Binding energy of an off-center donor in cylindrical quantum-well wires under intense laser fields

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Calculation of the binding energy of an off-center donor hydrogenic impurity in a cylindrical quantum wire, in the simultaneous presence of an intense high frequency laser field and a static magnetic field, is reported. Different geometries concerning the size of quantum wire, the donor impurity position, as well as the polarization direction of the applied laser field with respect to the quantum structure, were considered. We found that in the strong confinement regime the presence of the linearly polarized laser radiation resolves partially the degeneracy of donor states corresponding to symmetrical position of the impurity.

1. Introduction

The understanding of the properties of impurity energy levels in low-dimensional semiconductor structures is a subject of interest due to possible technological applications in electronic devices associated with these systems. In nanostructures, besides Coulombic interaction, the impurities are affected by confining potential which is more important as the dimension of the system is reduced. In the past decades, the study of the hydrogenic-shallow impurities in semiconductor quantum wells (QWs), quantum-well wires (QWWs) and quantum dots (QDs), has received much attention from both theoretical and technological points of view ([1-10] and references therein). More recently, such studies have been extended to low-dimensional semiconductor heterostructures under intense electric fields, created by a high-intensity THz laser [11-22]. Oliveira et al. [11] have studied the interaction of a laser field with QWs and QDs. They have reported that the strong localization of the electronic states, due to the quantum confinement, is further enhanced by laser interaction with semiconductor heterostructures. The theoretical studies on effect of an intense laser field radiation (LFR) on the optical properties of semiconductor quantum wells [12] and quantum wires [13] considering the laser-dressed potential energy have been performed. In these structures, blue shifts of the electronic energy levels dependent upon the device size are observed, thus allowing a new approach for controlling the optical emission wavelengths of quantum structures. A systematic study on the influence of two intense, long-wavelength, non-resonant laser fields on the electron energy levels and density of states in quantum wells has been performed within a Green's function approach by Enders et al. [14].

The laser field dependence of the intersubband optical absorption in a graded quantum well, under an applied electric field has been calculated in the effective mass approximation by Ozturk et al. [15]. The influence of a laser-field on the exciton binding energy and interband optical transitions in quantum-well wires with [16] and without [17] an external magnetic field has been investigated by Kasapoglu et al. They found that the additional confinement of the particles in the quantum wires offers a greater variety of electronic properties dependence on the intense laser field and magnetic field in comparison to three and two-dimensional materials.

Special attention has been given to the electronic confinement due to both an intense laser field and dimensionality effects on the shallow-donor located at the center of low-dimensional quantum structures. Using a variational method, Sari et al. [18] have calculated the laser-field dependence of binding energy and the polarizability of shallow-donor impurities in graded quantum wells under an external static electric field. Kasapoglu et al. [19] have studied the laser field and electric field effects on the donor-impurity-related photoionization cross-section and impurity binding energy in GaAs-GaAlAs graded quantum-well wires. Fanyao et al. [20] have reported calculation of the binding energy of an axial donor impurity in an ideal, infinite, cylindrical quantum wire placed in an intense, high-frequency laser field. By making use of a non-perturbative theory that "dresses" both the potential of the impurity and the confinement potential in the wire, they have observed a decrease of the binding energy with the increase of field intensity. In a spherical QD placed in an intense, high-frequency laser field, the theoretical studies [21-22] also predicted a rapid decrease of the binding energy of an on-center donor impurity, for both infinite and finite potential barriers, with increasing field amplitude.

However, the impurities could be located anywhere in the quantum structures. The problem of an off-center impurity is more general and leads to a series of effects that do not exist in nanostructures with an impurity located in the center. Thus, even in the absence of an intense LFR, in a strong confinement regime, a large spread of the ground-state energy is observed as the impurity position varies [3, 8, 23].

To our knowledge, there have been no calculated results about the energy levels of off-center donors in nanostructures under intense laser radiation. In this paper we studied the positional dependence of the ground donor state in a cylindrical QWW with a finite barrier height in the simultaneous presence of intense high-frequency laser and static magnetic fields.

2. Theory

We consider the donor impurity in a cylindrical QWW under the action of a magnetic field applied parallel to the wire axis and monochromatic electromagnetic radiation (of frequency ω), linearly polarized in a direction perpendicular to the axis of the wire (polarization vector $\mathbf{n}$). The Schrödinger equation for a particle moving under the combined forces of potential $V(\mathbf{r})$ and a radiation field was obtained by Kramers [24] as follows:

$$\left\{ \frac{\mathbf{p}^2}{2m*} + V[\mathbf{r} + \mathbf{a}(t)] \right\} \Psi = i\hbar \frac{\partial \Psi}{\partial t}. \qquad (1)$$

Here

$$\mathbf{a}(t) = \mathbf{a_0}\, sin(\omega t)\ , \qquad (2)$$

where $\mathbf{a_0} = a_0\, \mathbf{n}$, with $a_0 = \dfrac{e\,A_0}{m*\omega}$ the laser-dressing parameter, and A_0 the vector potential amplitude. $V[\mathbf{r} + \mathbf{a}(t)]$ is the "dressed" potential energy; for the Coulomb case $V(\mathbf{r}) = -\dfrac{e^2}{4\pi\varepsilon|\mathbf{r}|}$, the "dressed" potential has the form [25]:

$$V_0(\mathbf{r},\mathbf{a}) = -\frac{e^2}{4\pi\varepsilon} \frac{1}{2} \left[\frac{1}{|\mathbf{r} + \mathbf{a_0}|} + \frac{1}{|\mathbf{r} - \mathbf{a_0}|} \right] (3)$$

Within the framework of an effective-mass approximation, the Hamiltonian of the hydrogenic donor in a cylindrical QWW under the action of a magnetic field applied parallel to the wire axis, Oz, and the laser-field, is given by:

$$H = \frac{(\mathbf{p} + e\mathbf{A})^2}{2m*} + V_c(\mathbf{r}) + V_0(\mathbf{r},\mathbf{a_0}). \qquad (4)$$

Here $\mathbf{A} = (\mathbf{B} \times \mathbf{r})/2$ is the vector potential of the magnetic field,

$$V_c(\rho) = \begin{cases} 0, & \rho \leq R \\ \Delta E_c, & \rho > R \end{cases} \qquad (5)$$

is the confinement potential and R is the radius of the quantum wire.

We choose $\mathbf{n}$ direction perpendicular to the axis of the wire, so that:

$$V_0(\boldsymbol{\rho},z,\mathbf{a_0}) = -\frac{e^2}{4\pi\varepsilon} \frac{1}{2} \left[\frac{1}{\sqrt{(\boldsymbol{\rho} - \boldsymbol{\rho_i} + \mathbf{a_0})^2 + z^2}} + \frac{1}{\sqrt{(\boldsymbol{\rho} - \boldsymbol{\rho_i} - \mathbf{a_0})^2 + z^2}} \right] \quad (6)$$

In equation (6) ε is the dielectric constant of the wire material, and ρ_i gives the impurity's location. In our calculation, the donor position was chosen along the x axis. Following the procedure of Ref. [26], we take into account the cylindrical confining symmetry, the presence of the magnetic field, and the hydrogenic impurity potential by choosing a trial envelope variational wave function:

$$\Psi(\mathbf{r},\lambda) = \Phi(\rho,B)\, f(\boldsymbol{\rho},z,\lambda). \qquad (7)$$

Here $\Phi(\rho,B)$ is the radial solution of an electron in a cylindrical wire in the presence of the magnetic field [26]:

$$\Phi(\rho,B) = \begin{cases} \exp[-\xi/2]\ F(-\beta + 1/2, 1; \xi); & \rho < R \\ A\exp[-\xi/2]\ U(-\beta' + 1/2, 1; \xi); & \rho > R \end{cases}, (8)$$

where $\xi = \dfrac{eB}{2\hbar}\rho^2$, $\beta = \dfrac{m* E_0}{\hbar\, e\, B}$, $F(a,b;z)$ is the confluent hypergeometric function, and $U(a,b;z)$ is the Kummer function. The parameters A, β and β' are determined from the continuity of the wave function and its derivate at the boundary of the QWW, by using the relation between β and β':

$$\beta - \beta' = \frac{m*}{\hbar\, e\, B} V_0. \qquad (9)$$

$f(\boldsymbol{\rho},z,\lambda)$ is a laser field modulated trial wave function [20]:

$$f(\boldsymbol{\rho},z,\lambda) = \exp\left[-\frac{\lambda}{2}(|\mathbf{r_1}| + |\mathbf{r_2}|) \right], \qquad (10)$$

where

$$\mathbf{r_1} = \sqrt{(\boldsymbol{\rho} - \boldsymbol{\rho_i} + \mathbf{a_0})^2 + z^2} \qquad (11a)$$

$$\mathbf{r_2} = \sqrt{(\boldsymbol{\rho} - \boldsymbol{\rho_i} - \mathbf{a_0})^2 + z^2} \qquad (11b)$$

and λ is the variational parameter.

The laser "dressed" binding energy $E_b(B,\boldsymbol{\rho_i},\boldsymbol{\alpha_0})$ of the hydrogenic impurity is defined as:

$$E_b(B,\boldsymbol{\rho_i},\mathbf{a_0}) = E_0 - \min_\lambda \frac{\langle \Psi|H\Psi \rangle}{\langle \Psi|\Psi \rangle} \quad (12)$$

where E_0 is the ground-state energy of the system without the impurity.

3. Results and discussion

We have performed a numerical calculation for GaAs-$Ga_{1-x}Al_xAs$ QWWs with $\Delta E_c = 347,5 \text{ meV}$, corresponding to an Al concentration of $x \cong 0,4$. In what follows, we present our results in reduced effective units of energy, Ry*. For donors in GaAs, $\text{Ry*} \cong 5,7 \text{ meV}$.

In Fig. 1 we show the binding energy of an on-center donor as a function of the applied magnetic field and for different values of the laser parameter. Two different values of the radius wire, (a) $R = 50 \text{ Å}$ and (b) $R = 200 \text{ Å}$, are considered.

We have chosen the a_0 range so that $a_0' = \dfrac{a_0}{R} \leq 0,5$.

Notice that in the case of $a_0 = 0$ (no laser field), our results are quite similar to those obtained by Branis et al. [26].
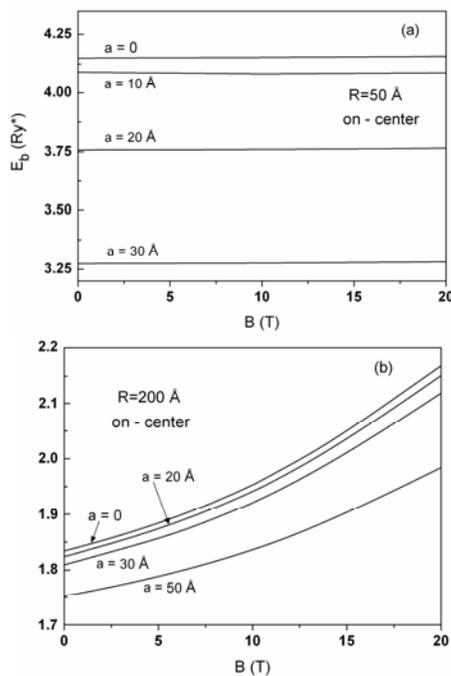

Fig. 1. Variation of the binding energy of an on-center donor as a function of the magnetic field for several values of the laser parameter.

We observe that the magnetic field has almost no influence on the binding energy for small R values ($R \leq 100 \text{ Å}$), but in the "large" R region the electron becomes more centered near the wire axis due to the squeezing by the applied magnetic field. Therefore, by

increasing the radius of the QWW the magnetic confinement predominates and the ground-state energy becomes less sensitive to the laser-field.

In Fig. 2 we plot the binding energy for on – center donor vs. a_0 for different wire radii and various magnetic fields. For $B = 0$ we have obtained the same dependence on the laser parameter as that of Fig. 2 in Ref. [20]. As expected, for a given value of B the binding energy of the impurity decreases with a_0. For large values of laser field parameter the wave function of the particle start to spill over into the barrier material, i.e., the electron becomes less confined, which leads to a smaller Coulomb interaction and therefore a lower binding energy. This is confirmed by the inset of figure 2(a), where the extents of the electron along the radial and longitudinal direction, respectively are shown as functions of a_0 for $R = 50 \text{ Å}$. Note that the laser-field polarization is along the radial direction and has no direct influence on the donor behavior in the z direction. In the ρ direction, the laser field increases electron-impurity separation. This implies a weaker Coulomb interaction and this effect should also be seen in the z direction. This is the case for the mean quadratic longitudinal extent, $\left\langle z^2 \right\rangle^{1/2}$ (Fig. 2(a)).
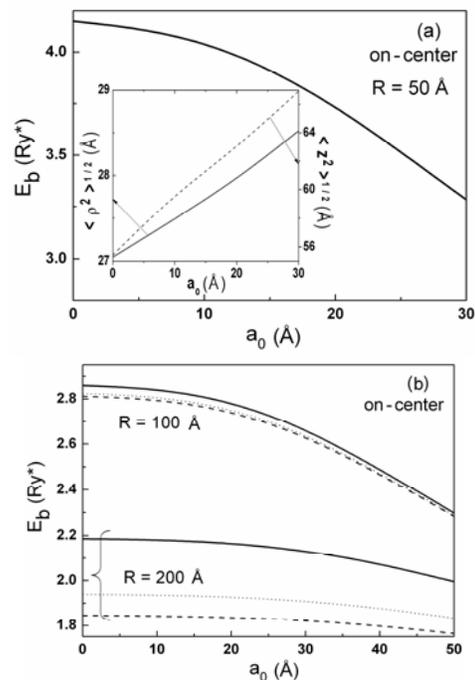

Fig. 2. Binding energy for on-center donor in GaAs-$Ga_{0.6}Al_{0.4}As$ QWWs as a function of the laser field parameter for different values of the wire radius and for three values of the axial magnetic field. B=0: dashed curves; B=10T: dotted curves; B = 20T: solid curves.

On the other hand, it is clear from Fig. 2 that for small R values the binding energy of an on-center impurity is more sensitive to the laser-field parameter a_0. This is in agreement with results obtained for the on-center donor in QWs [18] and QWWs [20].

The behavior of the binding energy of an off-center donor in a cylindrical GaAs-Ga$_{0.6}$Al$_{0.4}$As QWW is shown in figures 3-4.

We remark that as $\boldsymbol{\rho}_i$ increases, even for large R values, the binding energy is only slightly influenced by the magnetic field (Fig. 3). We found that for on-edge donors, as the wave function of the electron shift its amplitude toward the barrier, E_b is completely insensitive to the increase of the magnetic field for the values used here. Note that in the numerical calculations we considered two polarization directions, $\theta = 0^0$ and $\theta = 90^0$ respectively, where θ is the angle between $\boldsymbol{\rho}_i$ and $\mathbf{a}_0$.
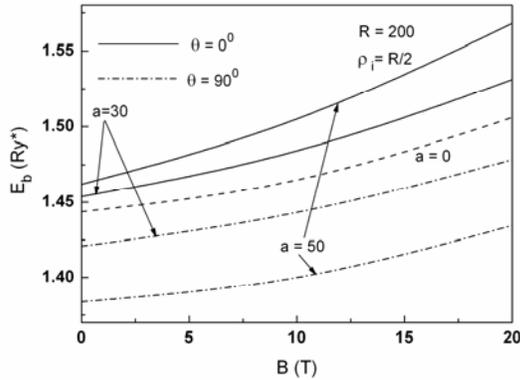

Fig. 3. Off-center donor binding energy as a function of the magnetic applied field for different values of the parameter laser field.

The dependence of the binding energy of a shallow donor impurity in a cylindrical GaAs-Ga$_{0.6}$Al$_{0.4}$As QWW as a function of the laser parameter for different impurity positions along the x axis is shown in Figs 4(a)-(c).
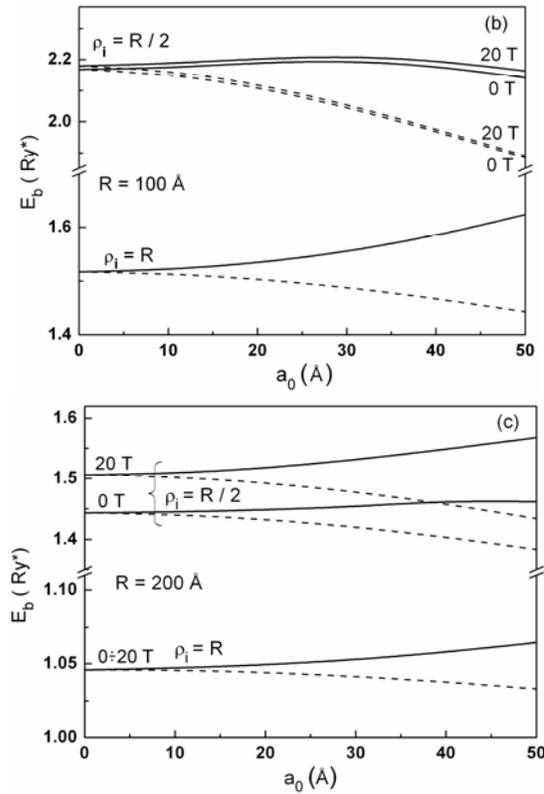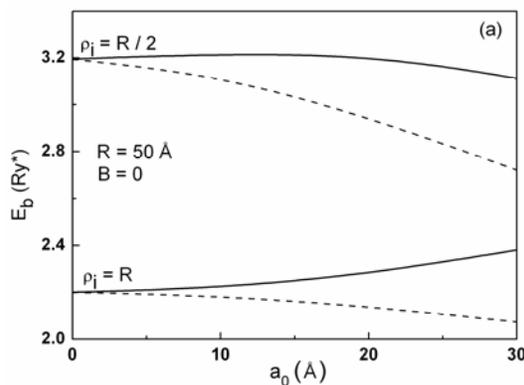

Fig. 4. Binding energy for off-center donor as a function of the laser field parameter for different values of the wire radius and for two polarization directions of LFR. $\theta=0^0$: solid curves; $\theta=90^0$: dashed curves.

We observed that that in narrow QWWs there is a considerable change of the binding energy for varying polarization directions of LFR. For a given value of $\boldsymbol{\rho}_i$, E_b increases (decreases) with a_0 when $\theta=0^0$ ($\theta=90^0$). This behavior is associated with the laser-field-induced deformation of the electron wave function and the competition between the effects of the laser field and of the barrier constraint. For $\theta=0^0$ (x-polarization) we found that the probability for finding the electron inside the wire increases with a_0, which agrees with the increase of the binding energy. For $\theta=90^0$, the confinement in the quantum structure is reduced as a_0 increases and the barrier penetration effect becomes predominant.

The behavior of the donor binding energy as the impurity position changes along the wire radial direction is shown in figure 5 for several values of the laser-field parameter.
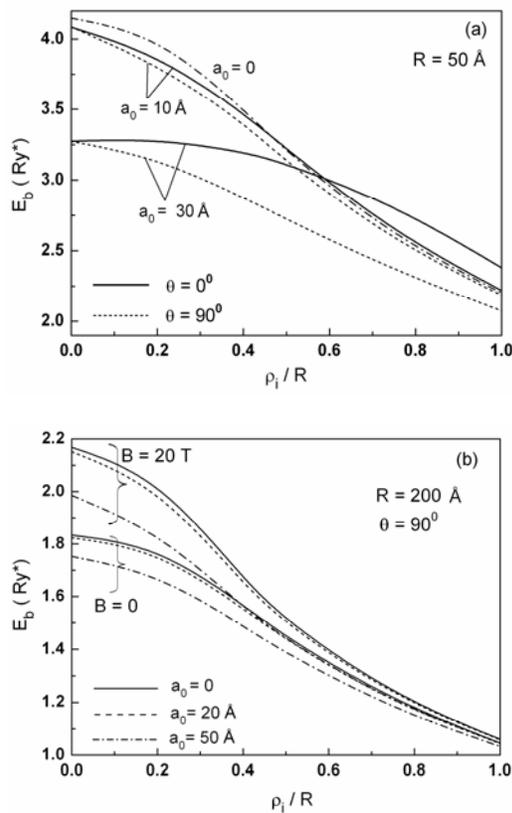
Fig. 5. Donor binding energies as functions of the impurity position for different values of the laser field parameter.

i) the experimental value for the binding energy of impurities in these structures could *not* be compared with the on-center impurity value. Thus the evaluation of center of gravity of the impurity band may be very important [27] when interpreting experimental data in low-dimensional systems under intense laser radiation. We intend to investigate this aspect.

ii) in QWWs, especially for small wire dimensions, by tuning the intensity and the polarization direction of the laser field we can obtain significant effects on the electronic and optical properties.

We have tested the accuracy of our variational approach by performing calculations for the binding energy in cylindrical GaAs-GaAlAs QWWs with the hydrogenic-like wave function given by equation (10), and a Gaussian-type orbital function [19], $f(z, \lambda) = exp\left[-\lambda z^2\right]$, respectively. Calculated results for $R = 100$ Å are displayed in figure 6. It appears that for the studied cases the hydrogenic-like variational function leads to better results, but the theoretical values for E_b with these different trial wave functions differ at most by 2%.
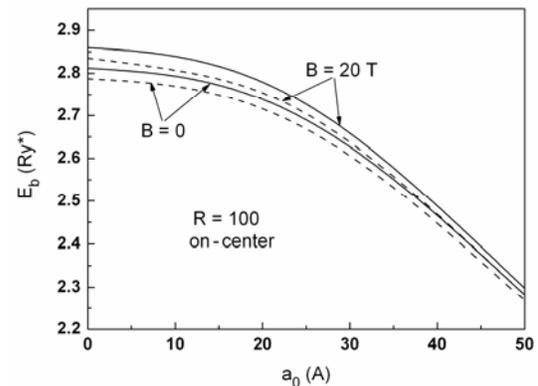
For the values of magnetic field used here, the electron tends to follow the impurity ion as a consequence of the Coulomb attraction. As the donor approaches the wire boundary, E_b decreases due to the increase in the kinetic energy as the electron wave function is compressed by the wire potential barrier. This is in agreement with the results obtained for the donors in QWW in the absence of the laser-field [3]. This effect is clearly pronounced for $\theta = 90^0$ (y-polarization of LFR), when the leakage of the wave function into the barrier region becomes more important (Fig. 5(a)). Since for the large wire dimensions the binding energy is relatively insensitive to the polarization of LFR, in Fig. 5(b) we plotted the variation of E_b with the donor position ρ_i, in a $R = 200$ Å QWW, only for $\theta = 90^0$. In this limit of large wire radius, for on-edge donors the energy is independent of the magnetic field strength and of the laser-field parameter.

In Fig. 5(a) it is also observed that, for small wire dimensions, the presence of laser field partially resolves the degeneracy of impurity states corresponding to symmetrical positions of the impurity. The confinement effects in QWWs in intense laser field lead to a large spreading of impurity levels, which depend very much not only upon the impurity position but also upon the polarization direction of LFR. Therefore,

Fig. 6. Comparison between the binding energy for an on-center donor in a R = 100 Å QWW, calculated by using the hydrogenic-like wave function (solid lines), with those obtained using the Gaussian type orbital function (dashed curves).

4. Conclusions

We studied the influence of the intense laser field on the binding energy of a shallow donor impurity in a cylindrical GaAs-GaAlAs QWWs under the action of an axial magnetic field. We used the effective-mass approximation within a variational scheme. For the first time, the donor-impurity position within the structure was taken into account. The study of the effects of laser field on the energy levels of the impurity suggests that the electronic properties of the quantum structures can be tuned by varying the laser field parameter and the polarization direction. This kind of optical control may be of great interest for optoelectronic devices based on low-dimensional systems.

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