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DOUBLE ACCEPTOR INTERACTION IN SEMIMAGNETIC QUANTUM DOT

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The effect of geometry of the semimagnetic Quantum Dot on the Interaction energy of a double acceptor is computed in the effective mass approximation using the variational principle. A peak is observed at the lower dot sizes as a magnetic field is increased which is attributed to the reduction in confinement.

Keywords: *DOUBLE ACCEPTOR, SEMIMAGNETIC QUANTUM DOT, COULOMB INTERACTION ENERGY, SHAPE EFFECT.*

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1. INTRODUCTION

Semimagnetic Quantum Dots like CdTe/$Cd_{1-x}Mn_xTe$ is widely studied because increase of composition Mn ion [1] or magnetic field [2] causes a transition from Type I to Type II superlattice. A slight deformation which is treated as perturbation can cause a change in shape of a Quantum Dot (QD) leading to the lifting of the degeneracy in the energy levels. The spectra of electron and donor states in a QD on proper size and shape have been studied by Zia-Lin Zhu, et al. [3]. Thus the geometry of the Quantum Dot plays a vital role on the binding energy of the donor [4] as well as on the diamagnetic susceptibility as the donor wavefunction is altered. The study of shape effect of QD may be useful in understanding physical phenomenon and designing materials and devices in QD structures. The study of double donor [5] /acceptor [6] impurities had been carried out widely on GaAs systems and the Coulombic interaction energies had been calculated for both with [7] and without magnetic field [8]. In this work we calculate the hole-hole Coulombic interaction energy in CdMnTe/CdTe Quantum dot in the effective mass approximation using variational principle for various geometries. As the confining potential in semimagnetic nanostructures can be manipulated by an externally applied magnetic field, one expects the Coulombic interaction studies in such material to be important for device applications.

2. THEORY

The Hamiltonian of the hydrogenic double acceptor impurity in the CdTe Cubical Quantum Dot (CQD) system of $Cd_{1-x}Mn_xTe$ / CdTe superlattice in the effective mass approximation in the presence of magnetic field applied along the growth direction is given as

$$H_1 = -\nabla_1^2 - \nabla_2^2 - \frac{2}{r_1} - \frac{2}{r_2} + V_B(\vec{r}_1) + V_B(\vec{r}_2) \tag{1}$$

$$H_2 = +\gamma L_{z1} + \frac{\gamma r_1^2 \sin^2 \vartheta_1}{4} + \gamma L_{z2} + \frac{\gamma r_2^2 \sin^2 \vartheta_2}{4} + \frac{2}{|\vec{r}_1 - \vec{r}_2|} \tag{2}$$

$$H = H_1 + H_2 \tag{3}$$

Using effective Bohr radius $a_B{}^* = \hbar^2\varepsilon_0/m^*e^2$ as unit of length, effective Rydberg $R^* = e^2/2\varepsilon_0 a_B{}^*$ as unit of energy and the strength of the magnetic field parameter $\gamma = \hbar\omega_c/2R^*$ where ω_c is the cyclotron frequency and $r_1 = \sqrt{x_1^2 + y_1^2 + z_1^2}$, $r_2 = \sqrt{x_2^2 + y_2^2 + z_2^2}$. The confining potential for $Cd_{1-x1}Mn_{x1}Te$ quantum dot is given by

$$V_B = \begin{cases} 0 & |x| \le \frac{L_x}{2}, |y| \le \frac{L_y}{2}, |z| \le \frac{L_z}{2} \\ V_0 & |x| \le \frac{L_x}{2}, |y| \le \frac{L_y}{2}, |z| \le \frac{L_z}{2} \end{cases} \tag{4}$$

where L_x, L_y and L_z is the length of the sides in x, y and z directions of the dot respectively and $V_0 = 0.3\Delta E_g^B$ where ΔE_g^B is the band gap difference with magnetic field and is given by [12].

$$\Delta E_g^B = \Delta E_g^0 \left[\frac{\eta \exp(\zeta\gamma) - 1}{\eta - 1} \right] \tag{5}$$

where ΔE_g^0 is the band gap difference between CdTe and $Cd_{1-x}Mn_xTe$ without magnetic field and $\eta = \exp(-\zeta\gamma_0)$, where ζ is a parameter(= 0.5) and γ_0 is the critical magnetic field which depends upon the value of the composition x. The band gap of $Cd_{1-x}Mn_xTe$ is given to be $1.606 + 1.587x$ eV. The critical magnetic field is given as $B_0 = A\exp(nx)$ Tesla with $A = -0.57$ and $n = 16.706$ which is a best fit to the extrapolated experimentally available critical fields.

The trial wavefunction for the singlet ground state of the double acceptor hole in a CQD is given by

$$\psi_1 = N \cos(\alpha x_1) \cos(\alpha y_1) \cos(\alpha z_1) \cos(\alpha x_2) \cos(\alpha y_2) \cos(\alpha z_2) \tag{6}$$

$$\psi_i = \psi_1 \exp\left(-\lambda |r_1 - r_2|\right) \tag{7}$$

$$\psi_0 = NB \exp\left[-\beta(x_1 + y_1 + z_1)\right] \exp\left[-\beta(x_2 + y_2 + z_2)\right] \exp\left[-\lambda |r_1 - r_2|\right] \tag{8}$$

$$\psi(r_1, r_2) = \begin{cases} \psi_i & |x| \le \frac{L_x}{2}, |y| \le \frac{L_y}{2}, |z| \le \frac{L_z}{2} \\ \psi_0 & |x| \le \frac{L_x}{2}, |y| \le \frac{L_y}{2}, |z| \le \frac{L_z}{2} \end{cases} \tag{9}$$

where N is the normalisation constant, $\alpha = (2m^*E/3)^{1/2}$ and $\delta = (2m^*(V_0 - E)/3)^{1/2}$, λ is the variational parameter and B is obtained from the continuity condition. E is the lowest energy without the acceptor impurity. The minimum of the Hamiltonian $\langle H \rangle_{\min}$ is evaluated and the variational parameter λ is fixed in the wave function $\psi(r_1, r_2)$ and this wavefunction is used to evaluate the hole-hole interaction energy

$$E_{hh} = \left\langle \psi(r_1, r_2) \right| \frac{2}{\left| \vec{r}_1 - \vec{r}_2 \right|} \left| \psi(r_1, r_2) \right\rangle \tag{10}$$

3. RESULTS AND DISCUSSIONS

The various cross sectional geometries of the QD are defined as $G_j(x, y, z)$: G1(L, L, L), G2(L, $L/2$, L) and G3($L/2$, $L/4$, L).

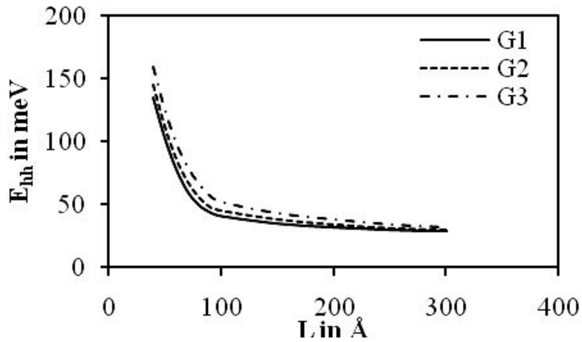

Fig. 1 – *E_{hh} vs L for $\gamma = 0$ and $x = 0.3$*

The variation of E_{hh} with respect to the radius of the Quantum Dot for different geometries, for $x = 0.3$ is presented in Fig. 1. It is seen that E_{hh} increases drastically as we go from G1 to G3. The increase is larger for small well widths than for larger well widths. It is seen that for smaller QD radius the E_{hh} reduces as the magnetic field is increased as shown in Fig. 2.

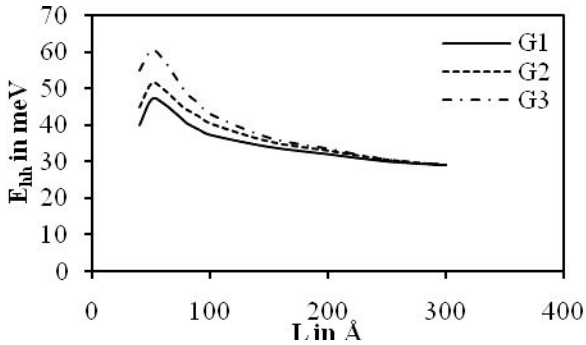

Fig. 2 – *E_{hh} vs L for $\gamma = 0.075$ and $x = 0.3$*

This is due to the fact that in semimagnetic QD, the barrier height is decreased as the applied magnetic field is increased and as the radius of the QD tends to the bulk limit there is no appreciable difference in E_{hh} value. It is also observed that for smaller QD radius at higher magnetic field there is a turnover in the E_{hh} value. We attribute this turnover to the reduction in barrier height due to magnetic field and the confinement of the acceptors a characteristic of finite barrier at lower well widths. To conclude, Coulomb interaction between the two holes lead to a strong correlation effect which depends on the shape of the QD. Such study may throw some light in understanding the two − hole spectra.

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