

# Confinement-induced reduction of the effective exchange parameters in semimagnetic semiconductor nanostructures

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We present a theoretical study of the effect of reduced dimensionality on the Zeeman splittings of the electron and hole states. It is based on the effective mass approximation for the confined states and the wave vector dependence of the  $sp-d$  exchange interaction parameters in the bulk semimagnetic semiconductor. We find that the ratio of the exciton Zeeman splitting to the magnetization in a nanostructure is reduced with respect to the bulk by a factor  $\rho$  that depends on the degree of confinement. The effect is relatively small (a few percent) in quantum wells, but  $\rho$  as a function of the well width shows a minimum, in qualitative agreement with experimental data in  $\text{Cd}_{1-x}\text{Mn}_x\text{Te}/\text{Cd}_{1-x-y}\text{Mn}_x\text{Mg}_y\text{Te}$  heterostructures. In small-size quantum dots of  $\text{Cd}_{1-x}\text{Mn}_x\text{Te}$  the predicted reduction is drastic:  $\rho \approx 0.5$  for the dot radius  $R = 10 \text{ \AA}$ ; it increases rapidly with  $R$  and then saturates to about 0.84. We account for the available magnetoabsorption data in the wurtzite-structure nanocrystals of  $\text{Cd}_{1-x}\text{Mn}_x\text{Se}$ , where uniaxial anisotropy also contributes to a reduction of the average Zeeman splitting. [S0163-1829(98)03547-4]

## I. INTRODUCTION

Semimagnetic or diluted magnetic semiconductors (DMS's) such as  $\text{Cd}_{1-x}\text{Mn}_x\text{Te}$  are known for strong magneto-optical effects related to the large Zeeman splittings of the band states that result from the  $sp-d$  exchange interactions between the band electrons and the Mn ions. In the mean-field framework the Zeeman splittings are proportional to the magnetization of the Mn spin system, allowing an experimental determination of the exchange parameters.<sup>1</sup> An interesting question concerns the low-dimensional structures of DMS materials: How does the confinement affect the exchange parameters? The magnetoabsorption data in  $\text{Cd}_{1-x}\text{Mn}_x\text{Se}$  nanocrystals<sup>2</sup> indicate a reduction of the Zeeman splitting with respect to the bulk. Indeed, in a previous theoretical study<sup>3</sup> of DMS quantum dots (QD's), where we neglected the wave vector dependence of exchange interaction in the bulk, the confinement-induced mixing between the light- and heavy-hole band states was shown to yield a reduction of the effective exchange parameter for the four-fold hole ground state. In the wurtzite-structure  $\text{Cd}_{1-x}\text{Mn}_x\text{Se}$  nanocrystals, a further reduction of the average Zeeman splitting results from the uniaxial anisotropy. Thus, assuming the same magnetization as in the bulk, we accounted for the magnetoabsorption data in these QD's. On the other hand, heterostructures containing DMS's have been extensively investigated, basically revealing effects related to the magnetic-field tuning of band offsets, including interface anomalies. Recently, Mackh *et al.*<sup>4</sup> reported a study that focused on the effect of one-dimensional confinement per se. They studied single quantum wells (QW's) of  $\text{Cd}_{1-x}\text{Mn}_x\text{Te}/\text{Cd}_{1-x-y}\text{Mn}_x\text{Mg}_y\text{Te}$ , with a substantial band offset ( $y \sim 0.25$ ), but no discontinuity in the fractional Mn concentration across the interfaces. Apparently, there is no discontinuity in the  $sp-d$  or  $d-d$  exchange interactions either.<sup>5</sup> The Zeeman splitting of the heavy-hole exciton was found to be reduced with respect to the bulk by a factor that

depends on the well width ( $L_w$ ), showing a minimum of about  $\sim 0.9$  at  $L_w = 45 \text{ \AA}$ . The authors presented an explanation of their data by invoking the wave vector dependence of the  $sp-d$  exchange interactions in the bulk, previously investigated by us.<sup>6</sup>

In this paper we present a general treatment of the Zeeman effect for confined states, based on the effective mass approximation and the wave vector dependence of exchange. The confinement potential is assumed to be independent of the magnetic field. We show that the effective exchange parameters, defined in terms of the ratio of the Zeeman splittings to the magnetization, are indeed reduced with respect to the bulk. We explicitly consider the cases of QW's and QD's and compare our results with available experimental data. In QW's the reduction effect is quantitatively rather small, but the reduction factor  $\rho$  for the heavy-hole exciton does show a minimum as a function of  $L_w$ , in qualitative agreement with experiment. In the case of QD's the present treatment generalizes our earlier work<sup>3</sup> and yields a strong size dependence of  $\rho$  in small-size nanocrystals.

## II. THEORETICAL MODEL

The Kondo exchange Hamiltonian for the interaction between a band electron and a set of localized spins can be written in the Bloch function basis as

$$\langle \phi_{\nu', \mathbf{k}', \sigma'} | H_{\text{ex}} | \phi_{\nu, \mathbf{k}, \sigma} \rangle = -\delta_{\nu' \nu} \sum_i e^{i(\mathbf{k}-\mathbf{k}') \cdot \mathbf{R}_i} J_{\mathbf{k}' \mathbf{k}}^{\nu} (\mathbf{s} \cdot \mathbf{S}_i)_{\sigma' \sigma}. \quad (1)$$

Here  $\nu$ ,  $\mathbf{k}$ , and  $\sigma$  denote the band index, wave vector, and the  $z$  component of spin ( $\mathbf{s}$ ), respectively.  $\mathbf{R}_i$  and  $\mathbf{S}_i$  represent the position and spin of the  $i$ th Mn ion. In the effective-mass or envelope-function approximation the  $n$ th electron (conduction band) state in a nanostructure can be written as

$$\psi_{n,m}^e(\mathbf{r}) = f_n(\mathbf{r}) u^c(\mathbf{r}) |m\rangle, \quad (2)$$

where  $f_n(\mathbf{r})$  is the envelope function,  $u^c(\mathbf{r})$  the  $s$ -like conduction band Bloch function at  $\mathbf{k}=0$ , and  $m=s_z$ . The Zeeman components in a magnetic field along the  $z$  direction (neglecting the small direct contribution proportional to the  $g$  factor) are given by the expectation values of  $H_{\text{ex}}$ :

$$E_{n,m}^e = \sum \langle \psi_{n,m}^e | \phi_{\nu',\mathbf{k}',\sigma'} \rangle \langle \phi_{\nu',\mathbf{k}',\sigma'} | H_{\text{ex}} | \phi_{\nu,\mathbf{k},\sigma} \rangle \times \langle \phi_{\nu,\mathbf{k},\sigma} | \psi_{n,m}^e \rangle. \quad (3)$$

Inserting Eq. (1) into Eq. (3) and making the usual mean-field and virtual-crystal approximations we obtain

$$E_{n,m}^e = Nx \langle S_z \rangle \sum_{\nu,\mathbf{k},\sigma} \sigma J_{\mathbf{k}\mathbf{k}}^\nu |\langle \phi_{\nu,\mathbf{k},\sigma} | \psi_{n,m}^e \rangle|^2, \quad (4)$$

where  $N$  is the total number of primitive cells in the crystal,  $x$  the fractional concentration of Mn and  $\langle S_z \rangle$  the average Mn spin. Note that the virtual crystal approximation used to derive Eq. (4) implies a spatially uniform magnetization in the applied field. This seems well justified in specially designed heterostructures such as the ones of Ref. 4. In QD's the expected spatial fluctuations of  $\langle S_z \rangle$  in the surface layers should not significantly affect the Zeeman splittings, because the carrier wave function approaches zero in the region concerned. However, the average magnetization need not be the same as in the bulk. On the other hand, in a magnetic polaron<sup>7</sup> the spatial variation of the exchange field is of crucial importance, so that the effective exchange reduction factors deduced in the present work can be used only in the saturation limit.

Now, for small  $k$ ,

$$\phi_{c,\mathbf{k},\sigma}(\mathbf{r}) \approx \frac{1}{\sqrt{V}} u^c(\mathbf{r}) e^{i\mathbf{k}\cdot\mathbf{r}} |\sigma\rangle, \quad (5)$$

where  $V$  is the volume of the crystal. Using Eqs. (2) and (5) in (4) we have

$$E_{n,m}^e = N_0 x \langle S_z \rangle m \sum_{\mathbf{k}} J_{\mathbf{k}\mathbf{k}}^c |\tilde{f}_n(\mathbf{k})|^2, \quad (6)$$

where  $N_0 \equiv N/V$  and

$$\tilde{f}_n(\mathbf{k}) \equiv \int e^{-i\mathbf{k}\cdot\mathbf{r}} f_n(\mathbf{r}) d\mathbf{r}. \quad (7)$$

The conduction band Zeeman energies at  $\mathbf{k}=0$  in the bulk semiconductor are given by  $N_0 x \langle S_z \rangle \alpha m$ , where  $\alpha \equiv J_{00}^c/V$ . Thus, if the magnetization remains unchanged, the Zeeman splitting in the nanostructure would be reduced by the factor

$$\rho_n^e = \frac{1}{(2\pi)^3} \int \mathcal{J}^c(\mathbf{k}) |\tilde{f}_n(\mathbf{k})|^2 d\mathbf{k}, \quad (8)$$

because  $\mathcal{J}^c(\mathbf{k}) \equiv J_{\mathbf{k}\mathbf{k}}^c/J_{00}^c$  is a decreasing function of  $k$ . This describes a reduction of the effective exchange parameter. Note that in the absence of any wave vector dependence of the conduction band exchange, i.e., if  $\mathcal{J}^c(\mathbf{k})=1$ , there is no reduction for the electron states.

Let us now focus on the nanostructure hole states. In the strong spin-orbit coupling limit, the confined hole states can be built out of the four  $\Gamma_8$  valence band states:

$$\psi_\mu^h(\mathbf{r}) = \sum_\nu F_{\nu\mu}(\mathbf{r}) u_\nu^v(\mathbf{r}), \quad (9)$$

where  $\mu$  and  $\nu$  run through  $3/2$ ,  $1/2$ ,  $-1/2$ , and  $-3/2$ . Note that we have dropped the level index  $n$  for simplicity. Following the procedure developed above for the electron states, the Zeeman components are given by

$$E_\mu^h = Nx \langle S_z \rangle \sum_{p,\mathbf{k},\sigma} \sigma J_{\mathbf{k}\mathbf{k}}^p |\langle \phi_{p,\mathbf{k},\sigma} | \psi_\mu^h \rangle|^2, \quad (10)$$

where  $p=1,0,-1$  for the three  $p$ -like valence bands (in the absence of spin) which correspond to  $\Gamma_5$  at  $\mathbf{k}=0$ . For small  $k$ ,

$$\phi_{p,\mathbf{k},\sigma}(\mathbf{r}) \approx \frac{1}{\sqrt{V}} e^{i\mathbf{k}\cdot\mathbf{r}} \sum_{q=-1}^1 D_{qp}(\mathbf{k}) u_q^v(\mathbf{r}) |\sigma\rangle. \quad (11)$$

Here  $D(\mathbf{k})$  is a unitary transformation that diagonalizes the  $3 \times 3$   $\mathbf{k}\cdot\mathbf{p}$  matrix. By neglecting the dependence of exchange on the subband index  $p$ ,  $J^p \approx J^v$ , and using the unitarity of  $D$  matrices, we obtain

$$E_\mu^h = N_0 x \langle S_z \rangle \sum_{\mathbf{k},\nu} (\nu/3) J_{\mathbf{k}\mathbf{k}}^v |\tilde{F}_{\nu\mu}(\mathbf{k})|^2, \quad (12)$$

where  $\tilde{F}_{\nu\mu}(\mathbf{k})$  represent the Fourier transforms defined as in Eq. (7). The reduction factor  $\rho^h$  for the effective exchange that results from Eq. (12) will be derived separately for the two types of nanostructures considered.

### A. Quantum wells

For an idealized single QW of width  $L_w$  with  $z$  as the growth axis, the electron states are given by

$$f(\mathbf{r}) = \chi(z) \frac{e^{i\mathbf{k}_\perp \cdot \mathbf{r}_\perp}}{\sqrt{S_\perp}} \quad (13)$$

in the usual notations. The ground state corresponds to the even function

$$\begin{aligned} \chi(z) &= C \cos k_w z, \quad |z| \leq \frac{L_w}{2} \\ &= C \cos\left(\frac{k_w L_w}{2}\right) e^{-\kappa_b(|z| - L_w/2)}, \quad \text{otherwise,} \end{aligned} \quad (14)$$

where  $C$  is the normalization constant. Assuming the same effective mass  $m^*$  in the two media,  $\kappa_b^2 = (2m^*/\hbar^2) V_b - k_w^2$ , where  $V_b$  is the barrier height, and  $k_w$  the lowest solution of the transcendental equation:  $k_w \tan(k_w L_w/2) = \kappa_b$ . Also,  $C^2 = \kappa_b / (1 + \kappa_b L_w/2)$ .

Using this envelope function in Eq. (8), we obtain

$$\rho^e = \frac{1}{2\pi} \int \mathcal{J}^c(\mathbf{k}_\perp, k_z) |\tilde{\chi}(k_z)|^2 dk_z, \quad (15)$$

where

$$\tilde{\chi}(k) = \frac{2C \cos(k_w L_w/2)}{k^2 + \kappa_b^2} \left( \kappa_b \cos \frac{k L_w}{2} - k \sin \frac{k L_w}{2} \right) + C \left[ \frac{\sin[L_w(k+k_w)/2]}{(k+k_w)} + \frac{\sin[L_w(k-k_w)/2]}{(k-k_w)} \right], \quad (16)$$

and we shall assume  $\mathbf{k}_\perp = 0$ .

As for the hole states in a QW, with the growth axis along  $\langle 100 \rangle$ , the light- and heavy-hole states are uncoupled at  $\mathbf{k}_\perp = 0$ , and the effective masses are given by  $m_0/(\gamma_1 \pm 2\gamma_2)$ , respectively.<sup>8</sup> Thus, we can set  $F_{\nu\mu}(\mathbf{r}) = \delta_{\nu\mu} F_{|\mu|}(\mathbf{r})$  in Eq. (12), obtaining a reduction factor for each kind of hole, as in the case of electron. The corresponding ground-state envelope functions  $F(\mathbf{r})$  are given by Eqs. (13) and (14), with the appropriate masses and barrier potentials. Explicitly, we have

$$\rho^h = \frac{1}{2\pi} \int \mathcal{J}^v(0,0,k_z) |\tilde{\chi}_h(k_z)|^2 dk_z, \quad (17)$$

where we have used  $\mathcal{J}^v(\mathbf{k}) \equiv J_{\mathbf{k}\mathbf{k}}^v/J_{00}^v$ . Note that  $\beta = J_{00}^v V$  is the usual bulk valence-band exchange parameter at  $\Gamma$ . Finally, the ratio of the Zeeman splitting of the heavy-hole exciton (between the  $\sigma^-$  and  $\sigma^+$  components) to the magnetization is reduced by the factor

$$\rho = (\alpha\rho^e - \beta\rho^h)/(\alpha - \beta). \quad (18)$$

It is interesting to note that Eq. (18) remains valid when the excitonic binding effect is taken into account (by neglecting the  $e$ - $h$  exchange interaction), albeit with modified expressions for  $\rho^e$  and  $\rho^h$ . Assuming a separable variational exciton envelope function of the form<sup>9</sup>

$$\phi_{\text{exc}}(\mathbf{r}_e, \mathbf{r}_h) = C_{\text{exc}} \chi_e(z_e) \chi_h(z_h) e^{-|\mathbf{r}_{e\perp} - \mathbf{r}_{h\perp}|/\lambda}, \quad (19)$$

a straightforward calculation leads to

$$\rho^{e,h} = \frac{1}{\pi} \int_0^{2\pi/a} \mathcal{J}^{c,v}(k) |\tilde{\chi}_{e,h}^{\text{exc}}(k)|^2 dk, \quad (20)$$

with

$$|\tilde{\chi}_{e,h}^{\text{exc}}(k)|^2 \equiv 4\lambda^2 k^2 \int_0^1 \frac{|\tilde{\chi}_{e,h}(ku)|^2}{[1 + \lambda^2 k^2 (1 - u^2)]^3} du. \quad (21)$$

Here  $a$  is the lattice constant, and we have neglected the anisotropy of  $\mathcal{J}^{c,v}(\mathbf{k})$ . It should be emphasized that our treatment of QW's assumes identical  $sp$ - $d$  exchange interaction parameters  $J_{\mathbf{k}\mathbf{k}}^{c,v}$  in the well and barrier materials.

### B. Quantum dots

In a QD of radius  $R$  the electron ground-state envelope function is

$$f(\mathbf{r}) = \frac{1}{\sqrt{2\pi R}} \frac{\sin(\pi r/R)}{r}. \quad (22)$$

Using this in Eq. (8), we obtain the effective exchange reduction factor

$$\rho^e = \frac{4\pi}{R^3} \int_0^{2\pi/a} \mathcal{J}^c(k) |I_0(k, \pi/R)|^2 k^2 dk, \quad (23)$$

where

$$I_l(x, y) \equiv \int_0^R j_l(xr) j_l(yr) r^2 dr. \quad (24)$$

On the other hand, in the spherical approximation, the hole states can be written as the eigenstates of total angular momentum ( $J$ ) and its  $z$  component ( $M$ ):<sup>10</sup>

$$F_{\nu M}^J(\mathbf{r}) = \sum_L \left\langle L, M - \nu; \frac{3}{2}, \nu \middle| J, M \right\rangle R_L(r) Y_{L, M - \nu}(\theta, \phi), \quad (25)$$

where Clebsch-Gordan coefficients are used. The dipole-active ground state is of the  $S_{3/2}$  type ( $J = 3/2$  with  $L = 0, 2$ ). From Eq. (12) the Zeeman energies are

$$E_{JM}^h = (N_0 \beta/3) x \langle S_z \rangle \frac{1}{(2\pi)^3} \sum_L \delta_{JM}^L \int \mathcal{J}^v(k) |\tilde{R}_L(k)|^2 k^2 dk. \quad (26)$$

Here

$$\delta_{JM}^L \equiv \sum_\nu \nu \left| \left\langle L, M - \nu; \frac{3}{2}, \nu \middle| J, M \right\rangle \right|^2 \quad (27)$$

and

$$\tilde{R}_L(k) \equiv \int R_L(r) j_L(r) 4\pi r^2 dr. \quad (28)$$

Finally, in the case of  $S_{3/2}$  states,

$$\delta_{3/2, M}^L = M/(2L + 1). \quad (29)$$

Thus, the reduction factor for the hole ground state can be written as

$$\rho^h = \rho_0^h + \frac{1}{5} \rho_2^h, \quad (30)$$

where

$$\rho_L^h \equiv \frac{1}{(2\pi)^3} \int \mathcal{J}^v(k) |\tilde{R}_L(k)|^2 k^2 dk. \quad (31)$$

Equation (30) shows that there is a reduction even in the absence of any wave vector dependence of exchange; it results from the mixing of the light- and heavy-hole band states.<sup>3</sup> The radial functions are<sup>11</sup>

$$R_0(r) = D[j_0(\kappa r/R) - t j_0(\sqrt{\eta} \kappa r/R)], \\ R_2(r) = -D[j_2(\kappa r/R) + t j_2(\sqrt{\eta} \kappa r/R)]. \quad (32)$$

Here  $t \equiv j_0(\kappa)/j_0(\kappa\sqrt{\eta})$ ,  $\eta$  is the ratio of the light- and heavy-hole effective masses and  $\kappa$  is the lowest solution of  $j_0(\kappa)j_2(\kappa\sqrt{\eta}) + j_2(\kappa)j_0(\kappa\sqrt{\eta}) = 0$  for the ground state. Thus,  $\tilde{R}_L(k)$  can be written as a linear combination of the integrals  $I_l(k, \kappa/R)$  and  $I_l(k, \sqrt{\eta}\kappa/R)$ , defined in Eq. (24). Let us point out that our discussion of the QD's is limited to the strong-confinement regime, with  $R$  assumed smaller than

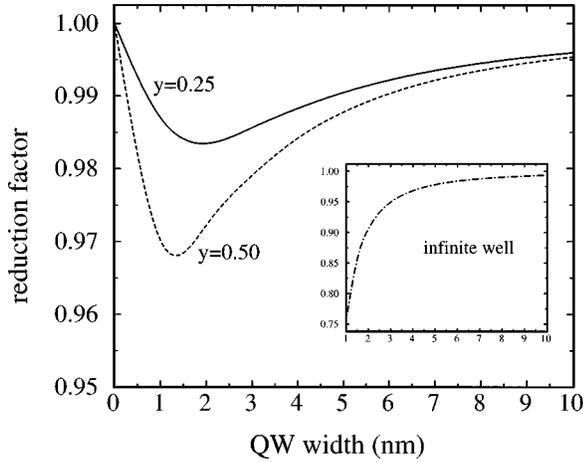


FIG. 1. Reduction factor  $\rho$  for the heavy-hole exciton as a function of the QW width (nm) in  $\text{Cd}_{1-x}\text{Mn}_x\text{Te}/\text{Cd}_{1-x-y}\text{Mn}_y\text{Mg}_y\text{Te}$  single QW's for  $y=0.25$  (solid curve) and  $0.50$  (dashed curve). The curve in the inset corresponds to the limit of infinite barrier height.

the bulk exciton Bohr radius. Thus, the effective exchange reduction factor for the Zeeman splitting between the strong components of the excitonic transition is simply given by Eq. (18).

### III. RESULTS AND DISCUSSION

In order to calculate the reduction factors in the different cases, we need to know  $\mathcal{J}^c(k)$  and  $\mathcal{J}^v(k)$ , describing the wave vector dependence of the  $sp-d$  exchange interactions in the bulk. We shall resort to a tight-binding model,<sup>6</sup> developed previously in order to account for the reduced excitonic Zeeman splitting at the  $L$  point of the Brillouin zone in bulk DMS's.<sup>12</sup> The model is recapitulated in the Appendix.

In Fig. 1 we present the calculated reduction factor  $\rho$  for the heavy-hole exciton in  $\text{Cd}_{1-x}\text{Mn}_x\text{Te}/\text{Cd}_{1-x-y}\text{Mn}_y\text{Mg}_y\text{Te}$  QW's. The results are based on the following parameters: the band gap difference  $\Delta E_g = 1.6y$  eV and the valence-band offset coefficient 0.3 (Ref. 13). In the absence of any data for the alloys, the effective mass parameters in both materials are assumed to be the same as those of CdTe:  $m_e^* = 0.096m_0$ ,  $\gamma_1 = 4.7$ ,  $\gamma_2 = 1.45$ , and  $\gamma_3 = 1.9$  (Ref. 14). Also,  $a = 6.48$  Å and  $\beta/\alpha = -4$ . We have plotted  $\rho$  as a function of the well width for  $y=0.25$  (solid curve) and  $0.50$  (dashed curve). The curve in the inset shows the limit of infinite barrier height. We see that  $\rho$  first decreases rapidly from 1, goes through a minimum and then increases slowly to 1. As the barrier height increases,  $\rho$  decreases and the position of the minimum shifts to a lower well width.

A comparison between the theoretical curve for  $y=0.25$  and the experimental data of Ref. 4 shows good qualitative agreement. But, quantitatively, the observed reduction at the minimum is  $\sim 10\%$ , while the calculated value is only  $\sim 2\%$ . The origin of this large discrepancy is not clear. We have examined the contribution of the two-dimensional confinement due to excitonic binding [see Eqs. (19)–(21)]. For example, at  $L_w = 30$  Å the variational calculation yields a binding energy of 17 meV and  $\lambda \approx 68$  Å, leading to a negligibly small reduction of the  $\rho$  value obtained without exciton effect. Moreover, the subband dispersion calculations<sup>8</sup>

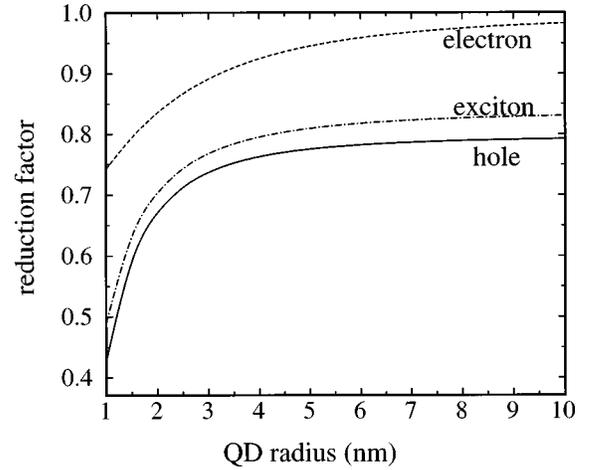


FIG. 2. Reduction factors for the electron, hole, and exciton ground states in  $\text{Cd}_{1-x}\text{Mn}_x\text{Te}$  QD's plotted against the QD radius (nm).

suggest that the mixing of light- and heavy-hole band states can indeed be neglected in the case of heavy-hole exciton. The correction due to the larger electron effective mass in the barrier is also negligible. It is tempting to attribute the discrepancy to a possible inadequacy of the simple model for the wave vector dependence of exchange. However, the applicability of our theory to  $\text{Cd}_{1-x}\text{Mn}_x\text{Te}/\text{Cd}_{1-x-y}\text{Mn}_y\text{Mg}_y\text{Te}$  heterostructures is also questionable. To our knowledge, no direct measurement of the exchange parameters  $N_0\alpha$  and  $N_0\beta$  in bulk  $\text{Cd}_{1-x}\text{Mn}_x\text{Mg}_y\text{Te}$  has yet been reported. While the Zeeman data of Ref. 5 suggest that  $N_0(\alpha - \beta)$  is the same as in  $\text{Cd}_{1-x}\text{Mn}_x\text{Te}$ ,  $N_0\alpha$  and  $N_0\beta$  separately need not be identical in the two systems, let alone the wave vector dependence. Finally, let us point out that the preliminary calculation presented in Ref. 4, which gave a reduction of  $\sim 3\%$ , implicitly assumed  $\tilde{\chi}(k) \propto \delta(k - k_w)$  for the heavy hole ground state; in fact, the maximum of the function  $\tilde{\chi}(k)$  is located at  $k=0$  [see Eq. (16)].

Figure 2 shows the results for  $\text{Cd}_{1-x}\text{Mn}_x\text{Te}$  QD's. The different reduction factors  $\rho^e$ ,  $\rho^h$ , and  $\rho$  are plotted against the QD radius. Clearly, as expected, the reduction effect is quantitatively much more important than in the case of QW's. The strong size dependence in small-size QD's results from the wave vector dependence of exchange. Note that  $\rho^h$  rapidly approaches the saturation value  $\rho_{\text{sat}}^h \approx 0.8$ , which simply corresponds to the effect of mixing between the light- and heavy-hole states, considered previously.<sup>3</sup> To our knowledge, no experimental data are available for  $\text{Cd}_{1-x}\text{Mn}_x\text{Te}$  QD's. Yanata *et al.*<sup>2</sup> reported magnetoabsorption data in  $\text{Cd}_{0.9}\text{Mn}_{0.1}\text{Se}$  nanocrystals of average radius 5 nm; in a magnetic field ( $B$ ) of 7 T the absorption spectrum at  $T=4.2$  K shows a redshift of  $\sim 40$  meV. We obtained 39 meV within the simplified model of Ref. 3, by taking the uniaxial anisotropy into account and assuming the same magnetization as in the bulk. Here, we reexamine this case in view of the present model. In Ref. 3, following Efros,<sup>11</sup> we assumed  $\eta=0.14$  for the ratio of the light- and heavy-hole masses in CdSe and obtained the size-independent reduction factor  $\rho_{\text{sat}}^h = 0.7$ . However, realistic CdSe band parameters<sup>15</sup> give  $\eta=0.28$ , leading to  $\rho_{\text{sat}}^h = 0.96$ . In the present model we obtain  $\rho^h$

$=0.94$  and  $\rho^e=0.95$  at  $R=5$  nm. But the larger value of  $\eta$  corresponds to a larger splitting between the light- and heavy-hole levels,<sup>11</sup> yielding a stronger anisotropy. Thus, averaging over the random orientation of the QD  $c$  axis with respect to the applied field, we now obtain 43.5 meV for the redshift in  $R=5$  nm nanocrystals, in reasonable agreement with experiment. Note that the redshift in the bulk is 58 meV when  $B\parallel c$ , indicating a reduction of  $\sim 25\%$  in the nanocrystals. However, the dominating factor is anisotropy; the reduction due to confinement per se is only  $\sim 5\%$  in this case.

#### IV. CONCLUDING REMARKS

We have presented a theoretical model for calculating the Zeeman splittings in low-dimensional DMS structures, when the confinement potential does not depend on the magnetic field. The effective exchange parameters, defined in terms of the ratio of the Zeeman splittings to the magnetization, are found to be reduced with respect to the bulk. The reduction factors depend on the degree of confinement and are related to the wave vector dependence of  $sp-d$  exchange interaction parameters in the bulk. There is a further reduction in the case of QD hole states, which results from the mixing between the light- and heavy-hole band states. For the Zeeman splitting of the heavy-hole exciton in  $\text{Cd}_{1-x}\text{Mn}_x\text{Te}/\text{Cd}_{1-x-y}\text{Mn}_x\text{Mg}_y\text{Te}$  QW's investigated by Mackh *et al.*,<sup>4</sup> the predicted reduction is too small. However, the variation of  $\rho$  with the well width, showing a minimum, is in good qualitative agreement with experiment. As expected, the confinement-induced reduction is stronger in QD's. Numerical results presented for  $\text{Cd}_{1-x}\text{Mn}_x\text{Te}$  indicate that  $\rho\approx 0.5$  for the QD radius 10 Å; it increases rapidly with size and then saturates to the value 0.84, determined by the ratio of the light- and heavy-hole effective masses. In the wurtzite-structure  $\text{Cd}_{0.9}\text{Mn}_{0.1}\text{Se}$  nanocrystals of average radius 50 Å studied by Yanata *et al.*<sup>2</sup> the uniaxial anisotropy plays a dominant role in reducing the average Zeeman splitting; we obtain a good agreement with the magnetoabsorption data. Small-size zinc blende nanocrystals of  $\text{Cd}_{1-x}\text{Mn}_x\text{Te}$  would be more suitable for an experimental investigation of the confinement-induced reduction of effective exchange parameters. The reduction should be also important in quantum wires; our calculation can be easily extended to this case.

#### APPENDIX

Here we recapitulate the model of Ref. 6 for the wave vector dependence of  $sp-d$  exchange interactions. The conduction band exchange  $J_{\mathbf{k}\mathbf{k}}^c$  is dominated by the on-site  $s-d$  exchange integral of the Coulomb potential. Using the four-orbital empirical tight binding model of Larson *et al.*<sup>16</sup> for  $\text{Cd}_{1-x}\text{Mn}_x\text{Te}$  band structure, we obtain the wave vector dependence

$$\mathcal{J}^c(\mathbf{k}) = 1 - \frac{B}{(A^2 + 2B) + A\sqrt{A^2 + 2B}} \quad (\text{A1})$$

with

$$A \equiv 2.52 - 0.92 \cos \frac{ka}{2}, \quad B \equiv 19.46 \left( 1 - \cos \frac{ka}{2} \right) \quad (\text{A2})$$

for  $\mathbf{k}$  along  $\langle 100 \rangle$ . Here  $a$  is the lattice constant. The valence band exchange  $J_{\mathbf{k}\mathbf{k}}^v$  mainly arises from the  $p-d$  hybridization and its  $\mathbf{k}$  dependence is dominated by the hopping interference term:

$$\mathcal{J}^v(\mathbf{k}) \propto \left| \sum_{\delta_1} e^{i\mathbf{k}\cdot\delta_1} + s \sum_{\delta_2} e^{i\mathbf{k}\cdot\delta_2} \right|^2, \quad (\text{A3})$$

where  $\delta_1$  and  $\delta_2$ , respectively, represent the position vectors of the first- and second-neighbor anions with Mn at the origin.  $s$  is the ratio between the first- and second-neighbor  $p-d$  hopping amplitudes. Explicitly,

$$\mathcal{J}^v(\mathbf{k}) = \frac{1}{2(1+3s)^2} \left[ (1+4s+5s^2) + (1+6s+7s^2) \cos \frac{ka}{2} + 2s(1+2s) \cos ka + 2s^2 \cos \frac{ka}{2} \cos ka \right] \quad (\text{A4})$$

for  $\mathbf{k}\parallel\langle 100 \rangle$ . As in Ref. 6, we assume  $s=0.1$ , which yields a satisfactory agreement with the magnetorefectivity data at the  $L$  point. While the variation of the conduction band exchange given by Eq. (A1) drastically overestimates the value at the  $L$  point, it is expected to provide a reasonable approximation for small  $k$ , most relevant in our present discussion.

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