_{n \mathbf{k} \sigma} | J S^\beta | u_{n' \mathbf{k}' \sigma'} \rangle \langle u_{n' \mathbf{k}' \sigma'} | J S^\alpha | u_{n \mathbf{k} \sigma} \rangle), \quad (8)$$

where the wave functions of the magnetic electrons ϕ are not shown explicitly. We note that we have used only the cell-periodic part of the Bloch wave function for $\Psi_{n \mathbf{k} \sigma}$. This approximation should not give rise to any appreciable error because the magnetic wave function ϕ is very localized and the change in the phase of the Bloch wave function is small over this short distance. Since the ground state of the $3d^5$ Mn electrons is in an orbital singlet ($S_{5/2}$ state), there are only two nonvanishing and independent exchange matrix elements

$$\langle S | J | S \rangle = J_s,$$

and

$$\langle Z | J | Z \rangle = J_p,$$

where J_s and J_p ($J_p = \langle X | J | X \rangle = \langle Y | J | Y \rangle$) are the exchange integrals for the s -like electrons of the Γ_6 band state, and the p -like electrons of the Γ_8 band state, respectively.

Due to the different quantization directions of the band states $u_{n\mathbf{k}\sigma}$ and $u_{n'\mathbf{k}'\sigma'}$ in the interband-exchange matrix element, there will be an additional angular factor generated in the interband-exchange matrix element between two basis functions belonging to the same space symmetry (e.g., s or p symmetry) but with different wave vectors $\mathbf{k}$ and $\mathbf{k}'$. A typical form of the exchange matrix element mentioned above, for example, between basis functions $b_c(\mathbf{k}') |R'_-\rangle_\uparrow$ and $c_n(\mathbf{k}) |Z\rangle_\uparrow$ is

$$b_c(\mathbf{k}')c_n(\mathbf{k})\langle R'_- | \uparrow J_s^z | Z \rangle_\uparrow = \frac{1}{2}b_c(k')c_n(k)\Omega_0 J_p d_{-1,0}^1(\theta) \quad (10)$$

where Ω_0 is the volume of the unit cell and θ is the angle between the wave vectors $\mathbf{k}$ and $\mathbf{k}'$, respectively. The angular factor $d_{m',m}^l(\theta)$ is the matrix element of the rota-

tional operator between spherical harmonic basis function $|l, m'\rangle$ and $|l, m\rangle$, and its value can be determined from the well-known transformation properties of spherical harmonics under rotation.²⁵ Other terms similar to that in Eq. (10) can be evaluated the same way. Then, from the discussion of the last paragraph, we can write the indirect exchange coupling constant $I^{a\beta}(\mathbf{R}_{ij})$ as

$$I^{a\beta}(\mathbf{R}_{ij}) = N_0^2 \sum_{\mathbf{k}, \mathbf{k}'} \sum_n \frac{e^{i(\mathbf{k}' - \mathbf{k}) \cdot \mathbf{R}_{ij}}}{\epsilon_c(\mathbf{k}') - \epsilon_n(\mathbf{k})} M_n^{a\beta}(\mathbf{k}', \mathbf{k}), \quad (11)$$

where $N_0 = 4/R_0^3$ is the number of unit cells per unit volume with R_0 the lattice constant. The nonvanishing terms of the interband-exchange matrix elements contributed by valence electrons from the light-hole (v_2) band and the split-off (v_3) band include the diagonal terms

$$\begin{aligned} M_n^{zz} &= [a_c(k')a_n(k)J_s + c_c(k')c_n(k)J_p \cos\theta - b_c(k')b_n(k)J_p \cos^2(\theta/2)]^2 \\ &\quad + \frac{1}{2}[c_c(k')b_n(k) - b_c(k')c_n(k)]^2 J_p \sin^2\theta, \\ M_n^{yy} &= [a_c(k')a_n(k)J_s + c_c(k')c_n(k)J_p \cos\theta + b_c(k')b_n(k)J_p \sin^2(\theta/2)]^2 \\ &\quad + \frac{1}{2}[c_c(k')b_n(k) + b_c(k')c_n(k)]^2 J_p \sin^2\theta, \\ M_n^{xx} &= [a_c(k')a_n(k)J_s + c_c(k')c_n(k)J_p \cos\theta - b_c(k')b_n(k)J_p \sin^2(\theta/2)]^2 \\ &\quad + \frac{1}{2}[c_c(k')b_n(k) + b_c(k')c_n(k)]^2 J_p \sin^2\theta \end{aligned} \quad (12)$$

and the symmetric off-diagonal terms

$$\begin{aligned} M_n^{xz} &= M_n^{zx} = \frac{1}{2}[c_c(k')b_n(k) - b_c(k')c_n(k)] \\ &\quad \times b_c(k')b_n(k)J_p^2 \sin\theta \end{aligned} \quad (13)$$

for $n = v_2$ and v_3 , respectively. The heavy-hole (v_1) band couples with the conduction band only through the hopping of p -like electrons, and the nonvanishing terms of $M_n^{a\beta}$ arising from this v_1 band are

$$\begin{aligned} M_{v_1}^{zz} &= \frac{1}{2}[c_c(k')J_p \sin\theta]^2 + [b_c(k')J_p \sin^2(\theta/2)]^2, \\ M_{v_1}^{yy} &= M_{v_1}^{xx} = \frac{1}{2}[c_c(k')J_p \sin\theta]^2 \\ &\quad + [b_c(k')J_p \cos^2(\theta/2)]^2, \\ M_{v_1}^{xz} &= M_{v_1}^{zx} = \frac{1}{2}c_c(k')b_c(k')J_p^2 \sin\theta. \end{aligned} \quad (14)$$

Due to the existence of the spin-orbit interaction, the indirect exchange interaction should also include various anisotropic contributions, such as the pseudodipolar interaction²⁶ and the antisymmetric Dzyaloshinsky-Moriya (DM) interactions.²⁷⁻²⁹ As the lack of inversion symmetry for the zinc-blende structure has been neglected, the DM interaction, averaged over the sample, reduces to zero and correspondingly the resulting indirect exchange interaction contains an isotropic and a symmetric pseudodipolar term.²⁶

For the case when the spin-orbit energy Δ reduces to zero, the band structure reduces correspondingly to doubly degenerate heavy-hole bands (v_1 and v_2 bands), and

only the conduction band and the lowest light-hole (v_3) bands are coupled by the kP interaction. In this case, the indirect exchange interaction reduces to the isotropic Heisenberg form

$$\Delta E = - \sum_{\substack{i,j \\ i>j}} I(\mathbf{R}_{ij}) \mathbf{S}_i \cdot \mathbf{S}_j, \quad (15)$$

and the interband-exchange matrix elements $M_n(\mathbf{k}', \mathbf{k})$ reduce correspondingly to¹⁹

$$M_{v_3} = [a_c(k')a_n(k)J_s + c_c(k')c_n(k)J_p \cos\theta]^2$$

and

$$M_n = \frac{1}{2}[c_c(k')J_p \sin\theta]^2, \quad n = v_1, v_2. \quad (16)$$

We have shown previously¹⁹ that the qualitative behavior of the indirect exchange coupling constant $I(\mathbf{R}_{ij})$ is determined mainly by the angular factor arising from the space symmetry of the basis functions and the s - p mixing of the band states which depends on the band structure. For direct energy-gap semiconductors with s - and p -band-edge states, for the case $R_{ij} > R_0$, the contribution to the indirect exchange from the lower valence (v_3) band which has strong s - p mixing with the conduction band is always ferromagnetic, but both of the degenerate heavy-hole bands will contribute antiferromagnetic terms.

In the double summations over $\mathbf{k}$ and $\mathbf{k}'$, the Brillouin zone of the fcc lattice is replaced by a sphere of radius $2\pi/R_0$. Because of the oscillating factor $e^{i(\mathbf{k}' - \mathbf{k}) \cdot \mathbf{R}_{ij}}$, im-

TABLE I. Calculated results for $I(R_{ij})$ as R_{ij} varies from R_0 to $3R_0$ for two configurations of $\text{Hg}_{1-x}\text{Mn}_x\text{Te}$ with $E_g = -0.3$ eV and $E_g = 0$ eV, respectively. Other band parameters are $\Delta = 1.0$ eV, $E_p = P^2/2m = 18.0$ eV, and lattice constant $R_0 = 12.1 a_0$, a_0 being the Bohr radius.

Configuration	x (%)	E_g (eV)	$I(R_0)$ (eV)	$I(2R_0)$ (eV)	$I(3R_0)$ (eV)
Negative gap	≈ 0	-0.303	-7.2×10^{-4}	-3.3×10^{-5}	-6.4×10^{-6}
Zero gap	$\approx 7.5\%$	≈ 0	-6.0×10^{-4}	-2.6×10^{-5}	-6.9×10^{-6}

posing a cutoff in the integration of $\mathbf{k}$ other than that provided by the actual Brillouin-zone boundary may result in spurious oscillations of $I^{ab}(\mathbf{R}_{ij})$ with interspin distance $\mathbf{R}_{ij}$. But with our particular choice of $2\pi/R_0$ as the integration limit for k and k' , this problem is avoided as long as the interspin distance is an integer multiple of the lattice constant R_0 . When this is not the case, a more realistic value for $I^{ab}(\mathbf{R}_{ij})$ may be calculated by interpolation. Because of the assumptions of isotropic energy bands and a spherical Brillouin zone, the indirect exchange coupling constants $I^{ab}(\mathbf{R}_{ij})$ depend only on the magnitude of $\mathbf{R}_{ij}$. The values of the exchange matrix elements $N_0 J_s$ and $N_0 J_p$ can be determined from the experimental results of the magnetooptic and magnetotransport measurements, and their values are approximately -0.05 eV and 1.0 eV, respectively.³⁰ With these values for J_s and J_p together with the band parameters of HgTe , i.e., $\Delta = 1.0$, $E_g = -0.30$, and $E_p = P^2/2m = 18.0$ (all in eV), the indirect exchange coupling constant at $R_{ij} = R_0$ is

$$\sum_{\alpha, \beta} I^{ab}(R_0) S_i^\alpha S_j^\beta = [-7.2 S_i^z S_j^z - 7.3 S_i^x S_j^x - 7.2 S_i^y S_j^y - 0.14(S_i^x S_j^z + S_i^z S_j^x)], \quad (17)$$

in units of 10^{-4} eV.

Comparisons between the present result and that of the case without consideration of the spin-orbit interaction¹⁹ show that the antiferromagnetic terms contributed by the higher valence bands (v_1, v_2) are still dominant but are reduced about 20% in magnitude. This reduction is due to the indirect mixing between the conduction and the light-hole (v_2) band by the coexistence of the spin-orbit interaction and the kP interaction. The indirect exchange coupling constant is approximately isotropic to within an error of less than 2% at $R_{ij} = R_0$. The deviation from isotropic behavior increases with the interspin distance R_{ij} and is estimated to be about 20% at $R_{ij} = 5R_0$. The calculated values of $I(R_{ij})$ with R_{ij} varying from R_0 to $3R_0$ for energy gaps $E_g = -0.3$ eV and $E_g = 0$ eV, corresponding to two typical configurations of $\text{Hg}_{1-x}\text{Mn}_x\text{Te}$, are given in Table I. Our investigation also shows that for $R_{ij} > R_0$, $I(R_{ij})$ decreases with R_{ij} according to a power law approximately as

$$I(R_{ij}) \approx R_{ij}^{-\delta} \quad (18)$$

with $3.8 < \delta < 4.6$ as R_{ij} varies from R_0 to $5R_0$.

IV. COMPARISON WITH EXPERIMENTAL RESULTS

A complete analysis of the magnetic properties of $\text{Hg}_{1-x}\text{Mn}_x\text{Te}$ requires detailed information about the distribution of Mn^{2+} ions in the crystal lattice. Experi-

mental investigations have shown an almost linear dependence of the Curie-Weiss temperature Θ on the Mn concentration x over a wide range ($0.1\% < x < 30\%$). It seems that the assumption of a completely random distribution of Mn^{2+} ions in the host lattice is a reasonable choice. However, various experimental results^{1,31} also indicate that the Mn ion distribution is not purely random, and there are no special magnetic clusters formed for low Mn^{2+} concentration cases such as that in $\text{Pb}_{1-x}\text{Mn}_x\text{Te}$.⁷

In order to compare our model with experiment, we need to calculate the magnetic susceptibility of $\text{Hg}_{1-x}\text{Mn}_x\text{Te}$. In the molecular-field approximation (high-temperature case), the magnetic susceptibility χ obeys the Curie-Weiss law

$$\chi^{-1} = a(T - \Theta) \quad (19)$$

with a negative paramagnetic Curie-Weiss temperature Θ which can be expressed in terms of the exchange coupling constant $I(\mathbf{R}_{ij})$ as

$$k_B \Theta = \frac{S(S+1)}{3N} \sum_{i,j} I(\mathbf{R}_{ij}), \quad (20)$$

where N is the total number of Mn ions, and the summations of i and j run over the actual positions of Mn ions, i.e., over $\mathbf{R}_i$ and $\mathbf{R}_j$, respectively. From the fact that even for very low Mn content ($x \approx 0.1\%$) the magnetic properties of $\text{Hg}_{1-x}\text{Mn}_x\text{Te}$ depart considerably from noninteracting spin behavior, and show an antiferromagnetic interaction between localized magnetic moments; we assume that, in the low- Mn^{2+} -concentration case, the nearest-neighbor couplings between Mn^{2+} ions can be neglected. There are two situations in which this assumption will be approximately valid. One is that, because the distribution of Mn^{2+} ions is not purely random and there are no special clusters formed, there are few chances for two Mn^{2+} ions to form a nearest-neighboring pair. The other possible situation is that the nearest-neighbor couplings between Mn^{2+} ions are locked in. A similar assumption was used by Kreitman *et al.*³² in their study of the magnetic susceptibility of Mn^{2+} in CdS and the effect of antiferromagnetic exchange. In their work, the experimental data provide clear evidence for isotropic antiferromagnetic exchange interactions between next-nearest-neighbor and even more distant pairs of Mn^{2+} ions. It seems that a similar exchange mechanism may be possible for Mn^{2+} ions in a HgTe lattice. With these assumptions, we can express the Curie-Weiss temperature Θ as

$$k_B \Theta = \frac{35x}{12} \sum_{\substack{\mathbf{R}_i \\ |\mathbf{R}_i| \geq R_0}} I(\mathbf{R}_i), \quad (21)$$

where the summation over $\mathbf{R}_i$ now runs over all the sites of a fcc lattice except the nearest-neighbor sites. By adopting $\delta \simeq 4.5$ for the exponent in Eq. (18), then the lattice sum of $R_i^{-\delta}$ over a fcc lattice in Eq. (21) can be evaluated.³³

The dependence of the energy gap E_g on Mn^{2+} concentration x is not known at present; we only know that $E_g \simeq 0$ occurs for $x \simeq 7.5\%$. So for the low- Mn^{2+} -concentration case, we will assume that E_g varies linearly with x . Finally, from Eq. (21) we get $\Theta = -7.8$ K for $x = 1\%$ and $\Theta = -35$ K for $x = 5\%$, respectively. These calculated values of the Curie-Weiss temperature are in good agreement with the experimental results, which give $\Theta_{\text{expt}} \simeq -6$ K for $x = 1\%$ and $\Theta_{\text{expt}} \simeq -30$ K for $x = 5\%$, respectively.

With the assumptions made in our model calculation, we think that the validity of the numerical results is restricted to the dilute impurity case. For the case of high Mn^{2+} concentration, the variation of cluster probabilities

for various Mn^{2+} clusters with Mn concentration may be important and complicated, and correspondingly the nearest-neighbor exchange couplings inside the clusters, which may be ferromagnetic as was assumed in our previous study of the magnetic properties of $\text{Pb}_{1-x}\text{Mn}_x\text{Te}$,³⁴ may play an important role. In making a comparison between theory and experiment we should mention that the intraband exchange due to the free carriers in semiconductors is usually not important as has been shown by several authors.^{13,15}

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