Electron-hole contribution to the apparent $s-d$ exchange interaction in III-V dilute magnetic semiconductors

Cezary Śliwa[1,*] and Tomasz Dietl[1,2,†]

[1]*Institute of Physics, Polish Academy of Sciences, Aleja Lotników 32/46, PL 02-668 Warszawa, Poland*

[2]*Institute of Theoretical Physics, University of Warsaw, ul. Hoża 69, PL 00-681 Warszawa, Poland and ERATO Semiconductor Spintronics Project, Japan Science and Technology, Aleja Lotników 32/46, PL 02-668 Warszawa, Poland*

(Received 29 August 2008; published 28 October 2008)

Spin splitting of photoelectrons in p-type and electrons in n-type III-V Mn-based diluted magnetic semiconductors is studied theoretically. It is demonstrated that the unusual sign and magnitude of the apparent s-d exchange integral reported for GaAs:Mn arises from exchange interactions between electrons and holes bound to Mn acceptors. This interaction dominates over the coupling between electrons and Mn spins, so far regarded as the main source of spin-dependent phenomena. A reduced magnitude of the apparent s-d exchange integral found in n-type materials is explained by the presence of repulsive Coulomb potentials at ionized Mn acceptors and a bottleneck effect.

DOI: 10.1103/PhysRevB.78.165205 PACS number(s): 75.50.Pp, 71.70.Gm, 71.55.Eq

I. INTRODUCTION

Owing to the possibility of gradual incorporation of magnetism to the well-known semiconductor matrices, diluted magnetic semiconductors (DMSs) (Refs. 1–4) offer unprecedented opportunity for examining *quantitatively* the origin of spin dependent couplings between band carriers and electrons localized on the open d shell. According to thorough studies of Mn-based II-VI DMSs, the spin-dependent coupling of the band-edge electrons and Mn spins is characterized by $N_0\alpha=250\pm60$ meV,[2] where N_0 is the cation concentration and α is the s-d exchange integral. The above value of $N_0\alpha$ is in a full accord with the notion that spin-dependent effects in the conduction band of a tetrahedrally coordinated DMS originate from the intra-atomic potential s-d exchange interaction. Indeed, the corresponding s-d exchange energy is 392 meV in the case of free Mn^{1+} ions,[5] and in a DMS it is a subject of up to twofold reduction by a covalent admixture of the anion s-type wave function to the Kohn-Luttinger amplitude at the conduction-band edge. In accord to this insight, $N_0\alpha=0.3$ eV results from *ab initio* computations for n-(Ga,Mn)As.[6]

Surprisingly, the recent comprehensive studies of quantum wells of highly dilute paramagnetic $Ga_{1-x}Mn_xAs$ ($x\leq0.13\%$) suggest *antiferromagnetic* $N_0\alpha=-23\pm8$ meV (Refs. 7 and 8) or -20 ± 6 meV (Ref. 9) for photoelectrons at the band edge. These observations have not been explained by the recent theory,[6] and appear to challenge the time-honored notion that the spin-dependent coupling between the electrons and Mn spins in a tetrahedrally coordinated DMS originates from the necessarily ferromagnetic intra-atomic potential s-d exchange.

The starting point of our approach is the realization that the density of Mn acceptors in the studied[8,9] quantum wells of GaAs was more than one order of magnitude lower than the critical value corresponding to the insulator-to-metal transition and the onset of the hole-mediated ferromagnetism in this system. Furthermore, a relatively high growth temperature resulted in a small concentration of compensating defects. Accordingly, the conduction-band photoelectrons interacted with complexes consisting of both Mn and hole spin, d^5+h, which are bound by the electrostatic potential and mutually coupled by a strong antiferromagnetic p-d exchange interaction. We develop here theory of the exchange interaction for such a case and show that it explains, with no adjustable parameters, the sign reversal of the apparent s-d exchange integral. Furthermore, we demonstrate that an assumption about the heating of the Mn spin subsystem, invoked in order to describe the observed dependence of electron-spin splitting on the magnetic field,[7,8] can be relaxed within the present theory.

Independently, much reduced spin splitting has been found for electrons injected to InAs quantum dots containing a neutral Mn acceptor.[10] This observation is consistent with the invoked here mutual cancelation of the s-d and s-p exchange energies.

Another case where the presence of bound holes is of primary importance is the Bir-Aronov-Pikus relaxation of electron spins. Surprisingly, it has recently been found[11] that the electron spin-relaxation time in GaAs:Mn is by two orders of magnitude longer comparing to GaAs:Ge, challenging a general belief that magnetic impurities are efficient spin coherence killers. This puzzling observation has been successfully interpreted[11] in accord to the theory presented here.[12]

While our model elucidates the origin of the anomalous sign and magnitude of the apparent s-d exchange integral for photoelectrons in p-type DMSs, it does not explain a reduced magnitude of this energy observed by electron-spin resonance in GaN:Mn,[13] and by electron spin-flip Raman scattering in GaAs:Mn.[14] We examine also this issue and demonstrate that the presence of a bottleneck effect and of a repulsive potential associated with ionized Mn acceptors in compensated III-V Mn-based DMSs leads to a sizable, Mn concentration dependent, reduction of the s-d exchange integral.

Our paper is organized as follows. In Sec. II we discuss a comparison of our theoretical results to experimental findings, delegating a detail description of the theory to subsequent sections. Thus, in Sec. III we present the adopted

model of the Mn acceptor in GaAs, including the form of the envelop functions and relevant Landé factors. This is followed by the derivation of the exchange integral J_{eh} describing the spin-dependent interaction between band electrons and bound holes, considering first the short-range (Sec. IV) and then the long-range part (Sec. V) of the electron-hole coupling. Finally, in Sec. VI we examine the effect of compensation on the magnitude of the apparent *s-d* exchange integral. Section VII contains a summary and outlook.

An important aspect of our theory is that the exchange integrals describing the coupling between conduction-band electrons and holes bound to acceptors can be expressed, with no adjustable parameters, by the acceptor envelop functions $f(r)$ and $g(r)$ as well as by the exchange splitting Δ and the longitudinal-transverse splitting Δ_{LT} of the bulk free excitons.

II. EXPLANATION OF THE OBSERVATIONS

The Mn acceptor complex can be described within the tight-binding approximation[15] or in terms of the Baldareschi-Lipari spherical model as proposed by Bhattacharjee and Benoit à la Guillaume[16] for GaAs:Mn and more recently employed to study impurity band effects.[17] We determine within this model how polarizations of a Mn spin $S=5/2$ and of a hole total angular momentum $J=3/2$ depend on the magnetic field B and temperature T. We then derive the form and magnitude of the exchange interactions between conduction-band electrons and holes bound by Mn acceptors, extracting relevant electron-hole *s-p* exchange parameters from the previous experimental studies of the free exciton in GaAs.

The Mn acceptor Hamiltonian for the magnetic field along z direction reads,

$$\mathcal{H} = \varepsilon \boldsymbol{J}\cdot\boldsymbol{S} + \mu_B B(g_{\mathrm{Mn}}S_z + g_h J_z), \tag{1}$$

where $\varepsilon=5$ meV is the experimentally determined *p-d* exchange energy in the Mn acceptor,[16] $g_{\mathrm{Mn}}=2.0$, and $g_h=0.75$ the is hole Landé factor derived in Sec. III. From the corresponding density matrix $\varrho=\exp[-\mathcal{H}/(k_BT)]$ we obtain $\langle S_z\rangle_{T,B}$ and $\langle J_z\rangle_{T,B}$. Within the molecular-field approximation, the exchange splitting of the conduction-band edge for uncompensated GaAs:Mn becomes

$$\hbar\omega_s(T,B) = xN_0[-\alpha\langle S_z\rangle_{T,B} + J_{\mathrm{eh}}\langle J_z\rangle_{T,B}], \tag{2}$$

where the second term arises from the coupling $(J_{\mathrm{eh}}/\mathcal{V})\boldsymbol{s}\cdot\boldsymbol{J}$ between the spin $\boldsymbol{s}$ of a band-edge electron and the angular momentum $\boldsymbol{J}$ of holes bound to Mn acceptors ($\mathcal{V}$ is the volume of the sample). As shown in Secs. IV and V, this interaction is characterized by the *s-p* exchange energy $N_0J_{\mathrm{eh}}=-0.51\pm0.17$ eV. Hence, for the expected values of $N_0\alpha$, the *s-p* exchange dominates over the *s-d* interaction. Furthermore, because of an antiferromagnetic sign of the *p-d* exchange interaction, $\langle S_z\rangle_{T,B}/\langle J_z\rangle_{T,B}<0$, the apparent coupling between the electron and Mn complex is antiferromagnetic. In particular, adopting $N_0\alpha=0.219$ eV we obtain the field dependence of electron-spin splitting shown in Fig. 1.

We recall that the data on the photoelectron precession frequency[7–9] were interpreted neglecting the presence of the bound holes ($J_{\mathrm{eh}}=0$) as well as by treating both $N_0\alpha$ and T in the Brillouin function $B_S(T,B)$ for $S=5/2$ as adjustable parameters.[7–9] Proceeding in the same way we can describe our theoretical results very well with $N_0\alpha^{(\mathrm{app})}=-20$ meV, $T_{\mathrm{eff}}=22$ K, as shown by dashed line in Fig. 1. We see that the present theory explains why the small antiferromagnetic apparent exchange energy $N_0\alpha^{(\mathrm{app})}=-20\pm6$ meV and enhanced temperature $T_{\mathrm{eff}}=20\pm10$ K were found experimentally.[8,9]

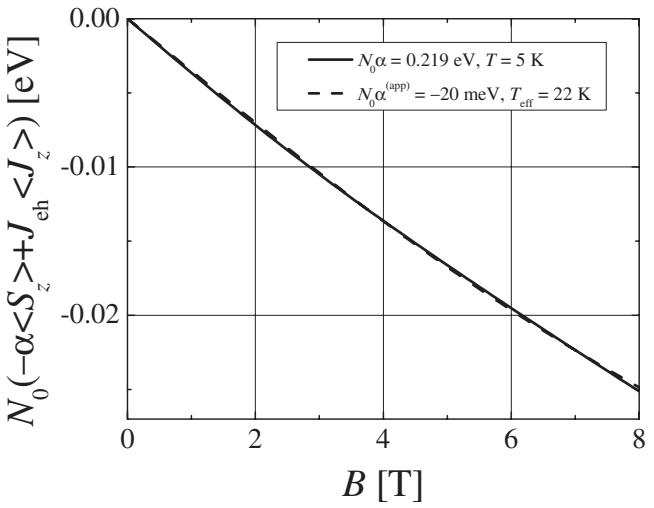

FIG. 1. Theoretical values of the electron spin-splitting energies $\hbar\omega_s(B)/x$ (solid line) computed as a function of the magnetic field at 5 K. Dashed line represents fitting to the solid line obtained by treating the apparent *s-d* exchange energy $N_0\alpha^{(\mathrm{app})}$ and temperature T_{eff} as adjustable parameters within the model that neglects the presence of the electron-hole exchange interaction ($J_{\mathrm{eh}}=0$).

It is worth noting that if the contributions of the two terms determining spin splitting compensate each other, the fitted values of $N_0\alpha^{(\mathrm{app})}$ and T_{eff} become correlated, so that only their ratio can be determined accurately. However, this correlation affects little the experimentally determined band-edge value of $N_0\alpha^{(\mathrm{app})}$ as it comes from the extrapolation of the data obtained for samples with finite quantum well width, in which the magnitudes of spin splitting are relatively large.

In addition to explaining the magnitude of spin splitting, the large value of the *s-p* exchange energy J_{eh} implied by our theory elucidates, as demonstrated recently,[11] why the spin-relaxation time in GaAs:Mn can be by two orders of magnitude longer than that in GaAs containing a similar concentration of Ge acceptors.

When the bound hole concentration is diminished by donor compensation, the relative importance of the *s-p* exchange decreases. This can be the case of a $Ga_{1-x}Mn_xAs$ sample with $x=0.1\%$, where $N_0\alpha^{(\mathrm{app})}=+23$ meV, according to spin-flip Raman scattering.[14] Even a lower value $|N_0\alpha|=14\pm4$ meV was found by analyzing the effect of the electrons on the Mn longitudinal relaxation time T_1 in n-$Ga_{1-x}Mn_xN$ with $x\leq0.2\%$.[13] The interpretation of the data was carried out[13] neglecting possible effects of the relaxation-time bottleneck,[18] which increases the apparent T_1. It can be shown, however, that for the expected magnitudes of electron spin-flip scattering times in wurtzite GaN:Mn,[19,20] this effect leads to an underestimation of the $|N_0\alpha|$ by less than a factor of 2. On the other hand, as dem-

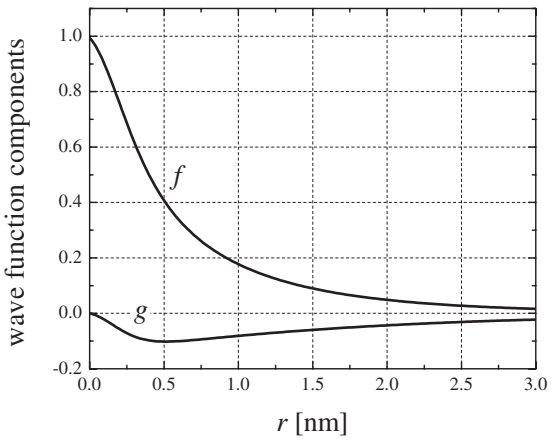

FIG. 2. The components of the acceptor wave function (see the main body of the text for the definition of the functions f and g).

onstrated in Sec. VI, the presence of positively charged donors shifts the electron wave function away from negatively charged Mn acceptors, which results in a rather strong reduction in the magnitude of the apparent s-d exchange integral in the relevant range of Mn concentrations in n-(Ga,Mn)N and compensated (Ga,Mn)As.

III. MODEL OF THE MANGANESE ACCEPTOR

The components $F_{\nu\mu}$ of the envelope function of the bound hole in the state $|\mu\rangle$, $\mu=\frac{3}{2},\frac{1}{2},-\frac{1}{2},-\frac{3}{2}$, are[16]

$$F_{\nu\mu}(\boldsymbol{r}) = \delta_{\mu\nu}R_0(r)Y_{00}(\theta,\phi) + \left\langle \frac{3}{2},\nu;2,(\mu-\nu)\middle|\frac{3}{2},\mu\right\rangle R_2(r)Y_{2,\mu-\nu}(\theta,\phi), \tag{3}$$

where $\nu=\frac{3}{2},\frac{1}{2},-\frac{1}{2},-\frac{3}{2}$ is the subband index (j_z). Accordingly, the spin-$\frac{3}{2}$ angular-momentum matrices j_α act on the index ν, while J_α act on the index μ. The radial functions $R_0(r)$ and $R_2(r)$ are obtained from the Baldareschi-Lipari equations by using a numerical solver of ordinary differential equations employing the standard values of the Luttinger parameters, $\gamma_1=6.85$, $\gamma_2=2.1$, $\gamma_3=2.9$, and $\kappa=1.2$ (Ref. 21). In order to model the Mn acceptor in GaAs we take $\varepsilon_\infty=10.66$ as the dielectric constant and the Gaussian central-cell potential with $r_0=2.8$ Å. The depth of the central-cell correction V_0 is chosen so that the binding energy without the exchange contribution is 86.15 meV (Ref. 16). We will use $f(r)=R_0(r)/\sqrt{4\pi}$, $g(r)=R_2(r)/\sqrt{4\pi}$, normalized as $\int_0^\infty 4\pi r^2[f(r)^2+g(r)^2]dr=1$. The functions $f(r)$, $g(r)$ are shown in Fig. 2.

Since both heavy and light hole masses are relevant, the spatial decay of the bound hole wave function is not characterized by a single exponent. An effective Mn acceptor Bohr radius calculated from the participation ratio is 0.76 nm for the wave function determined above. This agrees with the spatial extend of the probability density observed by scanning tunneling microscopy for the hole bound to Mn acceptor in GaAs.[15]

Now we calculate the Landé factor of the hole bound by the Mn acceptor, starting from the definition of the magnetic moment, $M_\alpha=-\partial\mathcal{H}_{\rm sph}/\partial B_\alpha|_{\boldsymbol{B}=0}$, where $\mathcal{H}_{\rm sph}$ is the hole Hamiltonian in the spherical approximation,

$$\mathcal{H}_{\rm sph} = \frac{\hbar^2}{m}\left\{\frac{1}{2}\gamma_1 k^2 - \bar{\gamma}\left[\left(j_x^2-\frac{1}{3}j^2\right)k_x^2 + c.p.\right] - 2\bar{\gamma}[\{j_x,j_y\}\{k_x,k_y\}+c.p.]\right\} - \frac{e\hbar}{m}\kappa\boldsymbol{j}\cdot\boldsymbol{B}, \tag{4}$$

in which $\{A,B\}=\frac{1}{2}(AB+BA)$, $\bar{\gamma}=(2\gamma_2+3\gamma_3)/5$, $k_\alpha=-i\frac{\partial}{\partial x_\alpha}-\frac{eA_\alpha}{\hbar}$, and the vector potential in the axial gauge is $A_\alpha=\varepsilon_{\alpha\beta\gamma}B_\beta x_\gamma/2$. We have

$$M_\alpha = \frac{e\hbar}{2m}\left\{\gamma_1\varepsilon_{\alpha\beta\gamma}x_\beta k_\gamma - 2\bar{\gamma}\left[\{j_\beta,j_\gamma\}-\frac{1}{3}\delta_{\beta\gamma}j^2\right]\varepsilon_{\alpha\delta\gamma}x_\delta k_\beta\right\} + \frac{e\hbar}{m}\kappa j_\alpha. \tag{5}$$

We substitute x_α and k_α in the spherical coordinates: $x=r\sin\theta\cos\phi$, $y=r\sin\theta\sin\phi$, $z=r\cos\theta$, $k_x=-i(\sin\theta\cos\phi\partial_r+\frac{1}{r}\cos\theta\cos\phi\partial_\theta-\frac{1}{r\sin\theta}\sin\phi\partial_\phi)$, $k_y=-i(\sin\theta\sin\phi\partial_r+\frac{1}{r}\cos\theta\sin\phi\partial_\theta+\frac{1}{r\sin\theta}\cos\phi\partial_\phi)$, $k_z=-i(\cos\theta\partial_r-\frac{1}{r}\sin\theta\,\partial_\theta)$. Finally, by acting with M_α on $F_{\nu\mu}$ and performing the integration over θ and ϕ we obtain

$$\langle\mu'|M_\alpha|\mu\rangle = \frac{e\hbar}{2m}\frac{4}{5}\int_0^\infty 4\pi r^2 dr \times\{g(r)[(\gamma_1-2\bar{\gamma})g(r)-\bar{\gamma}rf'(r)] + \bar{\gamma}f(r)[3g(r)+rg'(r)]\}J_{\alpha;\mu'\mu} + \frac{e\hbar}{m}\kappa\langle\mu'|j_\alpha|\mu\rangle, \tag{6}$$

where the value of the integral over r is -3.28. Therefore, $g_h=-[\frac{4}{5}\cdot(-3.28)+2\kappa\cdot 0.78]=0.75$, in a good agreement with the values given in Ref. 22 (observe the opposite sign convention). Moreover, substituting $g_1'=g_h$ and $g_2'=-0.07$ into the Eq. (3) of Ref. 23 yields $g_J=2.80$, in a good agreement with the experimental value of the complex g factor, $g_J=2.77$.

IV. SHORT-RANGE s-p EXCHANGE

We now derive a form of the short-range s-p exchange interaction between a conduction-band electron and a hole, which is valid for any localization radius of the hole. We make use of the known value of the free exciton exchange splitting Δ and the exciton Bohr radius a_X. Neglecting cubic terms of the form $j_x^3 s_x+j_y^3 s_y+j_z^3 s_z$, we obtain for the Hamiltonian of the short-range interaction a formula similar to Eq. 1 of Ref. 24,

$$\mathcal{H}^x = -\frac{1}{2}\pi a_X^3\Delta(\boldsymbol{s}\cdot\boldsymbol{j})\,\delta(\boldsymbol{r}_h-\boldsymbol{r}_e), \tag{7}$$

where $\Delta=0.006$ meV (Ref. 25, sign convention according to Ref. 26) and $a_X=12$ nm.

In the present case, we consider the coupling of a conduction-band electron to a hole bound to the Mn accep-

tor. Hence, we calculate the matrix elements $\langle \boldsymbol{k}_e,\sigma';\mu'|\mathcal{H}^x|\boldsymbol{k}_e,\sigma;\mu\rangle$, where $\boldsymbol{k}_e$ is the electron wave vector,

$$\langle \boldsymbol{r}_e|\boldsymbol{k}_e\rangle = \frac{1}{\sqrt{\mathcal{V}}}e^{i\boldsymbol{k}_e\cdot\boldsymbol{r}_e}, \tag{8}$$

σ is the electron spin, and μ numbers the spin states of the bound hole. Since

$$\langle \boldsymbol{k}_e|\delta(\boldsymbol{r}_h-\boldsymbol{r}_e)|\boldsymbol{k}_e\rangle = \frac{1}{\mathcal{V}} \tag{9}$$

and

$$\langle \mu'|j_\alpha|\mu\rangle = \left(\langle f^2\rangle + \frac{1}{5}\langle g^2\rangle\right)J_{\alpha;\mu'\mu}, \tag{10}$$

where $\langle f^2\rangle = \int_0^\infty 4\pi r^2 f(r)^2 dr$ etc., we obtain

$$\mathcal{H}_{SR} = -\frac{1}{2}\Delta\frac{\pi a_X^3}{\mathcal{V}}\left(\langle f^2\rangle + \frac{1}{5}\langle g^2\rangle\right)\boldsymbol{s}\cdot\boldsymbol{J}, \tag{11}$$

casting the short-range interaction into the required form involving $\boldsymbol{J}$, not $\boldsymbol{j}$. The numerical value is $\langle f^2\rangle + \frac{1}{5}\langle g^2\rangle = 0.78$. A similar reduction factor of the acceptor splitting was obtained previously for a variational wave function.[27] It appeared also in the case of DMS nanocrystals.[28] This value yields -0.28 eV as the contribution of the short-range interaction to $N_0 J_{\mathrm{eh}}$.

V. LONG-RANGE *s-p* EXCHANGE

The long-range interaction operator is given by[29]

$$\mathcal{H}^a_{m'n',mn}(\boldsymbol{r}_1'\boldsymbol{r}_2',\boldsymbol{r}_1\boldsymbol{r}_2) = -\sum_{\alpha,\beta} Q^{\alpha\beta}_{m'\mathcal{K}n,\mathcal{K}n'm}\frac{\partial^2 V(\boldsymbol{r}_1-\boldsymbol{r}_2')}{\partial r_{1\alpha}\partial r_{1\beta}} \times \delta(\boldsymbol{r}_1-\boldsymbol{r}_2)\delta(\boldsymbol{r}_1'-\boldsymbol{r}_2'), \tag{12}$$

$$Q^{\alpha\beta}_{m'\mathcal{K}n,\mathcal{K}n'm} = \frac{\hbar^2}{m^2E_g^2}p^\alpha_{m'\mathcal{K}n'}p^\beta_{\mathcal{K}nm}, \tag{13}$$

where $V(\boldsymbol{r}) = e^2/(4\pi\epsilon\epsilon_0 r)$ is the Coulomb potential. In particular, for an exciton with momentum $\boldsymbol{K}$ in the spin state j, the matrix element of this operator is

$$\langle j'\boldsymbol{K}'|\mathcal{H}^a|j\boldsymbol{K}\rangle = \frac{e^2}{\epsilon\epsilon_0}\frac{\hbar^2}{m^2E_g^2}\phi_{j'}\phi_j^*\delta_{\boldsymbol{K}\boldsymbol{K}'}, \tag{14}$$

where $\phi_j = \Sigma_{mn}[\Sigma_\alpha n_\alpha p^\alpha_{m\mathcal{K}n}]^* f^j_{\boldsymbol{K}mn}(0)$, $\boldsymbol{n} = \boldsymbol{K}/K$, and $f^j_{\boldsymbol{K}}(\boldsymbol{r})$ is the envelope function describing the relative motion of the electron and the hole in an exciton in the state $|j\boldsymbol{K}\rangle$.

We consider an exciton with the electron in the conduction band and the hole in the uppermost valence band of the Γ_8 symmetry. The canonical basis for the latter is $u_1 = |\frac{3}{2},\frac{3}{2}\rangle$, $u_2 = |\frac{3}{2},\frac{1}{2}\rangle$, $u_3 = |\frac{3}{2},-\frac{1}{2}\rangle$, $u_4 = |\frac{3}{2},-\frac{3}{2}\rangle$,

$$u_1 = -\frac{1}{\sqrt{2}}(X+iY)\uparrow, \tag{15}$$

$$u_2 = \frac{1}{\sqrt{6}}[-(X+iY)\downarrow + 2Z\uparrow], \tag{16}$$

$$u_3 = \frac{1}{\sqrt{6}}[(X-iY)\uparrow + 2Z\downarrow], \tag{17}$$

$$u_4 = \frac{1}{\sqrt{2}}(X-iY)\downarrow. \tag{18}$$

The time inversion operator acts as follows: $\hat{\mathcal{K}}u_i = \Sigma_j \mathcal{K}_{ji}u_j$, where the matrix $\mathcal{K}$ is

$$\mathcal{K} = \begin{pmatrix} 0 & 0 & 0 & i \\ 0 & 0 & -i & 0 \\ 0 & i & 0 & 0 \\ -i & 0 & 0 & 0 \end{pmatrix}. \tag{19}$$

It is convenient to use instead of $\alpha = x,y,z$ the index $a = -1,0,+1$, with $n_{+1} = -(n_x + in_y)/\sqrt{2}$, $n_0 = n_z$, $n_{-1} = (n_x - in_y)/\sqrt{2}$. Then we can express the momentum matrix elements in terms of Clebsch-Gordan coefficients:

$$\sum_\alpha n_\alpha p^\alpha_{m\mathcal{K}n} = P\sum_{n'}\sum_a \sqrt{\frac{4\pi}{3}}Y_{1a}(\boldsymbol{n})\left\langle 1,a;\frac{1}{2},m\middle|\frac{3}{2},n'\right\rangle \mathcal{K}_{n'n}, \tag{20}$$

where $P = \langle S|P_z|Z\rangle$. Assuming ground-state hydrogen wave functions for the envelope functions of the relative motion, we have $f^j_{\boldsymbol{K}mn}(0) = (\pi a_X^3)^{-\frac{1}{2}}\langle j|\frac{1}{2},m;\frac{3}{2},n\rangle$. Again, Clebsch-Gordan coefficients have been used and $|j\rangle = |J,J_z\rangle$, where $\boldsymbol{J}$ is the exciton spin $(J=1,2)$. We have $\phi_{|2,J_z\rangle} = 0$, $\phi_{|1,a\rangle} = (2i/\sqrt{3})P(\pi a_X^3)^{-\frac{1}{2}}n_a$. Therefore, $\|\phi\|^2 = \frac{4}{3}\frac{P^2}{\pi a_X^3}$ and we obtain the formula for the longitudinal-transverse exciton splitting,[26]

$$\Delta_{\mathrm{LT}} = \frac{4}{3}\frac{e^2}{\epsilon\epsilon_0}\frac{\hbar^2P^2}{m^2E_g^2}\frac{1}{\pi a_X^3}. \tag{21}$$

Now we can express the strength of the long-range interaction in terms of Δ_{LT},

$$Q^{\alpha\beta}_{m'\mathcal{K}n,\mathcal{K}n'm} = \frac{3}{4}\Delta_{\mathrm{LT}}\pi a_X^3\frac{\epsilon\epsilon_0}{e^2}\frac{p^\alpha_{m'\mathcal{K}n'}p^\beta_{\mathcal{K}nm}}{P^2}, \tag{22}$$

and calculate the matrix element

$$\langle \boldsymbol{k}_e,\sigma';\mu'|\mathcal{H}^a|\boldsymbol{k}_e,\sigma;\mu\rangle = \frac{1}{\mathcal{V}}\int d\boldsymbol{r}_1'd\boldsymbol{r}_2'd\boldsymbol{r}_1d\boldsymbol{r}_2 e^{-i\boldsymbol{k}_e\boldsymbol{r}_1'}F^*_{\nu'\mu'}(\boldsymbol{r}_2') \times \mathcal{H}^a_{\sigma'\nu',\sigma\nu}(\boldsymbol{r}_1'\boldsymbol{r}_2',\boldsymbol{r}_1\boldsymbol{r}_2)e^{i\boldsymbol{k}_e\boldsymbol{r}_1}F_{\nu\mu}(\boldsymbol{r}_2). \tag{23}$$

We use the following standard convention for the Fourier transform:

$$\tilde{f}(\boldsymbol{k}) = \int d\boldsymbol{r}e^{-i\boldsymbol{k}\cdot\boldsymbol{r}}f(\boldsymbol{r}). \tag{24}$$

Let

$$W_{\sigma'\nu,\nu'\sigma}(\boldsymbol{a}) = -Q^{\alpha\beta}_{\sigma'\nu,\nu'\sigma}\frac{\partial^2 V(\boldsymbol{a})}{\partial a_\alpha \partial a_\beta}, \tag{25}$$

$$\tilde{W}_{\sigma'\nu,\nu'\sigma}(\boldsymbol{q}) = \frac{3}{4}\Delta_{\mathrm{LT}}\pi a_X^3 \frac{q_\alpha q_\beta}{q^2}\frac{p^\alpha_{\sigma'\nu'}(p^\beta_{\sigma\nu})^*}{P^2}. \tag{26}$$

Then, using the properties of the Fourier transform, we can write the required matrix element as

$$\langle \boldsymbol{k}_e,\sigma';\mu'|\mathcal{H}^a|\boldsymbol{k}_e,\sigma;\mu\rangle = \frac{1}{\mathcal{V}}\{\tilde{W}_{\sigma'\nu,\nu'\sigma} * [(\tilde{F}_{\nu'\mu'})^* \cdot \tilde{F}_{\nu\mu}]\}(-\boldsymbol{k}_e), \tag{27}$$

where $*$ denotes the convolution

$$(\tilde{f} * \tilde{g})(\boldsymbol{k}) = \int \frac{d\boldsymbol{q}}{(2\pi)^3}\tilde{f}(\boldsymbol{q})\tilde{g}(\boldsymbol{k}-\boldsymbol{q}). \tag{28}$$

In particular, for $\boldsymbol{k}_e=0$,

$$\begin{aligned}\langle \sigma'\mu'|\mathcal{H}^a|\sigma\mu\rangle = \frac{3}{4}\Delta_{\mathrm{LT}}\frac{\pi a_X^3}{\mathcal{V}}\sum\int\frac{d\boldsymbol{q}}{(2\pi)^3} \\ \times [\tilde{F}_{\nu'\mu'}(\boldsymbol{q})]^*\frac{q^a}{q}\left\langle 1,a;\frac{1}{2},\sigma'\middle|\frac{3}{2},\xi'\right\rangle \mathcal{K}_{\xi',\nu'} \\ \times \mathcal{K}^*_{\xi,\nu}\left\langle 1,b;\frac{1}{2},\sigma\middle|\frac{3}{2},\xi\right\rangle\frac{(q^b)^*}{q}\tilde{F}_{\nu\mu}(\boldsymbol{q}),\end{aligned} \tag{29}$$

where the sum is over a,b,ν,ξ,ν',ξ'. To calculate this integral, Fourier transforms of the envelope functions in the spherical coordinates are needed. For $f(\boldsymbol{r})=f(r)Y_{lm}(\boldsymbol{r}/r)$, $\tilde{f}(\boldsymbol{k})=\tilde{f}(k)Y_{lm}(\boldsymbol{k}/k)$, where $\tilde{f}(k)=\int_0^\infty 4\pi r^2 dr f(r)Q_l(kr)$, and

$$Q_l(kr) = \frac{1}{2}\int_{-1}^{1} dx e^{-ikrx}P_l(x) = (-i)^l j_l(kr). \tag{30}$$

For $l=0$ and 2,

$$Q_0(kr) = \frac{\sin kr}{kr}, \tag{31}$$

$$Q_2(kr) = \frac{3kr\cos kr + (k^2r^2-3)\sin kr}{k^3r^3}. \tag{32}$$

The functions $\tilde{f}(k)$ and $\tilde{g}(k)$ are shown in Fig. 3. Now we can substitute the Fourier transforms into the integral and separate the radial and the angular integration.

By using the above results we obtain,

$$\mathcal{H}_{\mathrm{LR}} = -\frac{1}{6}\Delta_{\mathrm{LT}}\frac{\pi a_X^3}{\mathcal{V}}(\langle\tilde{f}^2\rangle - 2\langle\tilde{f}\tilde{g}\rangle + \langle\tilde{g}^2\rangle)\boldsymbol{s}\cdot\boldsymbol{J}, \tag{33}$$

where $\langle\tilde{f}^2\rangle=(2\pi)^{-3}\int_0^\infty 4\pi q^2\tilde{f}(q)^2dq$ etc. To compute $\langle\tilde{f}\tilde{g}\rangle$, one can use the identity $(r_1,r_2>0)$

$$\begin{aligned}\frac{1}{(2\pi)^3}\int_{k=0}^{\infty} 4\pi k^2 dk Q_0(kr_1)Q_2(kr_2) \\ = \frac{1}{4\pi}\left[\frac{\delta(r_2-r_1)}{r_1r_2} - \frac{3\theta(r_2-r_1)}{r_2^3}\right],\end{aligned} \tag{34}$$

from which it follows immediately that

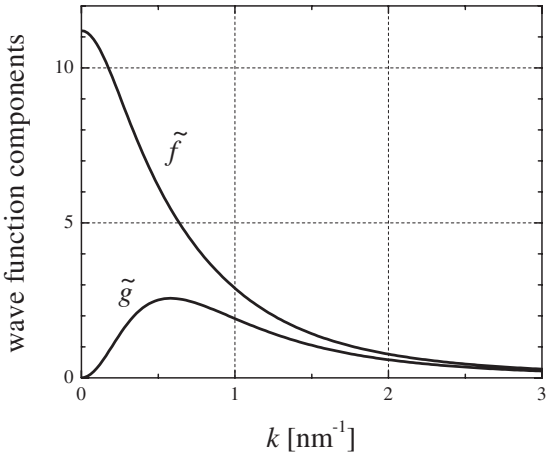

FIG. 3. The components of the acceptor wave function in the momentum representation (see the main body of the text for the definition of the functions $\tilde{f}$ and $\tilde{g}$).

$$\langle\tilde{f}\tilde{g}\rangle = \langle fg\rangle - 12\pi\int_0^\infty dr_2\int_0^{r_2} dr_1\frac{r_1^2}{r_2}f(r_1)g(r_2). \tag{35}$$

The numerical values are $\Delta_{\mathrm{LT}}=0.08\pm0.02$ meV (Refs. 30 and 31) and

$$\frac{1}{6}(\langle\tilde{f}^2\rangle - 2\langle\tilde{f}\tilde{g}\rangle + \langle\tilde{g}^2\rangle) = 0.024. \tag{36}$$

Hence, the contribution of the long-range s-p interaction to N_0J_{eh} is -0.23 eV, of the same order as the short-range part. Taking into account experimental uncertainty of the relevant parameters (we assume a 1 nm error of a_X and a 2 μeV error of Δ) we obtain the total magnitude of the electron-hole exchange energy $N_0J_{\mathrm{eh}}=-0.51\pm0.17$ eV.

For $\boldsymbol{k}_e\neq0$, the spherical symmetry is broken and $\mathcal{H}_{\mathrm{LR}}$ can no longer be cast into the form $\boldsymbol{s}\cdot\boldsymbol{J}$.

VI. APPARENT *s-d* EXCHANGE IN *n*-TYPE CASE

So far we have considered p-type systems, in which the interaction of photoelectrons with neutral Mn complexes is relevant. Now we examine compensated III-V Mn-based DMSs, in which the electron concentration n is greater than that of Mn impurities. In such samples of GaN:Mn and GaAs:Mn, strongly reduced magnitudes of the s-d exchange integral have been found by electron-spin resonance,[13] and by spin-flip Raman scattering,[14] respectively.

We note that in such samples Mn acceptors are ionized. Also ionized are donors, as the electron concentration corresponding to an insulator-to-metal transition is relatively low in the case of the conduction-band carriers. The presence of the corresponding repulsive and attractive Coulomb interactions means that the probability of finding a conduction-band electron at the core of the magnetic ion is reduced, and hence the *apparent* value of the exchange energy (the observed spin splitting) is diminished. It is worth noting that the possibility that the Coulomb potentials could affect the apparent value of the exchange integrals has already been mentioned in the

context of divalent Mn in GaN,[13] and trivalent Fe in HgSe.[32]

To evaluate a lower limit of the effect we neglect the presence of compensating donors and calculate the apparent *s-d* exchange integral $\alpha^{(\mathrm{app})}$ for an electron subject to the repulsive potential generated by the unoccupied Mn acceptors. We follow a Wigner-Seitz-type approach put forward by Benoit à la Guillaume *et al.*[33] to describe the interaction of the carrier spin with the Mn ions in the case of the strong-coupling limit, that is when the depth of the local Mn potential is comparable to the carrier bandwidth. It has been found in the subsequent works[34,35] that the corrections to the Wigner-Seitz approach caused by a random distribution of Mn ions are quantitatively unimportant.

We consider a Mn ion with the 5/2 spin $\vec{S}_i$ located at $\vec{R}_i$, which interacts with the carrier via the Heisenberg term $I(\vec{r}-\vec{R}_i)\vec{s}\cdot\vec{S}_i$. The form of the function $I(\vec{r}-\vec{R}_i)$ makes the interaction local: it vanishes outside the core of the Mn ion. For simplicity, $I(\vec{r}-\vec{R}_i)=a\theta(b-|\vec{r}-\vec{R}_i|)$. The exchange energy is then $\alpha=\int d^3\vec{r}I(\vec{r})=a\cdot\frac{4}{3}\pi b^3$. Moreover, in case of III-V compounds considered here, the impurity generates an electrostatic potential. If screening by the electrons is present, as in case of n-$Ga_{1-x}Mn_xN$, this potential is $e^2\exp(-\lambda r)/(4\pi\varepsilon\varepsilon_0 r)$, where ε is the static dielectric constant, and the screening parameter λ is given by $\lambda^2=e^2\mathcal{N}(\mathcal{E}_F)/(\varepsilon_0\varepsilon)$, where $\mathcal{N}(\mathcal{E}_F)=\frac{3}{2}n/kT_F$ (see Ref. 36, §5.2). For the $Ga_{1-x}Mn_xN$ samples,[13] $n\approx 10^{19}$ cm^{-3} corresponds to $T_F\approx 890$ K ($\mathcal{E}_F\approx 0.12$ eV), and therefore $1/\lambda\approx 1.6$ nm.

In the spirit of the Wigner-Seitz approach we assume that the carrier energy E and the envelope function $\psi(r)$ are given by the ground state s solution of the one-band effective-mass equation which contains the potential $U(r)$ created by the magnetic ion located at $r=0$. The standard one-impurity boundary condition $\psi(r)\to 0$ for $r\to\infty$ is replaced by the matching condition $\psi'(r)=0$ at $r=R$ to take into account the presence of other magnetic ions. The value R is determined by the concentration of the magnetic ions x according to the equation $(4\pi R^3/3)^{-1}=N_0 x$. The exchange interaction is modeled by a square-well potential $U\theta(b-r)$ superimposed on the electrostatic potential of an elementary charge located at $r=0$. The potential $U=\pm\frac{5}{4}a$ is, of course, different for spin-down and spin-up carriers.

We first ignore free-carrier screening, $\lambda\to 0$. The solution of the time-independent Schrödinger equation for the conduction-band electron in then

$$\psi(r)=c_0\exp(-\beta r)\Phi\left(1+\frac{A}{\beta};2;2\beta r\right)\equiv c_0 f \qquad (37)$$

for $0<r<b$, and the following linear combination for $b<r<R$

$$\psi(r)=c_1\exp(-\beta' r)\Psi\left(1+\frac{A}{\beta'};2;2\beta' r\right)+c_2\exp(\beta' r)\Psi\left(1-\frac{A}{\beta'};2;-2\beta' r\right)\equiv c_1 g+c_2 h, \qquad (38)$$

where $A=e^2m^*/(4\pi\varepsilon\varepsilon_0\hbar^2)$, $\beta=[2m^*(U-E)]^{\frac{1}{2}}/\hbar$, $\beta'=[2m^*(-E)]^{\frac{1}{2}}/\hbar$ (notice that changing the sign of β leaves ψ invariant, while changing the sign of β' interchanges c_1 with c_2; also, Φ and Ψ are not in general linearly independent). We used the symbols Φ, Ψ for the confluent hypergeometric functions ${}_1F_1(a;b;z)$, $U(a;b;z)$ (Ref. 37). The constants c_0, c_1, c_2 are determined by the continuity conditions $\psi(b^-)=\psi(b^+)$, $\psi'(b^-)=\psi'(b^+)$. Solving those two equations we obtain an equation for E,

$$\frac{w_{f,h}(b)g'(R)-w_{f,g}(b)h'(R)}{w_{g,h}(b)}=0, \qquad (39)$$

where by $w_{f,g}$ we denoted the Wronskian $fg'-f'g$.

We assume the following parameters for $Ga_{1-x}Mn_xN$: $m^*=0.22m_e$, $N_0=4.38\times 10^{22}$ cm$^{-3}=0.006495$ a.u., $\varepsilon=8.9$; and the following for $Ga_{1-x}Mn_xAs$: $m^*=0.067m_e$, $N_0=2.21\times 10^{22}$ cm$^{-3}=0.003281$ a.u., $\varepsilon=12.9$. In the experiments, samples were used with $0.01\%\le x\le 0.2\%$ of Mn in GaN,[13] and with $0.0006\%\le x\le 0.03\%$ of Mn in GaAs.[7] Those concentrations correspond to R up to about 75 a.u. for GaN and up to about 250 a.u. for GaAs.

To visualize the effect of the Coulomb term in the Mn potential, we have calculated the energies and wave functions including the additional Coulomb term for both GaN ($b=2$ a.u. ≈ 0.1 nm, $a=0.0371$ a.u. $=1.0$ eV) and GaAs ($b=2$ a.u. ≈ 0.1 nm, $a=0.0735$ a.u. $=2.0$ eV). These parameters correspond to $N_0\alpha=0.22$ eV. We have found that when calculating $\alpha^{(\mathrm{app})}/\alpha$, the details of the exchange potential (like the values of b and α within the expected range) are not quantitatively important.

In order to take into account the fact that the core and lattice polarizability decrease at small distances, $\varepsilon\to 1$ for $r\to 0$ we interpolate $\varepsilon(r)$ between $\varepsilon(0)=1$ and the macroscopic value attained at a distance of the bond length. The assumed dependence, presented in Fig. 4, is similar to that of the Thomas-Fermi model.[38] When $\varepsilon=\varepsilon(r)$ and/or free-carrier screening is included, we find the solution $\psi(r)$ of the Schrödinger equation for the given potential $U(r)$ numerically, as the Eqs. (37) and (38) are only valid for the Coulomb potential. Then, the spin splitting for a given value of x (or for the corresponding R) is evaluated as the difference of the energy E calculated for the spin-up and spin-down carriers from the equation $\psi'(R)=0$. Here, $\psi(r)$ is the numerical

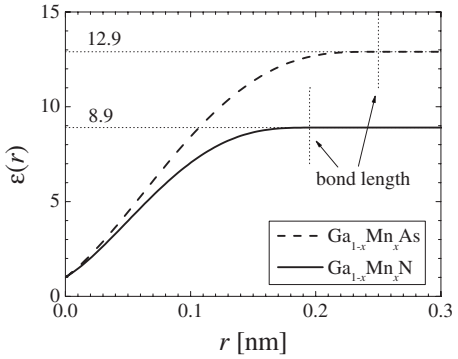

FIG. 4. The assumed dependence of the dielectric constant ε on the distance r to an ionized acceptor.

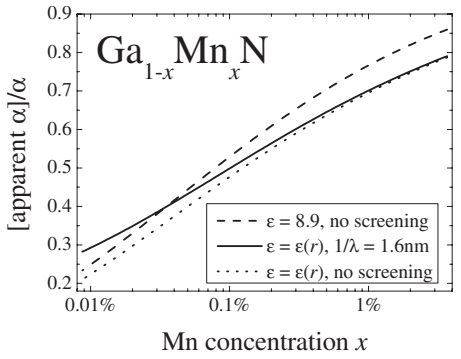

FIG. 5. The dependence of the ratio of the apparent and bare exchange energies α on x for for $Ga_{1-x}Mn_xN$ and various models of screening.

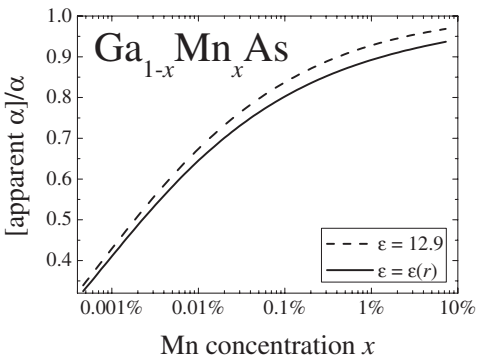

FIG. 6. The dependence of the ratio of the apparent and bare exchange energies α on x for $Ga_{1-x}Mn_xAs$.

solution of the Schrödinger equation with the potential that is different for spin-up and spin-down carriers.

The results of our calculations of $\alpha^{(app)}/\alpha$ as a function of the Mn ion concentration x are presented in Fig. 5 ($Ga_{1-x}Mn_xN$) and in Fig. 6 ($Ga_{1-x}Mn_xAs$). Independently of assumptions concerning screening, in both materials $\alpha^{(app)}/\alpha$ diminishes significantly when x decreases, up to factor of 3 in the experimentally relevant range of x. However, this reduction of $\alpha^{(app)}/\alpha$ is still smaller than that seen experimentally,[13,14] presumably because of an additional effect coming from the presence of attractive potentials brought about by compensating nonmagnetic donors.

VII. SUMMARY AND OUTLOOK

In order to understand the magnitude of the spin splitting of photoelectrons in Mn-based III-V DMSs, we have developed theory of the *s-p* exchange interaction between conduction-band electrons and holes localized on Mn acceptors, taking into account both short- and long-range contributions. According to our results, this exchange overcompensates the *s-d* interaction of the electrons with the Mn spins, making the resulting coupling to be antiferromagnetic. The theory describes, employing the standard value of the *s-d* exchange energy $N_0\alpha$=0.22 eV, the recent results on spin-splitting[7–9] and spin-relaxation time[11] of photoelectrons in GaAs:Mn with low Mn concentrations.

In view of our work, it would be remarkable to carry out Zeeman spectroscopy on nonmagnetic *p*-type semiconductors on the insulating side of the insulator-to-metal transition, where a large exchange splitting of the conduction band by the bound holes is predicted by the present theory. It would also be interesting to put forward an *ab initio* approach capturing such an effect. Finally, we note that the confinement-induced changes in the symmetry of the electron wave function explain,[6,9] via the *sp-d* kinetic exchange, the corresponding experimentally-revealed growth of the antiferromagnetic contribution to the exchange integral.[7–9] The question about the role of the simultaneously appearing *p-p* exchange is opened to further studies.

Furthermore, we have considered the interaction of conduction-band electrons with Mn ions in compensated *n*-type III-V DMSs, taking into account the electrostatic potential created by the magnetic ions. A substantial reduction in the magnitude of the apparent exchange energy has been found at low Mn concentrations, and interpreted as coming from the decrease of the carrier probability density at the core of the magnetic ion caused by the electrostatic repulsion. It has been suggested that this effect, enhanced by an attractive potential of compensating donors, accounts for reduced values of the exchange spin splitting observed experimentally in compensated III-V DMSs containing a minute amount of Mn.[13,14] In view of our findings, the presence of electrostatic potentials associated with magnetic ions makes that the apparent exchange energies should not be viewed as universal but rather dependent on the content of the magnetic constituent and compensating donors.

ACKNOWLEDGMENTS

We would like to thank W. Bardyszewski and R. Buczko for discussions. This work was supported in part by the EC project NANOSPIN (Grant No. FP6-2002-IST-015728).

*sliwa@ifpan.edu.pl
†dietl@ifpan.edu.pl

[1] *Diluted Magnetic Semiconductors*, Semiconductors and Semimetals, edited by R. K. Willardson and A. C. Beer, Vol. 25, edited by J. K. Furdyna and J. Kossut (Academic, New York, 1988).

[2] T. Dietl, in *Handbook on Semiconductors*, edited by T. S. Moss (North-Holland, Amsterdam, 1994), Vol. 3B, p. 1251.

[3] F. Matsukura, H. Ohno, and T. Dietl, in *Handbook of Magnetic Materials*, edited by K. H. J. Buschow (Elsevier, Amsterdam, 2002), Vol. 14, pp. 1–87.

[4] T. Jungwirth, J. Sinova, J. Mašek, J. Kučera, and A. H. MacDonald, Rev. Mod. Phys. **78**, 809 (2006).

[5] T. Dietl, C. Śliwa, G. Bauer, and H. Pascher, Phys. Rev. B **49**,

2230 (1994).
[6] G. M. Dalpian and S.-H. Wei, Phys. Rev. B **73**, 245204 (2006).
[7] R. C. Myers, M. Poggio, N. P. Stern, A. C. Gossard, and D. D. Awschalom, Phys. Rev. Lett. **95**, 017204 (2005).
[8] M. Poggio, R. C. Myers, N. P. Stern, A. C. Gossard, and D. D. Awschalom, Phys. Rev. B **72**, 235313 (2005).
[9] N. P. Stern, R. C. Myers, M. Poggio, A. C. Gossard, and D. D. Awschalom, Phys. Rev. B **75**, 045329 (2007).
[10] A. Kudelski, A. Lemaître, A. Miard, P. Voisin, T. C. M. Graham, R. J. Warburton, and O. Krebs, Phys. Rev. Lett. **99**, 247209 (2007).
[11] G. V. Astakhov, R. I. Dzhioev, K. V. Kavokin, V. L. Korenev, M. V. Lazarev, M. N. Tkachuk, Yu. G. Kusrayev, T. Kiessling, W. Ossau, and L. W. Molenkamp, Phys. Rev. Lett. **101**, 076602 (2008).
[12] C. Śliwa and T. Dietl, arXiv:0707.3542 (unpublished).
[13] A. Wołoś, M. Palczewska, Z. Wilamowski, M. Kamińska, A. Twardowski, M. Boćkowski, I. Grzegory, and S. Porowski, Appl. Phys. Lett. **83**, 5428 (2003).
[14] W. Heimbrodt *et al.*, Physica E (Amsterdam) **10**, 175 (2001).
[15] A. M. Yakunin, A. Yu. Silov, P. M. Koenraad, J. H. Wolter, W. Van Roy, J. De Boeck, J.-M. Tang, and M. E. Flatté, Phys. Rev. Lett. **92**, 216806 (2004).
[16] A. K. Bhattacharjee and C. Benoit à la Guillaume, Solid State Commun. **113**, 17 (2000).
[17] G. A. Fiete, G. Zaránd, K. Damle, and C. P. Moca, Phys. Rev. B **72**, 045212 (2005).
[18] S. Barnes, Adv. Phys. **30**, 801 (1981).
[19] M. Sawicki, T. Dietl, J. Kossut, J. Igalson, T. Wojtowicz, and W. Plesiewicz, Phys. Rev. Lett. **56**, 508 (1986).
[20] J. A. Majewski, Acta Phys. Pol. A **108**, 777 (2005); S. Schmult, M. J. Manfra, A. Punnoose, A. M. Sergent, K. W. Baldwin, and R. J. Molnar, Phys. Rev. B **74**, 033302 (2006); S. Cabañas, Th. Schäpers, N. Thillosen, N. Kaluza, V. A. Guzenko, and H. Hardtdegen, Phys. Rev. B **75**, 195329 (2007).
[21] T. Dietl, H. Ohno, and F. Matsukura, Phys. Rev. B **63**, 195205 (2001).
[22] A. V. Malyshev, I. A. Merkulov, and A. V. Rodina, Phys. Status Solidi B **210**, 865 (1998); see also, B. L. Gelmont and M. I. Dyakonov, Fiz. Tekh. Poluprovodn. (S.-Peterburg) **7**, 2013 (1973) [Sov. Phys. Semicond. **7**, 1345 (1974)].
[23] J. Schneider, U. Kaufmann, W. Wilkening, M. Baeumler, and F. Köhl, Phys. Rev. Lett. **59**, 240 (1987).
[24] H. Fu, L.-W. Wang, and A. Zunger, Phys. Rev. B **59**, 5568 (1999).
[25] E. Blackwood, M. J. Snelling, R. T. Harley, S. R. Andrews, and C. T. B. Foxon, Phys. Rev. B **50**, 14246 (1994).
[26] W. Ekardt, Solid State Commun. **22**, 531 (1977).
[27] J. Mycielski and C. Rigaux, J. Phys. (Paris) **44**, 1041 (1983).
[28] A. K. Bhattacharjee, Phys. Rev. B **51**, 9912 (1995).
[29] G. E. Pikus and G. L. Bir, Zh. Eksp. Teor. Fiz. **60**, 195 (1971).
[30] W. Ekardt, K. Lösch, and D. Bimberg, Phys. Rev. B **20**, 3303 (1979).
[31] R. G. Ulbrich and C. Weisbuch, Phys. Rev. Lett. **38**, 865 (1977).
[32] Z. Wilamowski, A. Mycielski, W. Jantsch, and G. Hendorfer, Phys. Rev. B **38**, 3621 (1988).
[33] C. Benoit à la Guillaume, D. Scalbert, and T. Dietl, Phys. Rev. B **46**, 9853 (1992).
[34] J. Tworzydło, Phys. Rev. B **50**, 14591 (1994).
[35] J. Tworzydło, Solid State Commun. **94**, 821 (1995).
[36] J. M. Ziman, *Principles of the Theory of Solids* (Cambridge University Press, London, 1972).
[37] L. J. Slater, *Confluent Hypergeometric Functions* (Cambridge University Press, Cambridge, England, 1960).
[38] R. Resta, Phys. Rev. B **16**, 2717 (1977).