Magnetopolaron Effects on the Intradonor 1s-2p$^+$ Transition Energies in a GaAs - AlGaAs Double Quantum Well

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In this work we present a calculation of the intradonor 1s-2p+ transition energies for an impurity donor present in a GaAs-AlGaAs Double Quantum Well structure as a function of an applied external magnetic field. In our calculation the impurity energy levels were obtained from a variational method by choosing a Gaussian trial wave function, and the energy corrections due to the polaronic effect were included by second order perturbation theory IWBPT as modified by Cohn, Larsen and Lax. We have considered only the GaAs bulk LO phonon in the electron-phonon coupling. A very good agreement between the theoretical and experimental results for a DQW consisting of two 100 Å well widths separated by a 100 Å potential barrier width was obtained.

Keywords: Intradonor 1s-2p+ transition; GaAs-AlGaAs Double Quantum Well; Magnetic field

I. INTRODUCTION

In recent years a great number of experimental works were devoted to the understanding of the nature of electron phonon coupling in doped GaAs heterostructures. These effects can be better studied in doped multiple quantum well structures (MQW) fabricated with low carrier density. As these systems are free of any screening process, they became extremely convenient in order to investigate the electron-phonon interaction (polaronic effect).

Magneto-optical measurements of intra-donor 1s-2p+ transition energies in doped GaAs-AlGaAs MQW were reported by several authors [1-4]. The kind of phonon present in the polaronic interaction was the main point of discussion. While some experimental works claim the observation of electron interaction with nonbulk phonons modes [1,2], other experimentalists claim that the electron interacts only with the bulk longitudinal optical (LO) phonon of GaAs [3,4].

Theoretical calculations treating the problem of a bound resonant magnetopolaron in GaAs structures were recently reported. Osório *et al*. [5-7] have calculated the intradonor 1s-2p+ transition energies as a function of the longitudinal magnetic field for a center impurity in a GaAs single quantum well (SQW), and a good agreement with the available experimental data has been obtained when the electron- LO phonon coupling is considered. Similar conclusions were obtained in references [7,8]. A good agreement between the theoretical calculations of Osório *et al*. [6] with the available experimental data occurs for an impurity placed inside the SQW. However, for impurities located in the potential barrier, the fit to the experimental results is not so good. The SQW approximation cannot correctly describe the MQW samples.

In this work we present a calculation of the 1s-2p+ transition energies for a donor impurity placed in a GaAs-$Al_xGa_{1-x}As$ double quantum well (DQW) structure in the presence of a uniform magnetic field applied in the DQW growth direction. The impurity levels are obtained through a variational method [6] and the electron-LO phonon interaction effects are included in the calculations by the Improved Wigner-Brillouin Perturbation Theory (IWBPT) as modified by Cohn, Larsen and Lax [10]. The calculations are performed for different positions of the impurity in the DQW and the conduction band non parabolicity effects are considered. The two level resonant process (1s-2p+) is considered and the behaviour of the transition energies pinning in the phonon energy is studied. Our results are compared with that obtained for a single quantum well (SQW) and with experimental data available.

II. THEORY

We consider a GaAs-$Al_xGa_{1-x}As$ DQW with a donor impurity located in the barrier between the two wells at the position z_I. A uniform magnetic field (B) is applied along the z direction perpendicular to the wells interfaces. Within the framework of the effective-mass approximation, the Hamiltonian of an impurity bound electron in this system interacting with the GaAs-bulk Longitudinal-optical (LO) phonon is described by,

$$H = -\nabla^2 - \frac{2}{r}Rp + \gamma^2\frac{\rho^2}{4} + \gamma L_Z + V(z) + \sum_{\vec{k}} b_{\vec{k}}^+ b_{\vec{k}} + + \sum_{\vec{k}}\left(V_k e^{i\vec{k}.\vec{r}} b_{\vec{k}} + V_k^* e^{-i\vec{k}.\vec{r}} b_{\vec{k}}^+\right) \quad (1)$$

where the parameters are: $\gamma = \frac{\hbar\omega_C}{2\hbar\omega_{LO}}$, $Rp = \left(\frac{Ry^*}{\hbar\omega_{LO}}\right)^{1/2}$, and $V_K = \frac{-i}{|\vec{k}|}\left(\frac{4\pi\alpha}{V}\right)^{1/2}$. ω_C and ω_{LO} are respectively the cyclotron frequency and LO phonon frequency, R_Y^* is the effective Rydberg (5,83 meV), α=0.068 is the Frölich electron-LO phonon coupling constant, L_Z is the z-component of the angular momentum operator and $b_{\vec{k}}$ ($b_{\vec{k}}^+$) is the annihilation (creation) operator of the k wave vector LO phonon.

The electron DQW confining potential is defined as,

$$V(z) = \begin{cases} 0 & d/2 < |z| < d/2 + L \\ V_0 & d/2 > |z| \text{ and } |z| > d/2 + L \end{cases} \quad (2)$$

where d and L are the barrier-width and the well-width, respectively.

In the absence of the polaronic effect, we calculate the electron binding energies of the impurity levels 1s, $2p^-$ and $2p^+$, through the variational method as the Schrödinger equation for this system cannot be solved analytically. The trial-wave function we choose to describe the j state is,

$$\psi_j(r) = C_j F(z) \rho^{|m|} e^{im\theta} \exp\left(-\frac{b_j \rho^2}{2}\right) \quad (3)$$

where j=1,2,3 are for the levels 1s, $2p^+$ and $2p^-$ respectively corresponding to magnetic quantum number m=0,1,-1. C_j is the normalization constant, b_j are the variational parameters, and $F(z)$ is the standard wave function along the z direction for the electron in the ground state of a DQW given by,

$$F(z) = \begin{cases} D_1 e^{K_2 z} & z < -L_1 \\ -A_4 sinK_1 z + B_4 \cos K_1 z & -L_1 < z < -\frac{d}{2} \\ C_3(e^{K_2 z} + e^{-K_2 z}) & -\frac{d}{2} < z < \frac{d}{2} \\ A_4 sinK_1 z + B_4 \cos K_1 z & -\frac{d}{2}_1 < z < L_1 \\ D_1 e^{-K_2 z} & z > L_1 \end{cases}$$

where $L_1 = d/2 + L$, $K_2 = \sqrt{2m_b(V_0 - E)/\hbar^2}$, and $K_1 = \sqrt{2m_b E/\hbar^2}$. m_b is the GaAs electron effective mass and $m_2 = (m_b + 0.083x)$ is the AlGaAs electron effective mass. D_1, A_4, B_4, and C_3 are normalization constants. K_1 and K_2 are determined by imposing the continuity conditions and current conservation at the interfaces of the wells. The j-level energy is obtained by minimizing the mean value of the unperturbed Hamiltonian $E_j = \langle \psi_j | H | \psi_j \rangle$.

The displacement on the energies E_j due to the electron LO-phonon interaction effects was obtained by second order perturbation theory,

$$\Delta E_j = \sum_{n=0}^{\infty} \sum_{\vec{K}} |V_K|^2 \frac{\left| \langle n | e^{-i\vec{K}.\vec{r}} | j \rangle \right|}{E_j + \Delta_j - E_n - 1} \quad (4)$$

where $|n>$ and $|j>$ are the eigenfunctions of the unperturbed Hamiltonian H, and the term $\Delta_j = \Delta E_j - \Delta E_1$ introduces the Improved Wigner-Brillouin Perturbation Theory (IWBPT). Note that for $j = 1$ ($m = 0$, 1s-level) Δ_j=0. This perturbation theory gives the correct pinning behavior in the weak coupling regime [11]. The summation over the eigenstates $|n>$ includes all donor states and makes impossible to evaluate it exactly. Here, we consider only the first three states 1s, $2p^-$ and $2p^+$ in the sum over n, following the work of Cohn, Larsen and Lax [9]. The equation (4) can be written as,

$$\Delta E = \frac{\alpha}{2\pi} \sum_{n=0} \int \frac{d^2K}{K} \frac{\left| \langle n | e^{-i\vec{K}.\vec{\rho}} | j \rangle \right|}{E_j + \Delta_j - E_n - 1} F_Q(K) \quad (5)$$

where, F_Q(K) is the quasi-two-dimensional form factor, which takes into account the dimensionality of the system in the z-direction,

$$F_Q(K) = \int dz \int dz' \left|F(z)\right|^2 e^{-K|z-z'|} \left|F(z')\right|^2$$

III. RESULTS AND DISCUSSION

Our numerical results are for a GaAs-$Al_xGa_{1-x}As$ DQW structure consisting of two 100 Å quantum wells separated by a potential barrier with 212,6 meV (aluminum concentration x=0.3). The impurity donor is placed in the center of the potential barrier. We calculate the intradonor 1s-2p+ transition energies as a function of the applied magnetic field for several barrier widths.

Figure 1 shows the 1s-2p+ transition energies versus the magnetic field strength for a 200 Å single quantum well (SQW) (top dotted curves) and for DQW with 25-Å barrier width (intermediate solid + symbol curves) and 200 Å barrier width (lower solid curves). As expected decreasing the barrier width the transition energies for the DQW approximates the SQW result. For thin potential barrier the inner impurity position practically does not change the transition energy, this fact can be observed in Fig.1 where the intermediate curves show the results for two impurities position, in the middle and at the corner of the barrier.

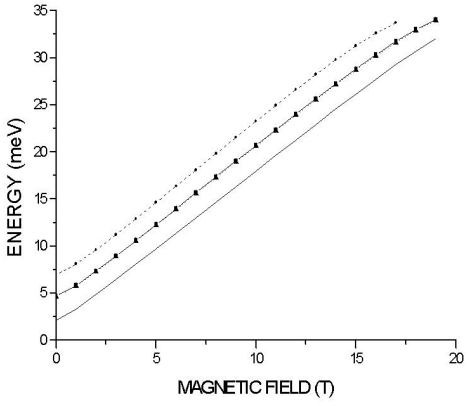

FIG. 1: 1s-2p+ transition energies as a function of the magnetic field strength for a 200 Å SQW (top curves) and for two DQW with barriers widths 25 Å (intermediate curves) and 200 Å (botton curve).

Figure 2 shows our theoretical results for the transition energy between the impurity levels 1s and 2p+ as a function of the magnetic field for a DQW consisting of two 100 Å wells separated by a 100 Å potential barrier. The impurity is located in the centre of the barrier. As it can be seen, the transition energy increases with increasing magnetic field strength and

a strong pinning of the transition energy occurs near the bulk-GaAs LO phonon energy.

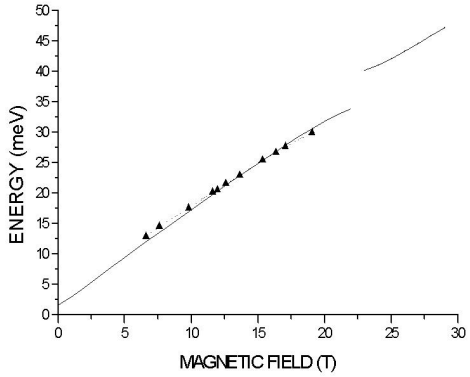

FIG. 2: 1s-2p+ transition energy as a function of the magnetic field for a DQW consisting of two 100Å wells separated by a 100Å potential barrier. The impurity is located in the centre of the barrier.

For B $>$ 20T a resonant splitting of the transition energy is observed. The set of triangles shows the experimental results obtained by Huant et al. [4] for a MQW sample with the impurities placed in the center of the potential barrier. The good agreement between the theoretical and experimental results only was possible when the transition energy was corrected by the conduction band nonparabolicity effect, included in the calculation through the Palik expression [10],

$$E_j^{NP} = E_j(1-\delta_2\frac{E_j}{E_G}) + \Delta E_j \qquad (6)$$

where δ_2 is the nonparabolicity parameter and E_G is the GaAs gap energy. In this work we use the typical value δ_2=0.95 [10]. From this figure we can see that for impurities located in the potential barrier the effect of the MQW structure must be taken into account.

IV. CONCLUSIONS

In this paper we calculate the transition energies between the impurity donor levels 1s and 2p+ present in a GaAs-AlGaAs DQW structures as a function of an applied external magnetic field. In our calculation the impurity energy levels were obtained by the variational method and the energies correction due to the polaronic effect was included by second order perturbation theory IWBPT as modified by Cohn, Larsen and Lax. We consider only the GaAs bulk LO phonon in the electron-phonon coupling. A very good agreement between the theoretical and experimental results for a DQW consisting of two 100 Å wells separated by a 100 Å potential barrier was obtained.

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