Donor binding energy under magnetic field in cylindrical nanotube with two GaAs/GaAlAs quantum wells

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Abstract. A systematic study of the binding energy of the ground state of a hydrogenic off-axis donor in a cylindrical quantum wire containing two quantum wells in a section of the tube layer is calculated in the presence of a uniform magnetic field applied parallel to the wire axis with different potential shape. We express the wave function as a product of combinations of s and p subband wave functions and an envelope function that depends only on the electron–ion separation. By using the variational principle we derive a differential equation for the envelope function, which we solve numerically. Two peaks in the curves for the dependence of the ground-state binding energies on the donor distance from the axis are presented and it is shown that the increasing the magnetic field increasing the binding energy while the impurity is located in the QW1, whereas the opposite occurs when the impurity is located in the QW2.

1. Introduction

The study of the behavior of the on-axis hydrogenic impurity center in quantum-well wires (QWWs) that represent a quasi-one-dimensional system has attracted considerable attention in the 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 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 experimentally obtained [3]. In our previous work we show that the low lying 1s and 2p_{x,y} 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

Neglecting the differences between material parameters, the dielectric constant \( \varepsilon = 12.53 \) and the electron effective mass \( m^* = 0.067 m_e \) of the well and those of the barrier, the Hamiltonians of the electron, \( H_0 \) and the donor, \( H \) in a heterostructure with cylindrical symmetry in the presence of an applied uniform magnetic field \( \vec{B} = B \hat{z} \) in the effective-mass approximation, can be written as:

\[
H = H_0 - \frac{2}{| \vec{r} - \vec{\xi} |}; \quad H_0 = -\nabla^2 + V(\rho) + \frac{1}{4} \gamma^2 \rho^2 - i \gamma \frac{\partial}{\partial \varphi}
\]

Where \( \vec{r} \) and \( \vec{\xi} \) are used to designate the electron and ion positions, respectively and we have introduced the effective Bohr radius \( a_0^* = \hbar / \sqrt{m^* \varepsilon} \) as the unit of length, the effective Rydberg \( R_0^* = \varepsilon^2 / 2a_0^* \varepsilon \) as the unit of energy and \( \gamma = \varepsilon h / 2m^* cR_0^* \) 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 \( \Phi(\vec{r} - \vec{\xi}) \) could be interpreted as a variational wave function:

\[
\psi(\vec{r}) = [\alpha f_{1s} + \sqrt{1 - \alpha^2} f_{2p}] \Phi(\vec{r} - \vec{\xi}).
\]

where \( \alpha \) is a variational parameter \((-1 < \alpha < 1) \) which gives the grade of the mixing of the subbands [4]. 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 \( H_0 f(\vec{r}) = E_0 f(\vec{r}) \) is separable and the electron wave function can be written as follows:

\[
f(\vec{r}) = e^{i \vec{k} \cdot \vec{r}} e^{i m \varphi} g(\rho),
\]

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:

\[
g^*(\rho) + \frac{1}{\rho} g'(\rho) + U(\rho) g(\rho) = 0; \quad g'(0) = 0; \quad g(\infty) = 0
\]

\[
U(\rho) = E_0 - \gamma m - k^2 - V(\rho) - \frac{\gamma^2 \rho^2}{4} - \frac{m^2}{\rho^2}
\]

The differential equation (4) is solved numerically using the trigonometric sweep method [5]. For modelling a nanotube containing two \( GaAs/Ga_{1-x}Al_xAs \) quantum wells (QWs), we use the confinement potential given by the following expression:
\[ V(\rho) = V_1(\theta(-\rho, -R_1, W)) + V_2(\theta(\rho, R_2, W)) - V_3(\theta(\rho, R_3, W)) + V_4(\theta(\rho, R_4, W)), \]

where:

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

is soft-edge version of the Heaviside function, \( R_i, V_i \) represent the radii and heights of the barriers, respectively; \( W \) is a parameter related to the width of the transition region (see Fig. 1).

Fig. 1 Confinement potential shape containing two GaAs/GaAlAs quantum wells (QWs), different magnetic field applied and potential concentric barrier \( V_{\text{Layer}} \). \( V_{\text{eff}} \) include the confinement potential plus the magnetic field induced potential due to the paramagnetic term in the eq. (1).

**3. Results and Discussion**

The peak position coincides approximately with the midpoint between the interior and exterior radii for QW1 and QW2, \((R_1 + R_2)/2\) and \((R_3 + R_4)/2\) respectively where the confinement is the largest. In addition, we display the variation of the binding energies as a function of the distance from the donor location to the axis for different values of the magnetic field parallel to the axis. Increasing the magnetic field decreases the cyclotron radius relative to the wire radius for the electron. Inconsequence, the binding energies of the donor located close to the axis increases, while for donors removed far from the axis the distance between the electron and the donor under the magnetic field grows and the binding energy decreases. This is why the order of the curves of the binding energies dependencies for different magnetic fields presented in Fig. 4 is inverted as the donor is removed from the axis. It is interesting that the crossovers of all curves related to the inversion of their order occur approximately at the same point, corresponding to a distance \( 2.2a_0^* \) from the axis of the nanotube. In this position of the donor binding energy is almost insensitive to the external magnetic field, while the binding energies of donors arranged closer or further from the axis increases or decreases respectively.

**4. Conclusions**

In this work using the effective mass-approximation within the variational approach and different values of the magnetic field applied parallel to the axis, we calculate the binding energy for the lowest state of the off-axis \( D^0 \) donors in a nanotube with two square wells, taking into account the variation of
the potential shape $W = 0.1a^*_0, 0.2, 0.5a^*_0$, square, soft and parabolic barrier, respectively. 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.

Fig. 4 D$^0$ ground state binding energies as a function of the donor displacement $\xi_0$ from the axis of the cylindrical nanotube with different values of the magnetic field and potential shape.

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