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Energy Level Calculations in Diluted Magnetic Semiconductor Core Shell Quantum Dots

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Abstract From the present experiment, it is clear that in small magnetic field, the energies of spin–up electron state increases with increasing magnetic fields and decreases for spin-down electron states with increasing magnetic fields. At small magnetic field, the energies are determined by the exchange interaction term for both spin up and spin down electron states. At large magnetic field, the exchange term approaches to a constant and the energies are determined mainly by the magnetic confinement term that is the Zeeman term. The analysis made in this research can be useful for predicting tunneling of electrons and holes from core to shell and can have applications in calculating the spin polarized current from the CSQDs.

Keywords *Semiconductor, Junction Semiconductors, Quantum Dots*

1. Introduction

Magnetic semiconductors are semiconductor materials that exhibit both ferromagnetism and useful semiconductor properties. Magnetic semiconductors would also allow control of quantum spin state (up or down). Furdyna J.K., (1988) for the first time reviewed the physical properties of diluted magnetic semiconductors (DMS) of the type $A^{II}1\text{-}xMnxB^{VI}$. Diluted magnetic semiconductors (DMSs), i.e. semiconducting crystals whose lattice is made up in part of substitutional magnetic ions (e.g. $Cd_{1-x}Mn_xTe$, $Hg_{1-x}Fe_xSe$, $Zn_{1-x}Co_xS$) (Samarth *et al*., 1990). A wide class of semiconducting materials is available, which are characterized by the random substitution of a fraction of the original atoms by magnetic atoms. Such materials are termed commonly as semimagnetic semiconductors (SMSC) or diluted magnetic semiconductors (DMS) (Balkanski and Wallis, 2000). The most common SMSC are II-VI compounds (like CdTe, ZnSe, CdSe, CdS, etc.), with transition metal ions (e.g. Mn, Fe or Co) substituting their original cations. There are also materials based on IV-VI (e.g. PbTe, SnTe) and recently III-V (e.g. GaAs, InSb) crystals. In some cases, the rare earth elements (e.g. Eu, Gd, Er) are also used as magnetic atoms in SMSC. These mixed crystals (semiconductor alloys) are thought to consider as containing two interacting subsystems. The first of these is the system of delocalized

conduction and valence band electrons (Kyrychenko and Kossut, 2000). The second is the random, diluted system of localized magnetic moments associated with the magnetic atoms. The fact that both the structure and the electronic properties of the host crystals are well known means that they are perfect for studying the basic mechanisms of the magnetic interactions coupling the spins of the band carriers and the localized spins of magnetic ions. The coupling between the localised moments results in the existence of different magnetic phases (such as paramagnets, spin glasses and antiferromagnets).

The manganese-based SMSC (i.e. with Mn as the magnetic cations) has provided a good understanding of the behavior of these semiconductors. The first of wide gap SMSC to be studied was CdMnTe. The extremely large Zeeman splittings of the electronic bands, and the giant Faraday rotation observed have been ascribed to the exchange interaction between the s, p band electrons and the d electrons associated with the Mn ions. A quantum dot (QD) is a nanoscale structure (Goronkin *et al*., 1999) consisting of one or more semiconducting materials in which the motion of fundamental charge carriers is confined in all spatial dimensions (Nicolas, 2006). Nanocrystals of group II-VI semiconductor quantum dots in which electron and holes are three dimensionally confined within the exciton Bohr radius of material are characterized by the optical properties such as broad absorption and sharp emission bands.

2. Materials and Methods

The experiment was carried as per the standard method of Luttinger (1995). Under spherical approximation the luttinger parameters for ZnSe are as $\gamma_1 = 3.94$, $\gamma_2 = 1.00$,and $\gamma_3 = 1.52$, the luttinger parameters for ZnS are $\gamma_1 = 1.77$, $\gamma_2 = 0.3$ and $\gamma_3 = 0.62$; Lande g-factor for electron, $g_e = 1.15$ and for hole $g_h = 1.62$; fitting parameters So and To are 0.41 and 3.6 respectively; effective mass of electron $m_e^* = o.17$ and the Luttinger parameter kappa $\kappa = 0.64$.

3. Results and Discussion

The frame work so far has the generality intact and is applicable to all magnetic doped II-VI semiconductor core shell quantum dots (CSQDs). The present results have been applied to a specific CSQDs of which core is made of Mn doped ZnSe and shell is ZnS. For numerical estimation, we have chosen Mn ions as the transition metal ions for doping and have accounted for the s-d and p-d exchange interaction. We considered very small DMS CSQDs in the strong confinement regime with both magnetic field and geometrical confinements influencing the optical properties of the CSQDs. More or less similar observations have been reported by Bergqvist *et al*., (2004). The authors demonstrated that the magnetic properties of diluted magnetic semiconductors are dominated by short ranged interatomic exchange interactions that have a strong directional dependence. In present experiment, the radius of the core of CSQDs is taken to be $2.5x10^{-9}m$ which is smaller than the exciton Bohr radius 5.2x10^{-9} m. The magnetic field was assumed to be applied along z-direction such that a symmetric magnetic confinement occurs in x-y plane.

The electron and hole energies are given by:

$$E^{\pm}{}_{e} = \frac{9}{4}\frac{\pi^2 A c^2 \hbar^2}{\sqrt{m_e{}^3 V_c}} \pm \frac{1}{2} g_e \mu_B B \mp A_{ex}$$

$$E_{hh}^{\pm} = \frac{\hbar^2}{2m_0 a^2} \pm \frac{3heB\kappa}{4m_0} \mp 3B_{ex}$$

The material parameters used in the calculation are the conduction and valence band offset which are 0.58ev and 0.03ev respectively. Kyrychenko and Kossut (2000) presented a theoretical study of the valence-band states in diluted magnetic semiconductor quantum wire structures. As a consequence of confinement in two directions, the hole states in a quantum wire are known to be mixtures of heavy- and light-hole components. Due to a strong p-d exchange interaction in diluted magnetic semiconductors, the relative contribution of these components is strongly affected by an external magnetic field, which lends complete support to our findings.

Luttinger parameters under spherical approximation are taken as 3.94, 1.00 and 1.52 for ZnSe while for ZnS the same Luttinger parameters are 1.77, 0.3 and 0.62. Lande g-factor for electron $g_e = 1.15$ and for hole $g_h = 1.62$, fitting parameters So and To be 0.41 and 3.6 respectively. Effective mass of electron $m_e = 0.17$ and the Luttinger parameter $\kappa = 0.64$. Using these parameters in equations 1 and 2 above, the electron energy as function of magnetic field have been plotted in Figure 1 for concentration (0.1, 0.2, 0.3) at temperature T=10k.

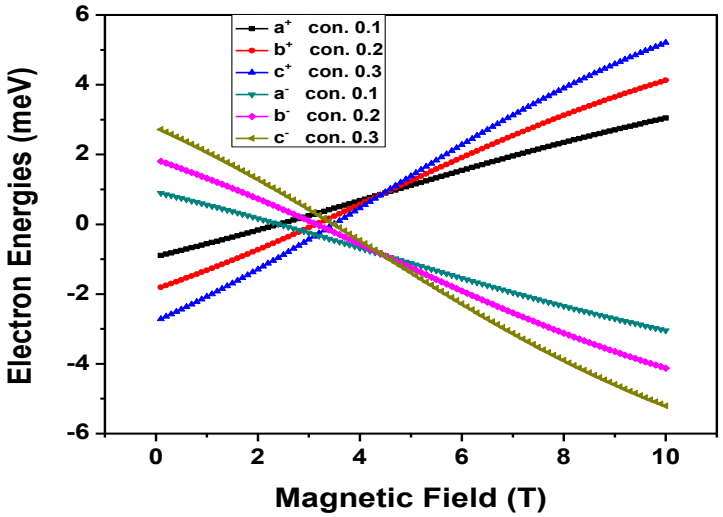

Figure 1: *Electron Energy as Function of Magnetic Field*

The curves $a^{\pm}, b^{\pm}, c^{\pm}$ are plotted for the dopant concentration 0.1, 0.2 and 0.3 respectively. The super scripts $\pm$ represent the electron spin up and spin down states.

From the Figure 1, it is clear that at small magnetic field, the energies of spin–up electron states increases with increasing magnetic fields and decreases for spin-down electron states with increasing magnetic fields. At small magnetic field, the energies are determined by the exchange interaction term for both spin up and spin down electron states. At large magnetic field, the exchange term approaches to a constant and the energies are determined mainly by the magnetic confinement term that is the Zeeman term. The reason for this is that at large magnetic fields, the doped Mn ions are aligned completely. This further reveals that the Zeeman splitting of electron dominates over the exchange splitting. Therefore, we find cross over point of both spin up and spin down states where the exchange term and the Zeeman term compensate.

Another interesting observation from Figure 1 is the occurrence of change of the sign of the splitting energy. The change in the sign splitting arises due to the fact that the exchange splitting opposes the Zeeman splitting and their orders of magnitude are same for the electrons. Also the splitting energies increase linearly with low fields, depending on doping concentration and shows non linear behavior at modest fields. The reason is that the low external magnetic field partially aligns the Mn spins, and at higher fields all the Mn spins are aligned completely. As the effective manganese concentration increases, the Zeeman splitting energies are getting larger.

In carrying out electron energy calculations, we incorporated s-d exchange interaction. In order to examine the effect of magnetic impurity doping on hole energies, p-d exchange interaction is incorporated. Using the physical parameters defined for ZnSe/ZnS CSQDs, we have obtained the variation in hole energies as a function of magnetic field at T=50k for 10, 20, 30 percent impurity concentration. Figure 2 exhibits hole energy variations as a function of magnetic field in arbitrary scale.

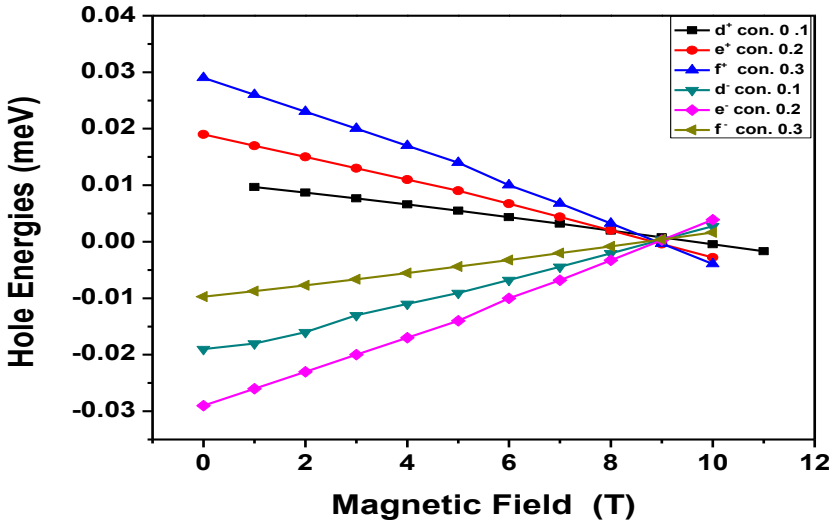

Figure 2: *Hole Energy as a Function of Magnetic Field*

The curves $d^{\pm}, e^{\pm}, f^{\pm}$ are plotted for the dopant concentration 0.1, 0.2 and 0.3 respectively. The super scripts $\pm$ represent the hole spin up and spin down states. The behavior of the energies of the hole states shown in Figure 2 is much more complicated as they decrease rapidly with increasing magnetic field and cross over at certain value of magnetic field where the Zeeman splitting is compensated by the exchange splitting.

The exchange splitting can be ascribed to the p-d exchange interaction. The splitting under such circumstances is approximately $6B_{ex} = \frac{N_0 \beta \langle S_z \rangle x}{6}$. If we consider an equivalent magnitude of Zeeman splitting for holes, then the intrinsic magnetic field which can generate such amount of Zeeman splitting can be found to be $\frac{2B_{ex} m_0}{e\hbar\kappa}$. Since B_{ex} is directly proportional to the dopant concentration, the magnitude of the intrinsic magnetic field can be seen to increase with the increasing Mn dopant concentration. Figure 2 also indicates that the exchange splitting of hole dominates over the Zeeman splitting which is reverse in case of electrons.

The hole states are more complicated than the electron states, because the wave function of the hole state consists of components of different J_z and l values and they mix with each other due to the contribution of the off- diagonal terms in the hole Hamiltonian.

The exchange interaction term and the Zeeman term cause splitting of the energies of these components at small magnetic field. At large magnetic field, the hole energy increases slightly due to the magnetic confinement, but is different for different states that have different orbital momentum (l). Also from Figure 2, the energy levels due to spin up and spin down hole states cross with each other. This is because the magnetic field due to exchange and the field due to magnetic confinement are applied simultaneously to ZnSe/ZnS CSQDs.

5. Conclusion

Conclusively, we calculated electron and hole energies in CSQDs in which the core is a diluted magnetic semiconductor by taking into account the s-d and p-d exchange interactions. The hole energies have been calculated using the Luttinger Hamiltonian. For this purpose, it was assumed that the electrons and holes are confined within the core of the quantum dot. The confinement energy being equal to the conduction and valence band offsets. In DMS the spin of electrons and holes is lifted due to s-d and p-d exchange interactions respectively. By using Luttinger Hamiltonian it was found that the Luttinger parameters modify due to exchange interactions in the presence of magnetic field. The analytical results are applicable to the entire II-VI semiconductor CSQDs. The numerical analysis has been carried out for ZnSe/ZnS CSQDs with core being doped by Mn ions. It was observed that the exchange splitting compensates the Zeeman splitting. The analysis made in this research can be useful for predicting tunneling of electrons and holes from core to shell and can have applications in calculating the spin polarized current from the CSQDs.

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