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EXCITED STATES OF A MAGNETIC POLARON IN A QUANTUM WELL

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The effect of magnetic field on the donor binding and spin polaronic shift of a donor in some low lying excited in a semimagnetic Quantum Well has been investigated in the effective mass approximation using the variational principle including the effect of non-parabolicity of the conduction band. The results are presented and discussed.

Keywords: *DONOR BINDING ENERGY, SPIN POLARONIC SHIFT, SEMIMAGNETIC QUANTUM WELL, NON-PARABOLICITY, EXCITED STATES.*

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1. INTRODUCTION

Due to the emerging technology in the synthesis and characterization of semiconductor nanostructures materials like $Cd_{1-x}Mn_xTe/CdTe$ provide a wide range of applications in various fields such as memory devices, optoelectronics, spintronics, etc. The possibility of tailoring the band offset with external perturbations like magnetic field and temperature, and also just by varying the magnetic ion concentration, Diluted Magnetic Semiconductors (DMS) such as $Cd_{1-x}Mn_xTe/CdTe$ with substitutional magnetic atoms provide a wide room for research to study electronic and magnetic properties simultaneously [1]. They also show a transition from type – I to type – II superlattice when the composition of Mn ion in $Cd_{1-x}Mn_xTe$ [2, 3] or magnetic field [4] is increased. Apart from these studies, the exchange interactions between the localized magnetic moments and the band electrons due to the presence of these substituitional magnetic ions [5], result in new physical effects such as large Faraday rotation [6], giant negative magneto resistance and magnetic polaron [7].

In the present work we investigate theoretically the donor bound magnetic polaronic shift to the impurity ionization energies using the mean field theory with modified Brillouin function of a donor in the low lying excited states like 2s, $2p_{\pm}$ and $2p_0$ in a $Cd_{1-x}Mn_xTe/CdTe$ Quantum Well in the effective mass approximation using variational principle. The effect of non parabolocity of conduction band has been included.

2. THEORY

Defining effective Bohr radius $a_B{}^* = \hbar^2\varepsilon_0/m^*e^2$ as unit of length and effective Rydberg $R^* = e^2/2\varepsilon_0 a_B{}^*$ as unit of energy and the strength of the magnetic field parameter $\gamma = \hbar\omega_c/2R^*$ (ω_c – cyclotron frequency), the Hamiltonian of the hydrogenic donor impurity in $Cd_{1-x2}Mn_{x2}Te/Cd_{1-x1}Mn_{x1}Te$ /$Cd_{1-x2}Mn_{x2}Te$

Quantum Well in the effective mass approximation in the presence of magnetic field applied along the growth direction is given as

$$\hat{H} = -\nabla^2 - \frac{2}{\varepsilon_0 \vec{r}} + V_B(z) + \gamma L_z + \frac{\gamma^2 \rho^2}{4}, \quad (1)$$

where $r = \sqrt{\rho^2 + z^2}$; ε_0 is the static dielectric constant of CdTe.

The confining potential for CdTe quantum well is given by,

$$V_B(Z) = \begin{cases} 0, & |Z| \le L/2; \\ V_0, & |Z| > L/2. \end{cases} \quad (2)$$

$V_0 = 70\ \%$ from ΔE_g^B; ΔE_g^B is the band gap difference with magnetic field [8] and is given,

$$\Delta E_g^B = \Delta E_g^0 \left[\frac{\eta e^{\zeta\gamma} - 1}{\eta - 1} \right], \quad (3)$$

where ΔE_g^B is the band gap difference without magnetic field given as $\eta = \exp(\zeta\gamma_0)$ with ζ as a parameter (0.5) and γ_0 as the critical magnetic field which depends upon the value of the composition x $(x_2 - x_1)$ which can be obtained from Zeeman splitting [9]. The critical magnetic field for different composition is given in Tesla as $B_0 = Ae^{nx}$ with $A = 0.734$ and $n = 19.082$ which gives the best fit to the extrapolated experimentally available critical fields. The band gap of $Cd_{1-x}Mn_xTe$ is given to be $1.606 + 1.587x$ eV. The trial wavefunctions for the donor electron in the low lying excited states are given by [10]

$$\begin{aligned} \Psi_{2p_0} &= N_{2p_0} Z f(Z) e^{-\alpha_{2p_0}\vec{r}}, \\ \Psi_{2S} &= N_{2S}(1 - \delta r) f(Z) e^{-\alpha_{2S}\vec{r}}, \\ \Psi_{2p_\pm} &= N_{2p_\pm} e^{\pm i\varphi} \rho f(Z) e^{-\alpha_{2p_\pm}\vec{r}}, \end{aligned} \quad (4)$$

where δ is the orthogonality parameter, N_{2s}, N_{2p0}, $N_{2p\pm}$ are the Normalization constants and α_{2s}, α_{2p0}, $\alpha_{2p\pm}$ are the variational parameters for the three states respectively. $f(Z)$ is the exact solution of a Quantum Well and is given by,

$$f(Z) = \begin{cases} \cos\alpha Z, & |Z| \le L/2; \\ Be^{-\tau|Z|}, & |Z| > L/2, \end{cases} \quad (5)$$

where $\alpha = E^{1/2}$ and $\tau = (V_0 - E)^{1/2}$, E is the subband energy which is obtained by solving the transcendental equation,

$$\tau = \alpha \tan(\alpha L/2). \quad (6)$$

The binding energy of the donor in the presence of magnetic field [11] is given by,

$$E_B = E + \gamma - \langle H \rangle_{\min} \quad (7)$$

2.1 Spin polaronic effect

The modified Brillouin function [12] to invoke the exchange interaction between the carrier and magnetic impurity in the presence of an external magnetic field B, yielding the magnetic polaronic shift given by,

$$E_{SP} = \tfrac{1}{2}\beta S N_0 \left\{ \left\langle \Psi_1 \left| x_1 B_S(y_1) \right| \Psi_1 \right\rangle + \left\langle \Psi_2 \left| x_2 B_S(y_2) \right| \Psi_2 \right\rangle \right\}, \quad (8)$$

where

$$B_S(y_\iota) = \frac{2S+1}{2S}\coth\frac{2S+1}{2S} y_\iota - \frac{1}{2S}\coth\frac{y_\iota}{2S},$$

$$y_\iota = \frac{S\beta \left|\Psi_\iota\right|^2}{2kT} + \frac{g\,\mu_B S\beta}{kT},$$

where β – exchange coupling parameter, S is the spin of Mn^{2+} (= 5/2), and xN_0 is the Mn ion concentration with $N_0 = 2.94 \times 10^{22}\ \mathrm{cm}^{-3}$ and $\beta N_0 = 220$ meV for CdTe. Also $g_{Mn} \approx 2$, and B is the strength of the external magnetic field, k is the Boltzmann constant and $B_s(y)$ is the modified Brillouin function.

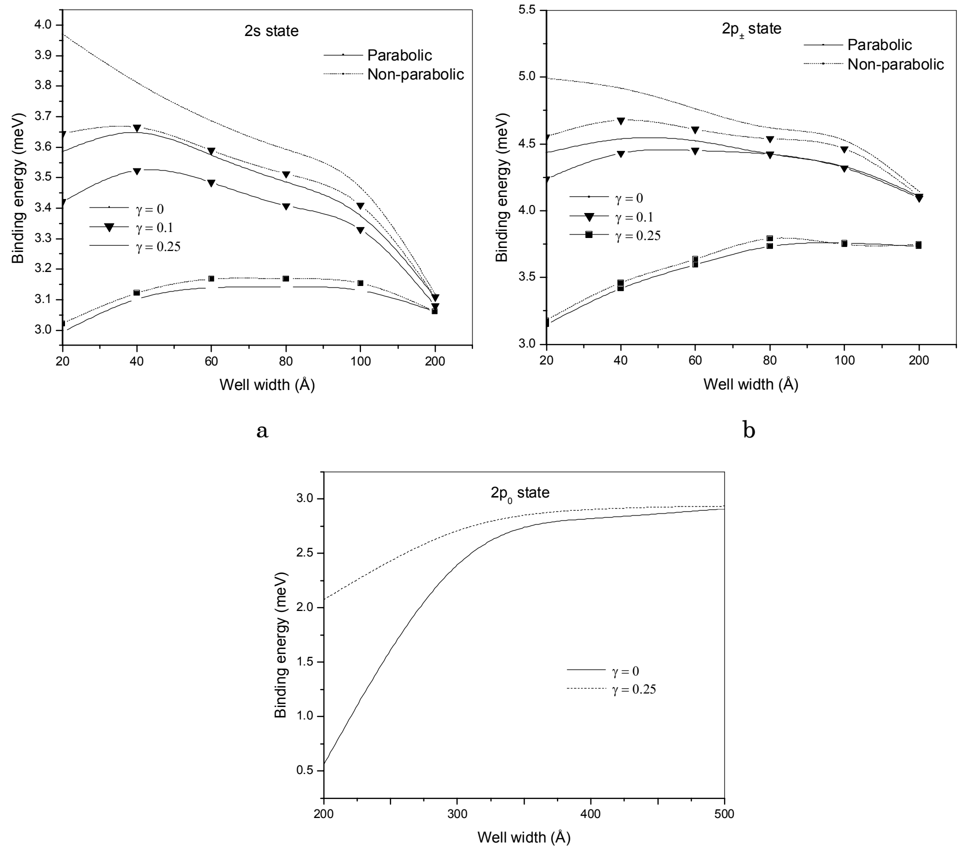
3. RESULTS AND DISCUSSION

The binding energy of the donor in the low lying excited states like 2s, $2p_{\pm}$ and $2p_0$ states have been computed for various magnetic fields for $x = 0.1$ and the variations are given in Fig. 1a-c respectively.

In the first two cases, it is observed that the donor binding decreases with increase in magnetic field. This is due to the reduction of potential barrier height on the application of magnetic field. We observe the characteristic 'turn over' of the peak value of donor binding in the lower well width region which is attributed to the transition of the system from strictly two dimensional to a quasi-two dimensional one. When the magnetic field is increased, the peak value of the binding energy shifts to the higher well width region.

Since there are no bound states below 180 Å for the $2p_0$ state, we could see the variation of binding energy only from 200 Å. The donor is almost in the bulk region and unlike the earlier cases, here, the binding energy increases with increase in magnetic field. This may be due to the reason, that in the higher excited state, the carrier gets decoupled from the magnetic moment of the impurity ion and behaves like a carrier in a non magnetic semiconductor [11].

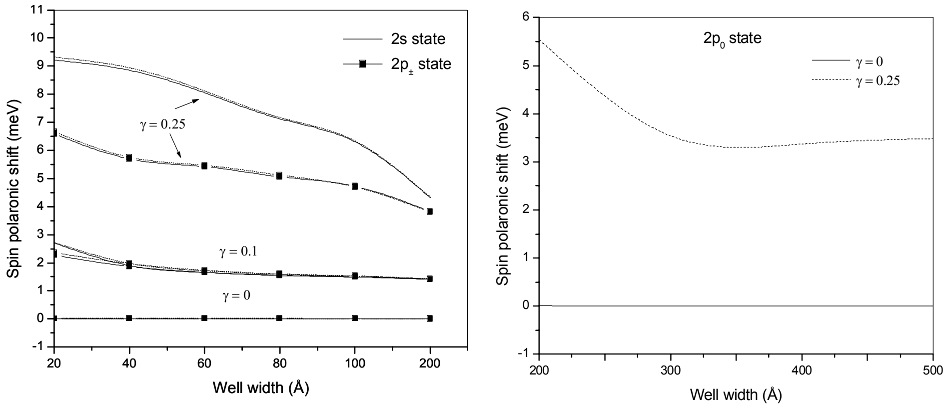
The variation of magnetic polaronic shift of the donor for 2s and $2p_{\pm}$ states for various magnetic fields is given in Fig. 2a and for $2p_0$.state in Fig. 2b. It is obvious from the figures that there is a drastic variation of magnetic polaronic shift with effective well width for higher magnetic fields in all the three states, which evidences the exchange interactions of the confined carrier with localized magnetic moments of the impurity magnetic ion. It is also observed that the magnitude of the shift decreases when the donor gets excited to higher level as expected.



c

***Fig. 1** – Variation of donor binding energy with well width for various magnetic fields for* 2s *(a),* $2p_{\pm}$ *(b) and* $2p_0$ *(c) states*

The effect of non-parabolicity enhances donor binding only in the lower well width region and becomes less significant for higher magnetic fields. As there is no bound state for the donor in $2p_0$ state for $L < 180$ Å, the well width is almost in the bulk region, the effect of non-parabolicity on donor is not quite appreciable. To conclude, the study of magnetic effect on a donor in the excited states in DMS is important since it is possible to investigate the various properties like magnetic excitations and other magneto optical transitions.



a b

Fig. 2 *– Variation of spin polaronic shift with well width for various magnetic fields in* 2s *and* $2p_\pm$ *states (a),* $2p_0$ *state (b)*

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