U.P.B. Sci. Bull., Series A, Vol. 70, No. 2, 2008 ISSN 1223-7027

BINDING ENERGY OF A SCREENED DONOR IN A CYLINDRICAL QUANTUM WIRE UNDER APPLIED MAGNETIC FIELDS

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În lucrare se prezintă un calcul variaţional al energiei de legătură al unui donor hidrogenoid ecranat, situat într-un fir cuantic de GaAs-$Al_{0.3}Ga_{0.7}As$*, în prezenţa unui câmp magnetic aplicat paralel cu axa firului. Se studiază dependenţa energiei de legătură de raza firului, de intensitatea câmpului aplicat şi de valorile parametrului de ecranare. Rezultatele arată că efectele variaţiei spaţiale a ecranării dielectrice sunt mai pronunţate pentru donorul situat pe axa firului decât pentru cel situat la marginea acestuia.*

By a variational method, we calculate the binding energy of a screened hydrogenic donor in a GaAs-$Al_{0.3}Ga_{0.7}As$ *quantum-well wire in the presence of a uniform magnetic field applied parallel to the wire axis. The binding energy is obtained as a function of the wire radius, the field strength and the screening parameter. Our results show that the effects of spatial variation of dielectric screening on edge wire donors are larger than those on center donors.*

Keywords: binding energy, screened donor, quantum-well wire, variational method

1. Introduction

The interest in the quantum size effects present in the low-dimensional structures has been primarily motivated by the fact that the optical and electronic properties of these structures are improved by the reduction of dimensionality. It is expected that the same properties be further improved by the reduction of dimensionality to quasi-one-dimensional quantum wires (QWW's).

An understanding of the physics of impurity states in semiconductor quantum wire structures is an important problem because the impurities play a central role in semiconductor technology. GaAs-AlGaAs structures are the most investigated systems, and a number of studies [1-3] concerned with impurity energy levels have been reported in the literature.

Extensive experimental and theoretical investigations of the behavior of energy levels of shallow impurities in quantum wires in the presence of a magnetic field have been carried out during the last years. For a field

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perpendicular applied to the modulated barrier quantum wires, Bayer *et al*. [4] have observed a magnetic field induced transformation of the quantization from quasi-one-dimensional quantum-wire states at low fields to fully quantized quasi-zero-dimensional states at higher fields. The diamagnetic shifts of the excitonic emission are measured in magneto-photoluminescence experiment, and they are important to obtain the dependence of the exciton binding energies on the wire width for InGaAs-GaAs system [5]. Using a variational procedure, within the effective-mass approximation, Latgé *et al*. [6] studied the intradonor infrared-absorption spectra in donor-doped GaAs-Ga_{1-x} Al_x As quantum wells under the presence of electric and magnetic fields. Zang *et al*. [7] calculated the energy levels of a hydrogenic impurity in a parabolic quantum well under applied magnetic field. The variational results of Zhu *et al*. [8] were in agreement with the experimental magneto-optical transition energies of D^0 and D^- centers in GaAs-Ga_{1-x} Al_x As quantum wells.

Screening in semiconductor nanocrystals is a fundamental issue, due to the large amount of technological applications of the nanostructures, but the phenomenon is still not fully understood. The presence of many papers recently published on this subject shows that there is a strong interest in this field [9, 10].

In this paper we report a study of the screening of point charges in GaAs-$Al_{0.3}Ga_{0.7}As$ quantum wire in magnetic fields applied parallel to the axis of the wire. The influence of radius size on the binding energy is also studied. We have performed the calculations using a variational method for finite confinement potentials. We report our results for ground state of a donor impurity located at the center and the edge of the wire, respectively.

2. Theory

In the effective-mass approximation, the Hamiltonian for a donor impurity in a cylindrical GaAs QWW with radius R, in the presence of a magnetic field applied along the axis of the wire, is:

$$H = -\frac{\hbar^2}{2m^*}\left[\frac{\partial^2}{\partial\rho^2} + \frac{1}{\rho}\frac{\partial}{\partial\rho}\right] - \frac{\hbar^2}{2m^*}\frac{\partial^2}{\partial z^2} + \frac{1}{8}\frac{q^2B^2}{m^*}\rho^2 - \\ - \frac{e^2\exp[-\alpha r]}{4\pi\varepsilon_0\varepsilon_r r} + V(\rho) \tag{1}$$

where α is the screening parameter. Here $V(\rho)$ is the potential-energy barrier that confines the carrier in the wire; we assume that

$$V(\rho)=\begin{cases}0 & \text{if } \rho < R\\ V_0 & \text{if } \rho > R\end{cases} \tag{2}$$

In Eq. (1) $r=\sqrt{(\rho-\rho_i)^2+z^2}$ is the electron-impurity distance, and $\vec{\rho}_i$ is the impurity position chosen along the y-axis.

We take the following trial wave function:

$$\psi_d = \psi_0(\rho, \vec{B})\exp\left[-\frac{\sqrt{(\rho-\rho_i)^2+z^2}}{\lambda}\right] \tag{3}$$

where λ is a variational parameter; $\psi_0(\rho, \vec{B})$ is the first subband wave function of the electron:

$$\psi_0(\rho, \vec{B}) = \mathrm{C}\, exp\left[-\frac{\xi}{2}\right] F\left[-\beta+\frac{1}{2}, 1, \xi\right] \tag{4}$$

where C is the normalization constant, $\xi=\frac{1}{2}\frac{qB}{\hbar}\rho^2$, $F(a,b,\xi)$ is the confluent hypergeometric function, $\beta=\frac{m^* E_0}{\hbar e B}$ with E_0 the lowest electron subband energy related to the $\psi_0(\rho, \vec{B})$ wave function. E_0 is the lowest solution of the equation:

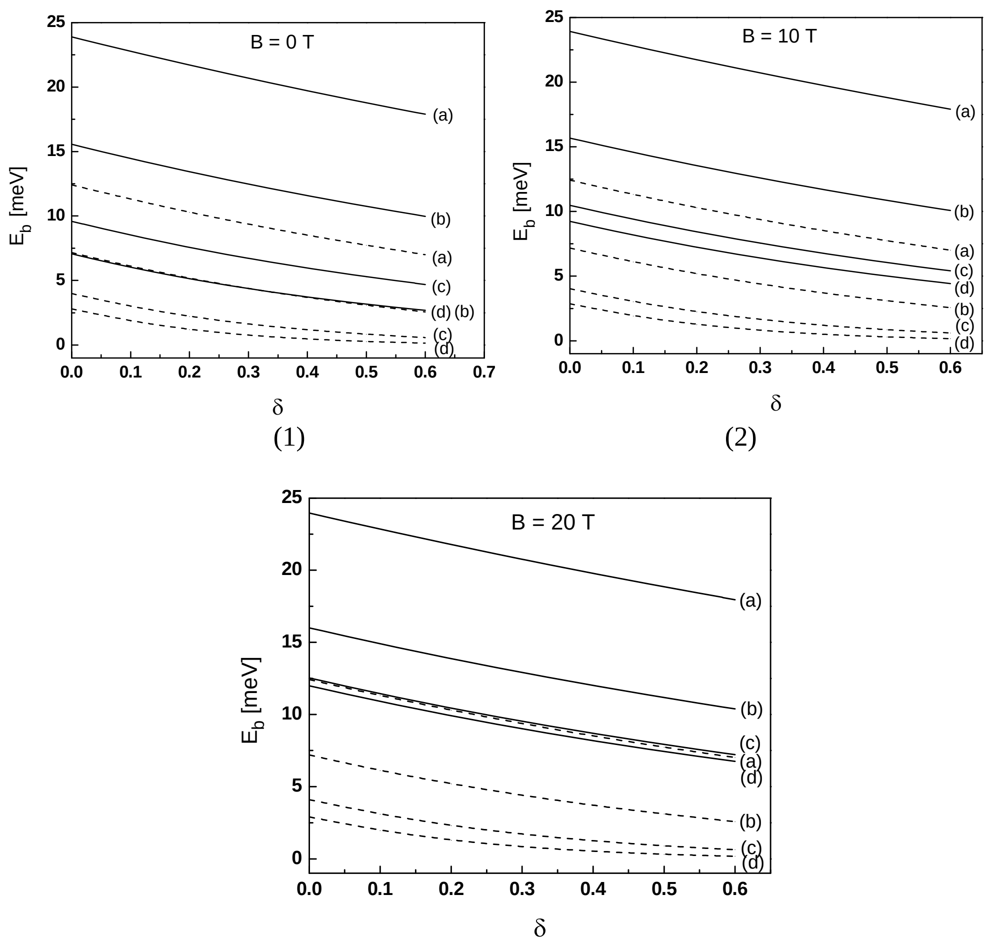
$$F\left[-\left(\beta-\frac{1}{2}\right), 1, gR^2\right]=0 \tag{5}$$

The donor energy E_d is obtained as $E_d = \min\limits_{\lambda} \frac{\langle\psi_d|H|\psi_d\rangle}{\langle\psi_d|\psi_d\rangle}$. The binding energy is given by: $E_b = E_0 - E_d$.

3. Results and discussions

We have performed a numerical calculation for GaAs-$Ga_{1-x}Al_xAs$ QWWs with $V_0 = 223\,\mathrm{meV}$, corresponding to an Al concentration of $x \cong 0.3$. We have taken $m^* = 0.0665\, m_0$ and we have calculated the binding energies as a function of the parameter $\delta = \alpha\, a_B{}^*$, where $a_B{}^* = \hbar^2 \varepsilon_0 / m^* e^2$ is the effective Bohr radius. For GaAs, $a_B{}^* \cong 99.3\,$Å.

In Fig. 1 we present the binding energy of screened on-center and on-edge donors, respectively. We plot the binding energies calculated for four wire radii (*R* = 50Å; 100Å; 200Å; 300Å) as a function of the screening parameter δ and different applied magnetic fields (*B* = 0T; 10T; 20T). The solid lines represent the binding energies for the screened on-center donor and the dash lines for the screened on-edge donor.



(3)

Fig.1. Screened on-center (solid lines) and on-edge (dash lines) donor binding energy as a function of the parameter δ for different values of the wire radius *R* (50Å – (a) lines; 100 Å – (b) lines; 200 Å – (c) lines and 300 Å – (d) lines) and three values of the magnetic field: (1) - *B* = 0T; (2) - *B* = 10T; (3) - *B* = 20T.

We observe that as the screening parameter becomes larger, the values of the binding energy decrease. This is because the screening reduces the attractive Coulomb interaction that binds the electron by the impurity ion for the both donor positions and for all the considered range of the applied magnetic field.

For the Figs. 2a and 2b we have selected the dependence of the binding energy as a function of the screening parameter only for R = 100Å and 300Å and for all the considered magnetic fields in the case of on-center donor. We want to emphasize that the binding energies decrease less when the wire radius is larger. Also, in Figs. 2b and 2c we show comparatively the decrease of the binding energy as the screening parameter increases for on-center donor (Fig.2b) and for on-edge donor (Fig.2c), for R = 300Å and for the three considered magnetic fields.

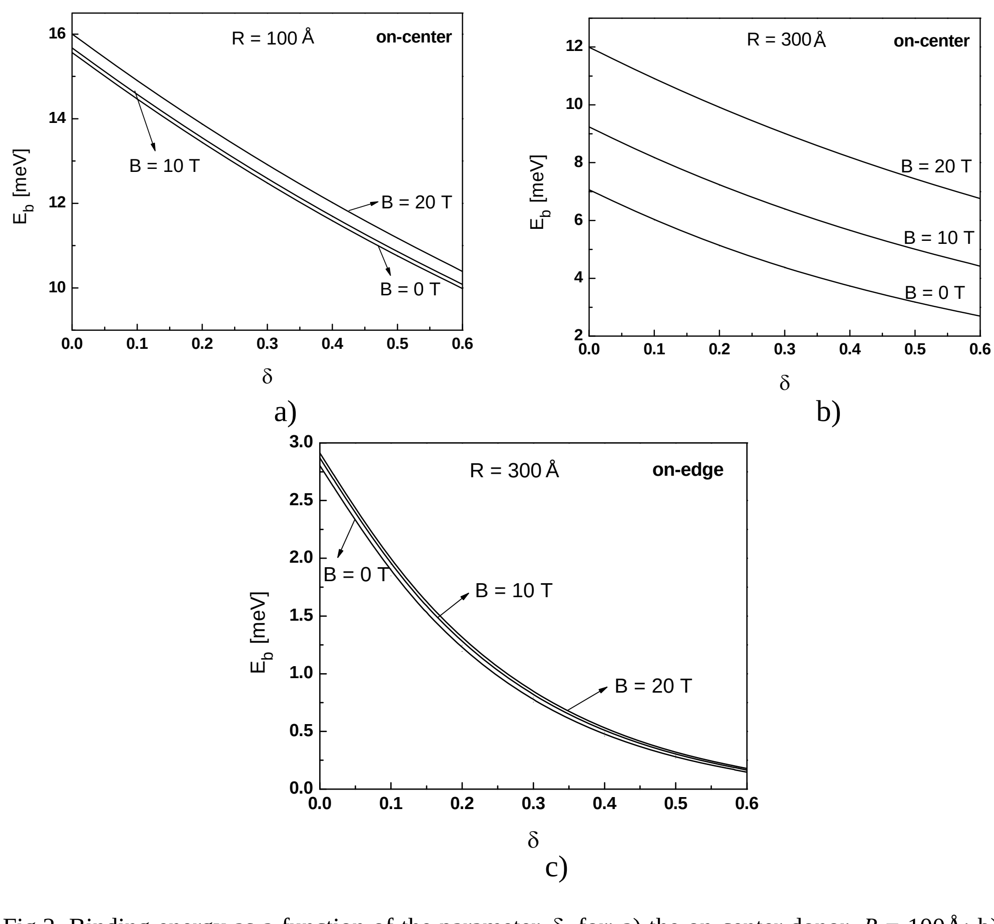
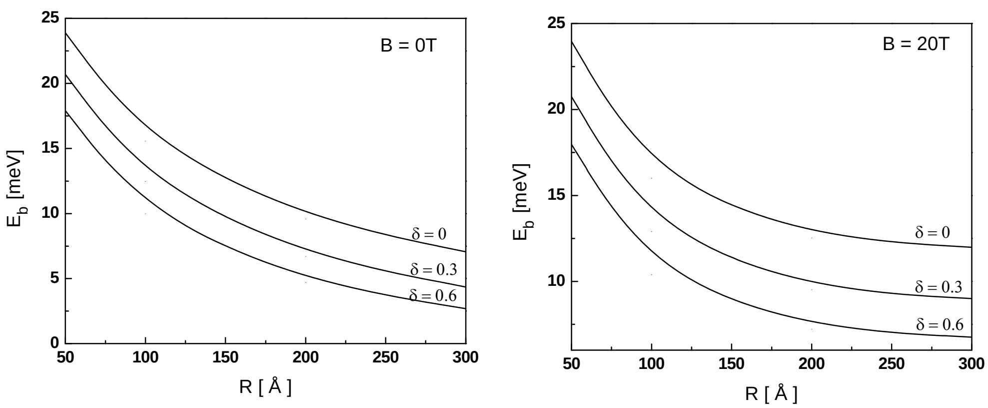


Fig.2. Binding energy as a function of the parameter δ for: a) the on-center donor, R = 100Å; b) the on-center donor, R = 300Å; c) the on-edge donor, R = 300Å.

When the impurity moves to the wire edge, because the magnetic field compresses the electron wave function near the wire axis, the Coulomb interaction is diminished. In this case, as Fig.2c shows, the dependence of the binding energy on the screening parameter is weaker.

Figs.3 and 4 show the dependence of the binding energy versus the wire radius in the absence (δ = 0) and in the presence (δ = 0.3; 0.6) of the screening and of the applied magnetic field. We observe that as the wire radius increases the binding energies decrease.

In the absence of the magnetic field, as the wave function is more spread, the binding energy is less sensitive on the screening parameter (Fig.3a and 3b).



a) b)

Fig.3. Binding energy as a function of the wire radius for different parameter δ values and for: a) B = 0T; b) B = 20T.

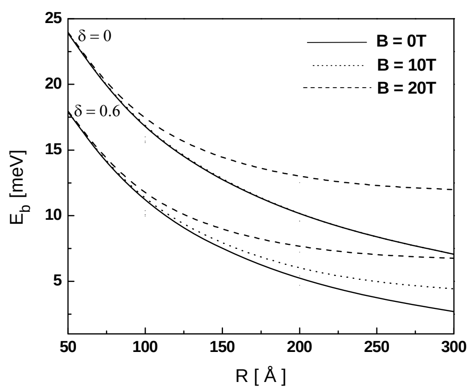


Fig.4. Binding energy of the donor as a function of wire radius and applied magnetic field for unscreening and strong screening cases.

In Fig.5 we present the average distance *r*, between electron and the impurity center

$$\langle r \rangle = \frac{\langle \psi_d | r \psi_a \rangle}{\langle \psi_a | \psi_d \rangle}$$

as a function of the screening parameter for different applied magnetic fields. Independent of the applied magnetic fields there is no influence of the screening parameter on the average distance for the on-center donor (the inset figure). For the on-edge donor the average distance increases with the screening parameter but decreases when the applied magnetic field has greater values. These dependences are in agreement with the behavior of the binding energy of the on-edge donor (Fig.2c).

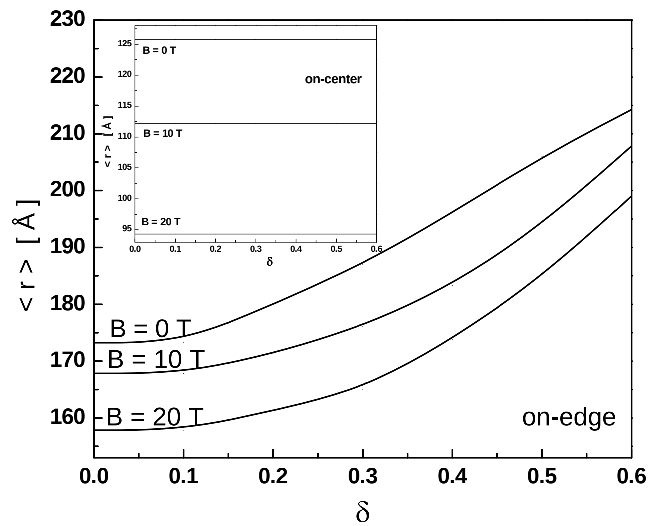


Fig.5. Electron-impurity average distance as a function of screening parameter for some applied magnetic fields. Inset: on-center donor.

4. Concluding remarks

We have calculated the binding energy of the ground state of a screened donor impurity in GaAs-$Al_{0.3}Ga_{0.7}As$ quantum wire in magnetic fields applied parallel to the axis of the wire. We have considered the donor impurity located at the center and the edge of the wire, respectively. Our results show that the binding energies decrease significantly when the screening parameter δ increases, for all the used wire radii, but increase for great values of the applied magnetic field. Also, the magnetic field influence is more pronounced for bigger wire radii and for on-center donors.

Concluding, for on-center donor the screening corrections are important and they must be taking into account for a precise calculation.

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