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Highly anisotropic Zeeman splittings of wurtzite $\text{Cd}_{1-x}\text{Mn}_x\text{Se}$ quantum dots

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The electronic structure and Zeeman splittings of wurtzite $\text{Cd}_{1-x}\text{Mn}_x\text{Se}$ quantum spheres are studied using the $k \cdot p$ method and mean-field model. It is interesting to find that the Zeeman splittings of some hole states in quantum spheres are highly anisotropic due to the spin-orbit coupling and wurtzite crystal structure. The anisotropy of the Zeeman splittings of hole ground states in large dots is large, while that in small dot is small because the hole ground states vary with radius. An external electrical field can change the Zeeman splitting significantly, and tune the g factor from nearly 0 to about 100. © 2007 American Institute of Physics. [DOI: 10.1063/1.2784192]

Nowadays, much of the research in semiconductor physics has been shifting toward diluted magnetic semiconductors (DMSs),¹⁻³ which have extensive applications in spintronics. Manganese-doped II-VI (Ref. 4) and III-V (Ref. 1) compound semiconductors have been widely studied. Meanwhile, the investigations of quantum confinement of carriers in spatially modulated semiconductor structures have been a field of intense activity over the past decades. High-quality CdSe quantum dots were synthesized recently.^{5,6} The electronic structure of these quantum spheres under magnetic field were theoretically studied.^{7,8} The method to dope Mn ions into CdSe quantum dots was achieved.⁹ DMS quantum dots were used as spin-polarized light-emitting diodes.¹⁰ The electron and hole states in zinc-blende DMS quantum dots were studied using $k \cdot p$ method.¹¹

The anisotropic Zeeman splitting was earlier found in the GaAs/AlAs quantum wells.¹² The fine structure of excitons in GaAs/AlAs quantum wells showed that the perpendicular (to the well plane) g factors of the heavy hole g_{hz} are in between 2 and 3, while the in-plane values g_{hx} and g_{hy} are smaller than 0.01. This strong anisotropy of the effective hole g value is a consequence of description of the heavy-hole states with $J_{hz} = \pm \frac{3}{2}$ by an effective spin $S_h = \frac{1}{2}$. From the spin Hamiltonian it can be seen that the in-plane splittings can only be due to the cubic hole Zeeman interaction terms. The small values of g_{hx} and g_{hy} correspond to a small q value in a bulk semiconductor. On the other hand, the bulk linear hole Zeeman splitting constant κ , which is about 1.2 for GaAs, results in a large g_{hz} value for GaAs layer samples.

Recently, the anisotropic Zeeman splitting has been found in ballistic one-dimensional hole systems.¹³ The splitting of the subband edges is shown in the transconductance gray scale plot when an in-plane magnetic field is applied parallel to the one-dimensional (1D) GaAs hole systems. In contrast, the transconductance gray scale shows that the degenerate 1D subbands are not affected by the perpendicular

magnetic field of up to 8.8 T, i.e., no Zeeman splitting is seen when the magnetic field is aligned perpendicular to the channel. This anisotropy of the effective g factor is a direct consequence of the one-dimensional confinement on a system with strong spin-orbit coupling.

It is expected that the anisotropic Zeeman splitting will also happen in quantum dots, which is very interesting and useful as the carriers' spins in quantum dots can be used as qubits for quantum information processing.¹⁴ In this letter, we use the six-band $k \cdot p$ method of semiconductor quantum dots, taking into account the p - d exchange interaction, to study the electronic structure, Zeeman splittings, and g factors of paramagnetic wurtzite $\text{Cd}_{1-x}\text{Mn}_x\text{Se}$ quantum spheres under external magnetic and electric fields.

We represent the six-band hole Hamiltonian under external magnetic and electric fields of DMS wurtzite quantum dots in the basis functions $|11\rangle \uparrow$, $|10\rangle \uparrow$, $|1-1\rangle \uparrow$, $|11\rangle \downarrow$, $|10\rangle \downarrow$, $|1-1\rangle \downarrow$ as

$$H_{\text{tot}} = - \begin{pmatrix} H_{h0} & 0 \\ 0 & H_{h0} \end{pmatrix} - H_{\text{so}} + V_{\text{Efield}} - H_{\text{mm},h} + H_{\text{asym}} + H_{\text{Zeeman},h} + H_{\text{pd}}. \quad (1)$$

H_{h0} is written as

$$H_{h0} = \frac{1}{2m_0} \begin{pmatrix} P_1 & S & T \\ S^* & P_3 & S \\ T^* & S^* & P_1 \end{pmatrix}, \quad (2)$$

where P_1 , P_3 , S , T , H_{so} , $H_{\text{mm},h}$, H_{asym} , $H_{\text{Zeeman},h}$, and the effective-mass parameters of CdSe were given in detail before.⁸ V_{Efield} is the electric field potential term. When the electric field F is applied along the x direction, $V_{\text{Efield}} = eFx$.

H_{pd} is the p - d exchange interaction Hamiltonian between the hole and magnetic ion, which is written as²

$$H_{\text{pd}} = \beta s_h \cdot \mathbf{M} / (g_{\text{Mn}} \mu_B), \quad (3)$$

where $g_{\text{Mn}} = 2$, s_h is the spin operator of the hole, β is the p - d exchange constant, $\beta N_0 = -1.11$ eV,³ N_0 is the number of

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FIG. 3. (a) Hole levels of $\text{Cd}_{1-x}\text{Mn}_x\text{Se}$ quantum spheres with $R=1.5$ nm and $x_{\text{eff}}=0.05$ at $F=0$ and $T=10$ K as functions of B ($B||z$). (b) Similar to (a) but $B||x$. (c) Hole g factor of $\text{Cd}_{1-x}\text{Mn}_x\text{Se}$ quantum spheres with $x_{\text{eff}}=0.05$ at $B=0.02$ T ($B||z$), $F=0$, and $T=10$ K as a function of R . (d) Similar to (c) but $B||x$.

the first excited states instead of the ground states have highly anisotropic Zeeman splitting. It is due to the change of hole ground states, as shown in Fig. 1(a). Figures 3(c) and 3(d) show the g_z and g_x of the hole ground states as functions of R . The sharp changes indicate the level crossing. We see that g_z is always big, while g_x is small when R is large. This significant change of g_x gives a way to test the interesting level crossing in wurtzite quantum dots which causes the dark exciton^{7,8} whose exciton recombination time is very long. This long living exciton is useful for investigating the properties of excitons, such as the Bose-Einstein condensation of excitons. As the spin states of the hole ground states of small ($R < 2.5$ nm) and large ($R > 2.5$ nm) quantum dots are different, we can use them as different types of qubits for quantum information processing.¹⁴

Therefore, the states which have very different space-wave functions have highly anisotropic Zeeman splitting. The former works on highly anisotropic Zeeman splittings^{12,13} focused on the heavy-hole states whose space-wave functions are different (such as $^0SX^+ \uparrow$ and $^0SX^- \downarrow$ in Fig. 1). Our explanation is applicable to their results and suggests investigation of the highly anisotropic Zeeman splitting of other states that have very different space-wave functions.

Figure 4 shows the hole levels and g factors of $\text{Cd}_{1-x}\text{Mn}_x\text{Se}$ quantum spheres with $R=5$ nm in the presence of magnetic field and electric field. The electric field induces state coupling [see Fig. 1(b)], and changes the spin states of the hole ground states. Thus, the Zeeman splittings are changed significantly by the electric field. Compared to the $F=0$ case (see Fig. 2), the Zeeman splitting of the hole ground states when $B||x$ is increased dramatically. The g factors can be tuned by the electric field, as shown in Figs. 4(c) and 4(d). g_z decreases and g_x increases with increasing electric field due to the state coupling. It is interesting to note that g_x varies from nearly 0 to larger than 100 as the electric field increases. Thus at a fixed magnetic field, we can use the electric field to tune the hole spin to be unpolarized ($g_x=0$) or polarized (g_x is large).

In summary, we studied the electronic structure, Zeeman splittings and g factors of wurtzite $\text{Cd}_{1-x}\text{Mn}_x\text{Se}$ quantum spheres using the six-band $k \cdot p$ method taking into account the p - d exchange interaction between the carrier and the magnetic ion. It is interesting to find that the Zeeman

FIG. 4. (a) Hole levels of $\text{Cd}_{1-x}\text{Mn}_x\text{Se}$ quantum spheres with $R=5$ nm and $x_{\text{eff}}=0.05$ at $F=15$ mV/nm ($F||x$) and $T=10$ K as functions of B ($B||z$). (b) Similar to (a) but $B||x$. (c) Hole g factor of $\text{Cd}_{1-x}\text{Mn}_x\text{Se}$ quantum spheres with $R=5$ nm and $x_{\text{eff}}=0.05$ at $B=0.02$ T ($B||z$) and $T=10$ K as a function of F ($F||x$). (d) Similar to (c) but $B||x$.

splittings of the hole states in quantum spheres can be highly anisotropic due to the spin-orbit coupling and the wurtzite crystal structure. The states which have very different space-wave functions have highly anisotropic Zeeman splitting. The anisotropy of the Zeeman splittings of hole ground states in large dots is large, while that in small dot is small, due to the change of hole ground states with radius, and this gives us a way to test the interesting level crossing in wurtzite quantum dots which causes the long living dark exciton.^{7,8} An external electrical field can change the Zeeman splitting significantly, and tune the g factor from nearly 0 to about 100 due to the coupling of hole states induced by the electric field. Under a fixed magnetic field, we can use the electric field to tune the hole spin to be unpolarized ($g_x=0$) or polarized (g_x is large).

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