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Effect of magnetic field on off-axis donor binding energy in a nanotube

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We analyze the effect of the mixing of the low-lying s and $p_{x,y}$ subbands on the ground-state binding energy of the off-axis donors in cylindrical nanotubes in the presence of a magnetic field parallel to the axis. 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. 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 effect of the subband mixing for off-axis donors in nanotubes is considerable. It is found that the magnetic field enhances the binding energies of donors located close to the axis whereas for donors located far from the axis the effect of the magnetic field on the binding energy is the opposite.

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 last two decades [1]. The effect of the magnetic field on the ground-state binding energy of the on-axis donor has been analyzed in Ref. [2]. The Bastard-type trial function without consideration of the effect of the subband mixing used in these calculations 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. This deficiency may be more essential in nanotubes (NT), the heterostructure with a repulsive core around the wire axis. In this case the confining potential along the cross section through the axis of the NT is similar to that of a symmetric double quantum well (DQW) for which, as has been demonstrated previously, the inclusion of the subband mixing plays an important role in correctly determining off-center donor binding energies [3]. In both cases the low-lying *s* and *p* subbands of the free electron become almost degenerate as the size of the center potential barrier increases and the mixing of these subbands in the presence of the off-axis donor may no longer be neglected.

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. In consequence, the separation between the electron and the ion increases whereas the binding energy decreases as the donor is removed from the axis. An additional increase of the electron–ion separation for off-axis donor should be observed in the presence of the external magnetic field oriented along the

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growth axis. Therefore one can expect that under strong magnetic fields the binding energy of the on-axis donor increases whereas the corresponding value for the off-axis donor located far from the axis decreases. The purpose of this paper is to study the effect of the mixing of the s and p subbands on the off-axis donors in QWW and NT in the presence of a magnetic field oriented along the growth axis.

To this end we use the variational procedure proposed previously [4] that provides a simple and efficient algorithm for calculating the binding energies of the off-center neutral and negatively charged donors in QWs, QWWs and QDs with a high degree of accuracy. In Ref. [5] this procedure has been applied for calculating the energies of the neutral, D^0 and negatively charged, D^- off-axis donors in nanotubes without taking into account the effect of the subband mixing. In this work we develop a variational formalism for the study of the off-axis donor ground state confined in the NT in the presence of the external magnetic field oriented along the axis, which permits us to take into account the effect of the subband mixing. We calculate the variation of the binding energy as a function of the distance from the donor position to the axis of the NTs with different exterior and repulsive core radii, and discuss how magnetic-field effects can vary depending heavily on the donor position.

2 Formalism

Neglecting the differences between material parameters, the dielectric constant ε and the electron effective mass m^* 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 $\boldsymbol{B} = B\hat{z}$ in the effective-mass approximation, can be written as [2, 3]:

$$H_0 = -\nabla^2 + V(\rho) + \frac{1}{4}\gamma^2\rho^2 - i\gamma\frac{\partial}{\partial\varphi}; \qquad H = H_0 - 2/|\boldsymbol{r} - \xi| \,. \tag{1}$$

Here, we scale all lengths in the effective Bohr radius $a_0^* = \varepsilon\hbar^2/m^*e^2$, all energies in the effective Rydberg $R_y^* = e^2/2a_0^*\varepsilon$ and the magnetic field strength in the first Landau level expressed in the effective Rydberg $\gamma = e\hbar B/2m^*cR_y^*$. The 3D vectors ξ and $\boldsymbol{r} = (\rho, z)$ in Eq. (1) designate the ion and the electron positions, respectively, and $V(\rho)$ is the confining potential that we consider to be zero in the well $(R_i < \rho < R_e)$ and to V_0 into the interior $(\rho < R_i)$ and the exterior $(\rho > R_e)$ barriers. If the interior radius, R_i is equal to zero this confining potential describes a cylindrical QWW otherwise a NT.

The wave equation for the electron, $H_0 f(\boldsymbol{r}) = E_0 f(\boldsymbol{r})$ in cylindrical coordinates is separable and the electron wave function can be written as follows:

$$f(\boldsymbol{r}) = \mathrm{e}^{ikz}\,\mathrm{e}^{im\varphi} g(\rho) \,, \tag{2}$$

where $m = 0, \pm 1, \pm 2, \ldots$ 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

$$g''(\rho) + \frac{1}{\rho}g'(\rho) + \left[E_0 - \gamma m - k^2 - V(\rho) - \frac{\gamma^2\rho^2}{4} - \frac{m^2}{\rho^2}\right] g(\rho) = 0; \qquad g'(0) = 0; \qquad g(\infty) = 0. \tag{3}$$

A general solution of Eq. (3) for a piecewise constant potential $V(\rho)$ can be expressed in terms of the confluent hypergeometric functions [2], but we prefer in our calculations to solve this eigenvalue problem numerically by using the trigonometric sweep method described in the paper [6]. The solutions of the boundary value problem (Eq. (3)) 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 in our notation the electron wave function, $f_{n,m}(\boldsymbol{r})$ and the energy $E_0(n,m)$ depend on two quantum numbers (n,m). In Fig. 1 we show the energies $E_0(0,0)$ and $E_0(0,1)$ and the radial parts of the wave functions, $g_{0,0}(\rho)$ and $g_{0,1}(\rho)$ of the electron lowest levels 1s and 1p in two NTs with the exterior radius $R_e = 1a_0^*$ and two different radii of the repulsive core $R_i = 0.1a_0^*$ in Fig. 1a and $R_i = 0.5a_0^*$ in Fig. 1b. It is seen that these

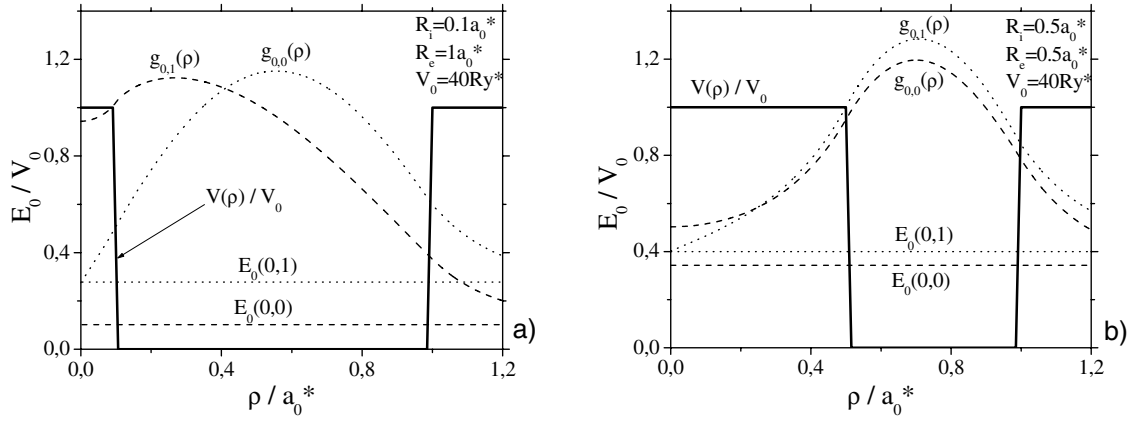

Fig. 1 Energies and wave functions of the two lowest levels, 1s and 1p of the electron in two NTs with different repulsive core radii, a) $R_i = 0.1a_0^*$ and b) $R_i = 0.5a_0^*$.

two levels become almost degenerate and the radial parts of the wave functions almost coincide as the width of the repulsive core increases.

The wave function $\Psi(\boldsymbol{r})$ of the donor is solved from the Schrödinger equation

$$\hat{H}\Psi(\boldsymbol{r}) = E\left(\mathrm{D}^0\right)\Psi(\boldsymbol{r}) , \tag{4}$$

where $E(\mathrm{D}^0)$ is the donor energy. We write $\Psi(\boldsymbol{r})$ in the following form to express the dependence on the distance between the electron and ion $|\boldsymbol{r}-\xi|$:

$$\psi(\boldsymbol{r}) = \left[\alpha f_{1\mathrm{s}}(\boldsymbol{r}) + \sqrt{1-\alpha^2}\, f_{1\mathrm{p}_x}(\boldsymbol{r})\right]\Phi(|\,\boldsymbol{r}-\xi\,|) , \tag{5}$$

where the first factor describes the mixing of the 1s and 1p subbands in the NT produced by the off-axis donor attraction, the second factor is an envelope function that describes the intrinsic properties of the donor and α is a variational parameter $(-1<\alpha<1)$ that gives the degree of mixing of the subbands. By choosing the trial function in the form of Eq. (4) we assume that the off-center donor located on the x-axis modifies the free-electron wave functions in such a way that it becomes more asymmetric in the x-direction due to mixing of the 1s, $f_{1\mathrm{s}}(\boldsymbol{r}) = g_{0,0}(\rho)$ and $1\mathrm{p}_x$, $f_{2\mathrm{p}}(\boldsymbol{r}) = g_{0,1}(\rho)\cos\varphi$ wave functions.

We consider the function $\Phi(r)$ as a variational wave function and using the method described in Ref. [4] we derive the following Euler–Lagrange equation:

$$-\frac{1}{J(r)}\frac{\mathrm{d}}{\mathrm{d}r}\left[J(r)\frac{\mathrm{d}\Phi(r)}{\mathrm{d}r}\right] + \left[\tilde{E}(r) - \frac{2}{r}\right]\Phi = E(\mathrm{D}^0)\,\Phi , \tag{6a}$$

where the radial part of the Jacobian, $J(r)$ and the averaged free electron local energy, $\tilde{E}(r)$ are given by:

$$J(r) = r^2 \sum_{i,k=0,1} \alpha^{2-i-k}\left(1-\alpha^2\right)^{(i+k)/2} P_{ik}(r) ; \tag{6b}$$

$$\tilde{E}(r) = r^2 \sum_{i,k=0,1} \alpha^{2-i-k}(1-\alpha^2)^{(i+k)/2} E_0(0,i)\, P_{ik}(r)/J(r) , \tag{6c}$$

$$P_{ik}(r) = \int_0^{2\pi}\int_0^{\pi} g_{0,0}^{2-i-k}(\tilde{\rho})\, g_{0,1}^{i+k}(\tilde{\rho})\left[1 - r^2\,\mathrm{sin}^2\,\theta\;\mathrm{sen}^2\varphi/\tilde{\rho}\right]^{i+k}\sin\theta\;\mathrm{d}\theta\;\mathrm{d}\varphi; \quad i,k = 0,1 , \tag{6d}$$

$$\tilde{\rho} = (r^2\sin^2\theta + \xi_\rho^2 + 2r\xi_\rho\sin\theta\cos\varphi)^{1/2} .$$

Here, ζ_ρ is the distance to the axis from the donor position. Equation (6a) coincides with the Schrödinger equation for a hydrogen atom in an effective space with the locally variable dimension [4]. Once the functions $g_{0,0}(r)$ and $g_{0,1}(r)$ are found, the functions $P_{ik}(r)$ $(i,k=0,1)$ may then be calculated in a straightforward way through Eq. (6d). Finally, to define the donor energy we solve Eq. (6a) by using the trigonometric sweep method [6].

3 Results and discussion

The values of the physical parameters pertaining to GaAs, $m^* = 0.067m_0$ and $\varepsilon = 12.5$, m_0 being the free-electron mass are 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 a GaAs/$Ga_{1-x}Al_xAs$ QWWs and NTs are presented in Figs. 2–5. 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/$Ga_{0.6}Al_{0.4}As$ QWW $(R_i = 0)$ for several values of the magnetic field calculated by us, with those obtained previously by Branis et al. [2] without subband mixing. In this calculation we intentionally choose the material parameters roughly corresponding 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.

For a given value of the magnetic field, the binding energy increases from its bulk value, equal to 1 Ry*, 1.84 Ry*, 2.27 Ry* and 2.84 Ry* for the magnetic fields 0, 100 kG, 200 kG and 400 kG, respectively, to its maximum value about 5.35 Ry*, as the wire radius R_e is reduced up to $0.2a_0^*$. 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 the barrier region under strong confinement [2, 3].

The calculation results for the D^0 binding energies in a GaAs/$Ga_{0.7}Al_{0.3}As$ nanotubes with the exterior radius $R_e = 3a_0^*$ and several repulsive core radii R_i as a functions of the donor displacement from the axis are presented in Fig. 3. The solid and dashed lines show our results obtained, respectively, for the models with and without mixing of the s and p subbands. It is seen that the effect of mixing is negligible when the donor is located close to the axis or it is moved far from the axis. In the intermediate case the binding energies of the off-axis donors enhanced due to including in the variational calculations the effect of the band mixing up to 5% in QWW $(R_i = 0)$ and up to 10% in nanotubes, where the effect of the subband mixing on the off-axis donors in an accurate calculation cannot be ignored.

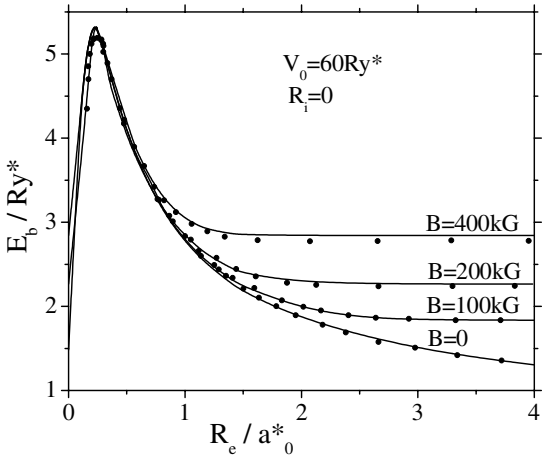

Fig. 2 On-axis donor-binding energies as a function of the QWW radius for several values of the magnetic field B parallel to the axis. The solid lines are our results and solid circles are by Branis et al. [2].

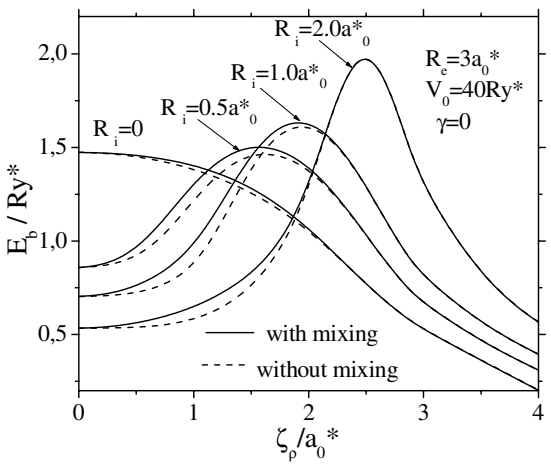

Fig. 3 Donor binding energies as a function of the distance from the axis in nanotubes with an exterior radius of $3a_0^*$ and several different repulsive core radii. The solid and dashed lines are, respectively, results with and without subband mixing included.

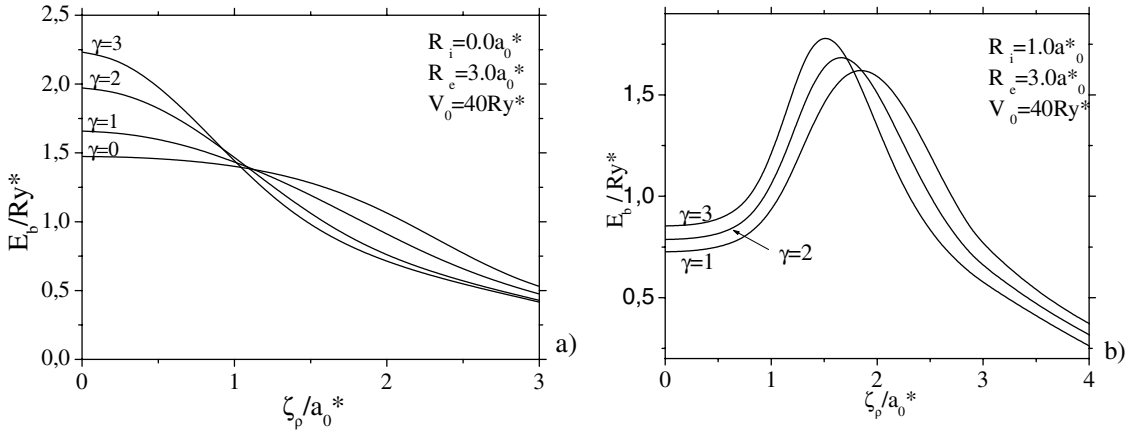

Fig. 4 Donor binding energies as a function of the distance from the axis in the GaAs/$Ga_{0.7}Al_{0.3}As$ a) QWW and b) NT for several values of the magnetic field parallel to the axis.

Also, one can observe a successive displacement of the curve peak position to the right with increasing core radius. The peak position for all the core radii coincides approximately with the midpoint between the interior and exterior radii, $(R_i + R_e)/2$, where the confinement is the largest. 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 contrary, for large core radii the electron can not penetrate into the central region, it is mostly located in the middle between the two barriers and when the donor is situated in the same position the electron–donor separation becomes very small.

In Fig. 4 we display the variation of the binding energies as a function of the distance from the donor location to the axis of a) the GaAs/$Ga_{0.7}Al_{0.3}As$ QWW with the radius $3a_0^*$ and b) the NT with the repulsive core and the exterior radii $1a_0^*$ and $3a_0^*$, respectively, for several 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. In consequence, 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 occurs approximately at the same point, corresponding to a distance $1a_0^*$ from the axis of the QWW or from the interior barrier in NT. 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 paper, we have presented a simple method of calculating of the binding energy for the lowest state of the off-axis D^0 donors in a nanotube in the presence of the magnetic field parallel to the axis, taking into account the effect of the mixing s and $p_{x,y}$ subbands. By using this procedure we calculate the D^0 binding energies in nanotubes with different radii of the repulsive core as a function of the distance from the donor location to the axis. It is shown that the inclusion of the subband mixing in the variational calculation provides an insignificant variation of the binding energy for donor positions close to the axis and far from the axis, whereas for intermediate donor positions the increase of the binding energies

reaches 10%. We found that the external magnetic field applied parallel to the axis increases the binding energies of donors located close to the axis and, conversely, decreases the binding energies of donors located far from the axis. The binding energies of donors remote from the interior barrier of a nanotube by a distance of about the effective Bohr radius are almost insensitive to the external magnetic field.

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