DONOR IMPURITY IN NANOTUBE WITH TWO GaAs/GaAlAs QUANTUM WELLS: MAGNETIC FIELD EFFECTS

J D González¹, R Escorcia¹ and J Sierra-Ortega¹

¹Grupo de Investigación en teoría de la Materia Condensada, Universidad del Magdalena, A.A. 731, Santa Marta, Colombia

Abstract. Micro-tubes containing two GaAs/GaAlAs quantum wells (QWs) in a section of the tube layer has been fabricated and optical properties of the embedded QWs has been studied. The ground state binding energy of an off-axis donor in a cylindrical nanotube, containing two GaAs/GaAlAs quantum wells (QWs) in the presence of a uniform magnetic field is calculated as a function of the donor location as well as the density of states. A trial function for describing the asymmetric electron charge distribution is taken as a product of the combination of 1s and 2pₓᵧ subband wave functions and an unknown function that depends only on electron-ion separation. We found that the increasing the magnetic field the increasing the binding energy while the impurity is located in the QW1, whereas the opposite occurs when the impurity is located in the QW2. Two peaks in the curves of the binding energy, as a function of the impurity position, are also found as well as in the density of impurity states.

E-mail: jdavid0831@gmail.com

1. Introduction

Recently, Prinz et al. demonstrated that multilayer structures including strained layers are useful to form nanotubes and nanocoils [1,2]. By using lattice-mismatched epitaxial layers that rolled up when freed from the substrate due to the built-in strain and a micro-tube including two GaAs/GaAlAs quantum wells (QWs) located at positions with different types of strain was fabricated and its optical properties before and after the fabrication process were investigated by photoluminescence (PL) spectroscopy. Micro-tubes containing two GaAs/AlGaAs quantum wells (QWs) in a section of the tube layer, and also the optical properties of the embedded QWs have been studied[3]. In our previous work we show that the low lying 1s and 2pₓᵧ subbands of the free electron in nanotube, become almost degenerated as the width of the repulsive core grows and the mixing of these subbands in the presence of the off-axis donor no longer should be depreciated [4].The purpose of this paper is to analyze the ground state energy of the off-axis neutral donor and the density of the impurity states in cylindrical nanotube with two GaAs/AlGaAs quantum wells with and without the presence of a magnetic field oriented along the growth axis.

2. Theory

We consider the problem of an off-axis neutral donor impurity in a cylindrical nanotube, which containing two GaAs/Ga₁₋ₓAlₓAs quantum wells (QWs) in the presence of a uniform magnetic field, as can see in figure 1. The material parameters m*, the conduction-band effective mass and ε, the
dielectric constant of the semiconductor heterostructure are assumed to be uniform throughout the heterostructure. The values of the physical parameters pertaining to GaAs ($m^*=0.067m_0$, and $\varepsilon=12.53$, where $m_0$ is the free-electron mass) are used in our calculations.

Fig. 1 Cylindrical nanotube, containing two GaAs/GaAlAs quantum wells (QWs)

Within the effective-mass approach, the dimensionless Hamiltonian for the donor can be written as

$$H = H_0 - \frac{2}{\bar{r} - \bar{\xi}}; H_0 = -\nabla^2 + V(\rho) + \frac{1}{4}\varepsilon^2\rho^2 - i\gamma\frac{\partial}{\partial\phi}$$

Where $\bar{r}$ and $\bar{\xi}$ are used to designate the electron and ion positions, respectively and we have introduced the effective Bohr radius $a_0^* = \varepsilon\hbar/m^*e^2$ as the unit of length, the effective Rydberg $Ry_0^* = e^2/2a_0^*\varepsilon$ as the unit of energy and $\gamma = eB/2m^*cRy^*$ as the dimensionless unit of the magnetic-field strength corresponding to the first Landau level.

To calculate the donor ground state energy, we choose a trial function as the product of a linear combination of the waves functions of the electron ground, $s$ and the first excited, $2p_{x,y}$ states, with an unknown isotropic function $\Phi(\bar{r} - \bar{\xi})$ could be interpreted as a variational wave function:

$$\psi(\bar{r}) = \sqrt{1-\alpha^2} \left\{ \Phi(\bar{r} - \bar{\xi}) \right\}, \quad (2)$$

where $\alpha$ is a variational parameter ($-1 < \alpha < 1$) which gives the grade of the mixing of the subbands [3]. One can see that in the particular case as $\alpha = 1$, there are not subband mixing and the trial function (2) becomes similar to the simple Bastard-type trial function. In general case, the mixing provided a decrease of the parameter $\alpha$. Greater the mixing the smaller is the parameter $\alpha$. In our calculations the parameter $\alpha$ decrease at to 0.8. Due to the inclusion of two quantum wells in the nanotube, appear the strong mixing subbands mostly in the central barrier. In this way, we must include the effect in our calculations.

For our model the wave equation for the free electron $H_{\text{f}} f(\bar{r}) = E_0 f(\bar{r})$ is separable and the electron wave function can be written as follows:

$$f(\bar{r}) = e^{ikz} e^{im\phi} g(\rho), \quad (3)$$

where $m = 0, \pm 1, \pm 2, \ldots$ is the angular momentum in $z$-direction, $k$ is the wave number corresponding to a free motion in $z$-direction ($-\pi < k < \pi$) and the function $g(\rho)$ is the solution of the one-dimensional boundary value problem:
\[ g^*(\rho) + \frac{1}{\rho} g'(\rho) + U(\rho) g(\rho) = 0; \quad g'(0) = 0; \quad g(\infty) = 0 \]  
\[ U(\rho) = E_0 - \gamma m - k^2 - V(\rho) - \frac{\gamma^2 \rho^2}{4} - \frac{m^2}{\rho^2} \]  
(4)

The differential equation (4) is solved numerically using the trigonometric sweep method [5]. For modelling a nanotube containing two GaAs/Ga\(_{1-x}\)Al\(_x\)As quantum wells (QWs), we use the confinement potential given by the following expression:

\[ V(\rho) = V_r(\rho, R_1, z) + V_r(\rho, R_2, z) - V_0 - W(\rho, W_1, W_2) + V_v(\rho, R_4, z), \]  
where:

\[ \theta(z, z_0, W) = \begin{cases} 
0 & ; z < z_0 - W \\
\left( z - z_0 \right)/W^2 - 1 & ; z - W \leq z < z_0 \\
1 & ; z \geq z_0 
\end{cases} \]  
(6)

is soft-edge version of the Heaviside function, \( R_1, V_i \) represent the radii and heights of the barriers, respectively; \( W \) is a parameter related to the width of the transition region (see Fig. 2).

Fig. 2. Confinement Potential in cylindrical Nanotube

The solutions of the boundary value problem (4) corresponding to the bottom of the subbands \((k = 0)\) with radial quantum numbers \( n = 0, 1, 2, \ldots \) and the angular momentum \( m \) we denote as \( g_{n,m}(\rho) \) and therefore in our notations the electron wave function, \( f_{n,m}(\vec{r}) \) and the energy \( E_{0}(n,m) \) depend on two quantum numbers \((n,m)\). If we assume that the off-center donor is located on the axis \( x \), then it modifies the free electron wave functions in such way that it becomes more asymmetric in the \( x \) direction. It is reason why in the trial function (2) should be chosen the electron wave functions which gives contribution in the mixing as \( f_{1s}(\vec{r}) = g_{0,0}(\rho) \) for the \( 1s \) state, and \( f_{2p}(\vec{r}) = g_{1,0}(\rho) \cos \phi \) for \( 2p \) state. Starting from the variational principle and using the method described in the papers [6] one can obtain the following Euler-Lagrange equation for the correlation function:

\[ -\frac{1}{J(r)} \frac{d}{dr} \left[ J(r) \frac{dF(r)}{dr} \right] + \left( \frac{\tilde{E}(r)}{r} \right)^2 \Phi = E(D^0) \Phi \]  
(7a)

Where \( E(D^0) \) represents the energy of the neutral donor, \( J(r) \) is radial part of the Jacobian and \( \tilde{E}(r) \) is the averaged free electron local energy, given by the followings expressions:

\[ J(r) = r^2 \sum_{i,j=0,1} \alpha^{2+i+j} \left( 1 - \alpha^2 \right)^{(i+1)/2} P_{ij}(r), \quad \tilde{E}(r) = r^2 \sum_{i,j=0,1} \alpha^{2+i+j} \left( 1 - \alpha^2 \right)^{(i+1)/2} E_0(0,i) P_{ij}(r)/J(r) \]  
(7b)
\[ P_{\lambda}(r) = \int_{0}^{2\pi} g_{0,0}^{2i-k}(\tilde{\rho}) g_{0,1}^{i+k}(\tilde{\rho}) \lambda^{i-k} \sin \theta d\theta d\phi ; i, k = 0,1 \quad \text{where} \quad \lambda = 1 - r^2 \sin^2 \theta \sin^2 \varphi / \tilde{\rho}^2 \]  

(7c)

In these relations \( \tilde{\rho} \) is the distance from the donor position to axis. Once the functions \( g_{0,0}(r) \) and \( g_{0,1}(r) \) are found, the functions \( P_{i,k}(r), (i, k = 0,1) \) and \( J(r) \) may then be calculated in a straightforward way through (7b) and (7c). Finally, to define the donor energy we solve the wave Eq. 7(a) by using the trigonometric sweep method [5]. To calculate the density of the impurity states we assume that the circular cross section of the nanotube is not too small in order that we might treat the impurity positions as a continuous random variable. In this case the density of the impurity states \( g(E) \) in a cylindrical nanotube is given by the following relation [4]:

\[ g(E_b) = \frac{2\pi \xi \rho(E_b)}{dE_b(\xi_\rho) / d\xi_\rho} \]  

(8)

In Fig. 3 and 4 we display the variation of the binding energy as a function of the distance from donor locations to the axis in a cylindrical nanotube with two square quantum wells and different values of the magnetic field parallel to the axis. Additionally, the different heights and small displacement to the right for minimum energy value in the second square well are shown due to increasing the magnetic field, for the lower it present a greater whereas larger are smaller, because the magnetic field provides additional confinements that tend to move the electron to the central region of the nanotube.

**Fig.3** \( D^0 \) ground state binding energies as a function of the donor displacement \( \xi_\rho \) from the axis of the cylindrical nanotube for different central barrier’s width and magnetic field \( \gamma = 0 \)

**Fig.4** \( D^0 \) ground state binding energies as a function of the donor displacement \( \xi_\rho \) from the axis of the cylindrical nanotube for different central barrier’s width and magnetic field \( \gamma = 20G \)
The figure 5 shows the additional maximums of the energy due to the inclusion of the two square quantum well such behavior of the donor binding energies is also reflected in the curves of density of impurity states in nanotube. It seen from the Fig. 6 that the two well causes the appearance of the singularities near the right-side and left-side threshold of the curves of the density of the impurity states and it middle part. These singularities are due to the existence of one minimum and one maximum in the binding energies dependence where the derivate $dE(\xi_\rho)/d\xi_\rho$ is equal to zero.

3. CONCLUSION

We have presented a simple method of calculation of the binding energy for the lowest state of the off-axis $D^0$ donors in a nanotube with two square wells in the presence of the magnetic field applied parallel to the axis, taking into account the effect of the mixing $s_y p_z$ subbands. We found that under external magnetic field applied parallel to the axis the binding energies of donors located close to the axis increases and located far from the axis decreases. Also we present new curves that show novels energy peaks and analyze the density of the $D^0$ impurity states for different magnetic fields.

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4. References

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