Donor binding energy under magnetic field with different radii and parabolic bottom potential

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Within the framework of the effective mass approximation we analyze a variation of the ground state energy of the off-axis neutral donor in a GaAs/Ga$_{1-x}$Al$_x$As cylindrical nanotube with a parabolic bottom potential under a uniform magnetic field directed along the symmetry axis. By using a variational principle and the functional derivative procedure, we derive a one-dimensional differential equation for the envelope function, which we solve numerically by using of the trigonometric sweep method. To take into account the mixing of the low lying subbands, we express the wave function as a product of the combination of $1s$ and $2p_{x,y}$ wave functions with an unknown envelope function that depends only on electron-ion separation. Results of the calculation of the ground state binding energy dependencies on the distance from the donor position to the axis and on the strength of the external magnetic field parabolic bottom potentials are presented. It is shown that the effect of the subband mixing for off-axis donors in the nanotube is considerable.

Keywords: Donor binding; energy parabolic potential.

1. Introduction

The Bastard-type trial function without consideration of the effect of the subband mixing, which is commonly used for calculating the ground state binding energy of donors located in such type of heterostructures, can be inadequate to describe the asymmetric electron charge distribution around the off-axis donor and can lead to a lower estimate of the binding energy. In the last two decades, there has been an increasing interest in the study of the peculiar physical properties of QWWs (Quantum Well Wires). The study of bound impurity states in such Q1D (One dimensional) structures is therefore considered to be a subject of fundamental interest and of significant attention [1]. Extensive theoretical investigation on the behavior of shallow impurities in QWW has been developed using the Bastard type trial function. In nanotubes, which are QWWs with a repulsive core around the wire axis, the confining potential along the cross section through the axis of the nanotube is similar to one of a symmetric double quantum well. As it has been previously demonstrated, the inclusion of the subband mixing plays an important role in correctly determining off-center donor binding energies in a double quantum well [2]. In our previous work, we showed that the low lying $1s$ and $2p_{x,y}$ subbands of the free electron in a nanotube, similarly to the case of a double quantum well, 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 [3]. In this work, we analyze the ground state energy of the off-axis neutral donor in a GaAs/Ga$_{1-x}$Al$_x$As cylindrical nanotube with a parabolic bottom potential shape in the presence of a uniform magnetic field applied along the symmetry axis. Due to the strong confinement in the radial direction, the electron bound to the off-axis donor tends to be localized mainly close to the axis cylindrical QWW, although the donor is moved from the axis. The trial function of the donor is taken as a product of the combination of $1s$ and $2p_{x,y}$ subband wave functions with an unknown envelope function that only de-
pends on electron-ion separation. Using the fractal dimension method [4] we find the one-dimensional differential equation for the envelope function, which we solve numerically.

2. Theory

Using the effective Bohr radius \( a_0 \) and the Rydberg \( R_y \) as units of length and energy, respectively, and neglecting differences between material parameters in the barrier and in the well, the dielectric constant \( \epsilon \) and the electron effective mass \( m^* \), the dimensionless Hamiltonian for a neutral donor impurity in a cylindrical nanotube, in the presence of an applied uniform magnetic field \( \vec{B} = B \hat{z} \) in the effective mass approximation can be written as:

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

where \( \vec{r} \) and \( \xi \) are used to designate the electron and ion positions, respectively. \( V(\rho) \) is the confinement potential with axial symmetry and with a repulsive core around the axis of the nanotube, and \( \gamma = eB/2m^*cR_y \) is the magnetic field strength corresponding to the first Landau level expressed in \( R_y \).

To calculate the donor ground state energy, we choose a trial function as a product of the linear combination of the wave functions of the electron ground s and the first excited \( 2p_{x,y} \) states, with an unknown one-dimensional function \( \Phi(|\vec{r} - \xi|) \)

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

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 when \( \alpha = 1 \), there is no subband mixing and the trial function (2) becomes similar to the simple Bastard-type trial function. In the general case, the mixing provided a decrease of the parameter \( \alpha = 1 \). The greater the mixing, the smaller the parameter \( \alpha \). In our calculations, the parameter \( \alpha \) decreases to 0.8. In our model, the wave equation for the free electron \( H_0 f(r) = E_0 f(r) \) is separable, and the electron wave function can be written as follows:

\[
f(\vec{r}) = e^{i k z} e^{i m \varphi} g(\rho) \quad (3)
\]

where \( m = 0, \pm 1, \pm 2, ... \) is the angular momentum in the \( z \)-direction, \( k \) is the wave number corresponding to a free motion in the \( z \)-direction \((-\pi < k < \pi)\), and the function \( g(\rho) \) is the solution of the one-dimensional boundary value problem:

\[
g''(\rho) + \frac{1}{\rho} g'(\rho) + U(\rho) g(\rho) = 0 \quad (4)
\]
\[
g'(0) = 0 \quad (5)
\]
\[
g'(\infty) = 0 \quad (6)
\]

The differential equation (4) is solved numerically using the trigonometric sweep method [5]. In our calculations we use the confinement potential, modelling a nanotube given by the following expression:

\[
V(\rho) = V_0 \theta(-\rho - R_i, W) + V_o \theta(\rho, R_e, W) \quad (8)
\]

where:

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

is a soft-edge version of the Heaviside function; \( R_i, \) \( V_i \) and \( V_o \) represent the radii and heights of the repulsive core and the barrier, respectively; \( W \) is a parameter related to the width of the transition region (see Fig. 1). In this particular case, we use function (5) to obtain the parabolic bottom potential shape. The solutions of the boundary value problem (4) corresponding to the bottom of the subbands \( (k = 0) \) with radial quantum numbers \( n = 0, 1, 2... \) 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 \( x \) axis, then it modifies the free electron wave functions in such a way that it becomes more asymmetric in the \( x \) direction. This is the reason why in the trial function (2) the electron wave functions which contribute to the mixing of \( f_{1s}(\vec{r}) = g_{0,0}(\rho) \) for the \( 1s \) state, and \( f_{2p}(\vec{r}) = g_{0,1} \cos \varphi \) for the \( 2p \) state should be chosen. Starting from the variational principle and using the method described in Ref. 6,

\[
U(\rho) = E_0 - \gamma m - k^2 - V(\rho) - \frac{\gamma^2 \rho^2}{4} - \frac{m^2}{\rho^2} \quad (7)
\]

Figure 1. Parabolic bottom potential confinement in a cylindrical nanotube. Additionally, the \( 1s \) (dotted curve) and \( 2p \) (solid curve) mixing are shown.
where \( E(D^0) \) represents the energy of the neutral donor, \( J(r) \) is the radial part of the Jacobian, and \( \bar{E}(r) \) is the averaged free electron local energy given by the following expressions:

\[
J(r) = r^2 \sum_{i,k=0,1} \alpha^{2-i-k}(1-\alpha^2)^{(i+k)/2}P_{i,k}(r)
\]

\[
\bar{E}(r) = \frac{\sum_{i,k=0,1} \alpha^{2-i-k}(1-\alpha^2)^{(i+k)/2}E_0(0,i)P_{i,k}(r)}{\overline{J(r)}}
\]

\[
P_{i,k}(r) = r^2 \int_0^{\infty} \int_0^{\infty} \rho g_{0,0}(\rho) g_{0,1}(\rho) \sin \theta d\theta d\varphi
\]

\[
i, k = 0, 1.
\]

\[
\lambda = 1 - r^2 \sin^2 \theta \sin^2 \varphi / \rho^2
\]

\[
\rho = (r^2 \sin^2 \theta + \xi^2 + 2r \xi \sin \theta \cos \varphi)^{1/2}
\]

In these relations, \( \xi \) is the distance from the donor position to the axis. Once the functions \( g_{0,0}(r) \) and \( g_{0,1}(r) \) are found, the functions \( P_{i,k} \), \( (i, k = 0, 1) \) and \( J(r) \) may then be calculated in straightforward way through (7b) and (7c). Finally, to define the donor energy, we solve the wave Eq.(6) by using the trigonometric sweep method [5]. In our calculations we use the material parameters for the GaAs/Ga_{0.7}Al_{0.3}As heterostructures given in Refs. 2. The curves in the inset of Fig. 2 show the values of the physical parameters pertaining to GaAs \( m^* = 0.067m_0 \) and \( \varepsilon = 12.5, m_0 \) being the free-electron mass used in our calculations. The results for the \( D^0 \) binding energy, defined as \( E_b(D^0) = E(0,0) - E(D^0) \), in GaAs/Ga_{1-y}Al_{y}As QWWs and NTs are presented in Figs. 2-4. In Fig. 2 we compare the binding energies of the on-axis donor as a function of the radius \( R_e \) of the cylindrical GaAs/Ga_{0.6}Al_{0.4}As As QWW \( (R_t = 0) \) of several values of the magnetic field calculated by u, with those previously obtained by Branis, Li and Bajaj [2] without subband mixing. In this calculation we intentionally chose the material parameters that roughly correspond to those from Ref. 2. The excellent agreement observed in all cases suggests that the effect of mixing on the on-axis donor binding energies independent of the strength of the magnetic field is negligible.

We also show the binding energy dependence on the donor as a function of the radius with several magnetic fields and a parabolic bottom potential. For a given value of the magnetic field, the binding energy increases from its bulk value, equal to 2.8\( \text{Ry}^* \), 3.4\( \text{Ry}^* \) and 3.7\( \text{Ry}^* \) for the magnetic fields 0, 100\( \text{kG} \) and 200\( \text{kG} \), respectively, to its maximum value of about 5.35\( \text{Ry}^* \), as the wire radius \( R_e \) is reduced to 0.2\( a_0^* \). As \( R_e \) further decreases, the binding energies begin to fall off rather rapidly to the bulk corresponding values. This is due to the leakage of the wave function into a barrier region under strong confinement.

The calculation results for the \( D^0 \) binding energies in a GaAs/Ga_{0.7}Al_{0.3}As nanotube with the exterior radius \( R_e = 3a_0^* \) and several repulsive core radii \( R_t \) as functions of the donor displacement from the axis are presented in Fig. 3. The solid and dashed lines show our results for the models...
and without mixing of the s and p subbands, respectively. It is seen that the effect of mixing is negligible when the donor is located close to the axis or when it is moved far from the axis. In the intermediate case, the binding energies of the off-axis donors are enhanced because of the inclusion in the variational calculations of the effect of the band mixing up to 7 in QWW ($R_i = 0$) and up to 11 in nanotubes, where the effect of the subband mixing on the off-axis donors in an accurate calculation cannot be ignored.

This effect is a considerable parabolic bottom potential. Besides, the height of these peaks falls as the core radius initially increases from 0 to $0.5a_0^*$, and further, when the core radius increases from $0.5a_0^*$ to $2.0a_0^*$, it grows rapidly. This is due to the fact that for small values of the core radius, the electron is mostly localized in the central region and therefore, the electron-donor separation increases with the donor displacement from the axis whereas the binding energy is lowered. On the other hand, for large core radii, the electron cannot penetrate into the central region; it is mostly located in the middle between two of the barriers, and when the donor

is situated in the same position, the electron-donor separation becomes very small.

3. Conclusion

We have presented a simple method of calculation of the binding energy for the lowest state of the off-axis $D^{13}$ donors in a nanotube with a parabolic bottom potential in the presence of the magnetic field applied parallel to the axis, taking into account the effect of the mixing s and $p_z$ subbands. We found that under an external magnetic field applied parallel to the axis, the binding energies of the donors located close to the axis increase, while those located far from the axis decrease.

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