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BINDING ENERGY OF AN OFF-CENTER DONOR IN CYLINDRICAL QUANTUM-WELL WIRES UNDER INTENSE LASER FIELDS

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In lucrare se studiază efectul radiației laser de înaltă frecvență asupra energiei de legătură a unei impurități hidrogenoide într-un fir cuantic din GaAs-AlGaAs, pentru diferite poziții ale impurității în fir. Valorile energiilor de legătură sunt obținute utilizând aproximația masei efective şi metoda variațională. Rezultatele obținute arată că prezența radiației laser ridică parțial degenearea pentru stările corespunzătoare unor poziții simetrice ale donorului în firul cuantic.

In this work, we have investigated the effect of the intense high frequency laser field on the ground-state binding energy of hydrogenic impurity in cylindrical GaAs-AlGaAs quantum well wires as function of the impurity position. The binding energies were obtained using the effective-mass approximation within a variational scheme. We have shown that in the strong confinement regime the presence of the linearly polarized laser radiation partially resolves the degeneracy of donor states corresponding to symmetrical position of the impurity.

1. Introduction

The ionisation of dopants (i.e., donor and acceptor impurities) provides the major source of carriers in semiconductors. The ionised dopants are also the major sources of electron-impurity scattering in semiconductor devices, which determine the transport and optical properties of the device systems at low-temperatures. Hence, the investigation of the impurities electronic structure (such as binding energies of donors and acceptors, transition energies, etc.) is fundamental in understanding almost all physically measurable properties in semiconductors. In the absence of an intense electro-magnetic radiation field, the binding energies of impurities in usual semiconductor materials are known [1] and the theoretical approaches to calculate these impurity states are well documented [2]. It should be noted that in semiconductor materials such as GaAs, Ge and Si, the binding energies of donor and acceptor impurities are of the order of terahertz photon energies so that an intense THz radiation can strongly affect the impurity states. With development and application of coherent, high-power, long-wavelength, frequency-tunable and linearly polarised radiation sources such as

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THz or far-infrared lasers, it has now become possible to measure the effect of an intense laser radiation on ionisation and perturbation of dopants (especially shallow impurities) in different semiconductor systems. The results obtained experimentally indicate that in the presence of intense laser radiation i) impurity states in different semiconductor systems are perturbated by the intensity and frequency of the THz laser fields [3-5]; ii) some interesting intense radiation phenomena, such as impact ionisation of dopants [3] and splitting and broadening of the impurity spectrum [5], can be observed. In order to understand these fundamentally new experimental findings and to predict new radiation phenomena, it is essential to calculate the effects of an intense laser field on the binding energies of impurities in semiconductors.

More recently, such studies have been extended to low-dimensional semiconductor heterostructures under intense electric fields, created by a high-intensity THz laser [6-17]. Oliveira *et al*. [6] 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. Theoretical studies on the effect of an intense laser field radiation (LFR) on the optical properties of semiconductor quantum wells [7] and quantum wires [8] considering the laser-dressed potential energy have been performed**.** In this 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, nonresonant 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*. [9].

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*. [10]. The influence of a laser-field on the exciton binding energy and interband optical transitions in quantum-well wires with [11] and without [12] an external magnetic field has been investigated by Kasapoglu *et al*.

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*. [13] 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.* [14] 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*. [15] 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 nonperturbative 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 [16-17] have 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 at the center. In this paper we have studied the positional dependence of the ground donor state in a cylindrical QWW with a finite barrier height in the presence of an intense high-frequency laser field.

2. Theory

We consider the donor impurity in a cylindrical QWW under the action of a 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 a potential $V(\mathbf{r})$ and a radiation field was obtained by Kramers [18] as follows:

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

Here

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

where $\mathbf{a_0}=a_0\,\mathbf{n}$, with $a_0=\frac{eA_0}{m^*\omega}$ the laser-dressing parameter, e and m^* are the electron charge, and the electron effective-mass, respectively, and A_0 is the vector potential amplitude. $\mathrm{V}[\mathbf{r}+\mathbf{a}(\mathrm{t})]$ is the "dressed" potential energy; in the Coulomb case $\mathrm{V}(\mathrm{r})=-\frac{\mathrm{e}^2}{4\pi\varepsilon|\mathbf{r}|}$, the "dressed" potential has the form [19]:

$$\mathrm{V}_0(\mathbf{r},\mathbf{a})=-\frac{\mathrm{e}^2}{4\pi\varepsilon}\frac{1}{2}\left[\frac{1}{|\mathbf{r}+\mathbf{a}_0|}+\frac{1}{|\mathbf{r}-\mathbf{a}_0|}\right] \tag{3}$$

Within the framework of an effective-mass approximation, the Hamiltonian of the hydrogenic donor in a cylindrical QWW under the action of the laser-field, is given by:

$$H = \frac{\mathbf{p}^2}{2m^*} + V_c(\mathbf{r}) + V_0(\mathbf{r}, \mathbf{a}_0). \tag{4}$$

Here

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

is the confinement potential obtained from the 60% rule of the total band gap discontinuity between $Ga_{1-x}Al_xAs$ and GaAs and R is the radius of the quantum wire.

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

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

In Eq. (6) ε is the dielectric constant of the wire material, and $\boldsymbol{\rho}_\mathrm{i}$ gives the impurity's location. In our calculation, the donor position was chosen along the x axis. We take into account the cylindrical confining symmetry and the hydrogenic impurity potential by choosing a trial envelope variational wave function:

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

Here $\Phi(\rho)$ is the radial solution of an electron in a cylindrical wire:

$$\Phi(\rho) = \begin{cases} J_0(k_1\rho) & \rho < R \\ A\, K_0(k_2\rho); & \rho > R \end{cases} \tag{8}$$

where

$$k_1^2 = \frac{2\, m^* E_0}{\hbar^2},\ k_2^2 = \frac{2\, m^*(\Delta E_c - E_0)}{\hbar^2}, \tag{9}$$

$J_0(x)$ is the Bessel function of the first kind, and $K_0(x)$ is the Bessel function of the second kind. The parameters A and E_0 are determined from the continuity of the wave function and its derivative at the boundary of the QWW. $f(\boldsymbol{\rho}, z, \lambda)$ is a laser field modulated trial wave function:

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

where

$$\mathbf{r}_1 = \sqrt{(\boldsymbol{\rho} - \boldsymbol{\rho}_\mathbf{i} + \mathbf{a_0})^2 + z^2} \tag{11a}$$

$$\mathbf{r}_2 = \sqrt{(\boldsymbol{\rho} - \boldsymbol{\rho}_\mathbf{i} - \mathbf{a_0})^2 + z^2} \tag{11b}$$

and λ is the variational parameter.

The laser "dressed" binding energy $E_b(\boldsymbol{\rho}_i, \boldsymbol{\alpha}_0)$ of the hydrogenic impurity is defined as:

$$E_b(\boldsymbol{\rho}_i, \mathbf{a}_0) = E_0 - \min_{\lambda} \frac{\langle \Psi | H\Psi \rangle}{\langle \Psi | \Psi \rangle} \tag{12}$$

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 $\Delta E_c = 347{,}5$ 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, Ry* $\cong$ 5.7 meV.

In Fig. 1 we show the binding energy of an on-center donor as a function of the laser parameter, for different values of the radius wire. We have chosen the a_0 range so that $a_0' = \frac{a_0}{R} \leq 0.5$. Notice that in the case of $a_0 = 0$ (no laser field), our results are quite similar to those obtained by Branis *et al*. [20]. In addition, for *R*=100 Å and 200 Å we have obtained the same dependence on the laser parameter as that of Fig. 2 in Ref. 15.

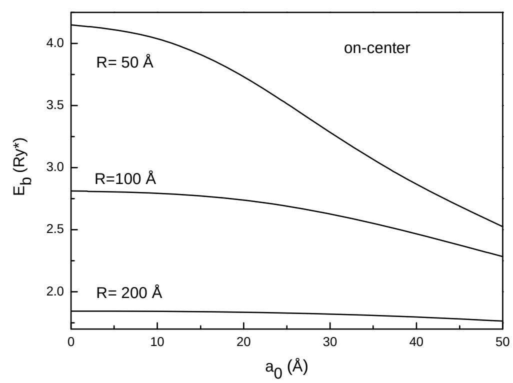

Fig. 1. Variation of the binding energy of an on-center donor in a cylindrical quantum wire as a function of the laser parameter for several values of the radius wire.

As expected, we observed that 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. On the other hand, it is clear from figure 1 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 [13] and QWWs [15].

The behaviour of the binding energy of an off-center donor in a cylindrical GaAs-$Ga_{0.6}Al_{0.4}As$ QWW is shown in figure 2.

Note that in the numerical calculations we considered two polarization directions, $\theta = 0°$ and $\theta = 90°$ respectively, where θ is the angle between $\boldsymbol{\rho}_i$ and $\mathbf{a}_0$.

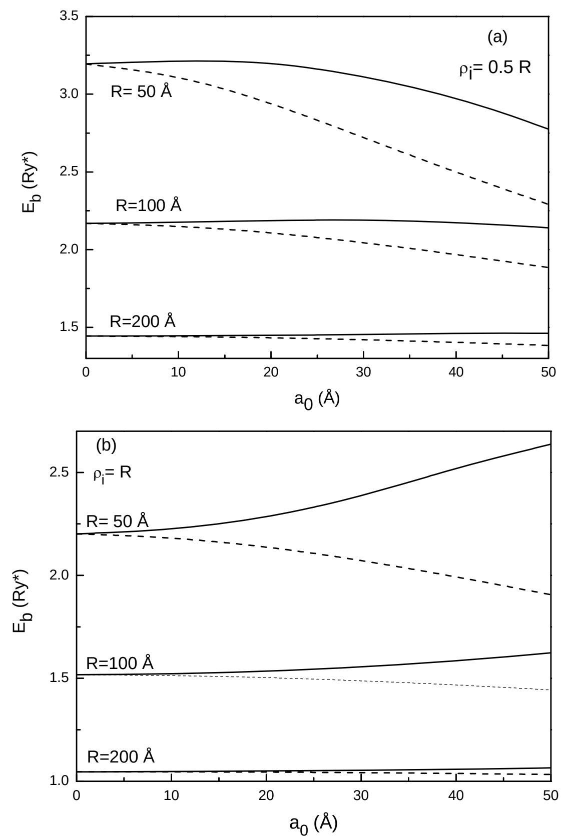

Fig. 2. Binding energy for an off-center donor as a function of the laser field parameter for different values of the wire radius and for two polarization directions of LFR. $\theta = 0°$: solid curves; $\theta = 90°$: dashed curves.

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 $\theta = 0°$ ($\theta = 90°$). 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 the barrier constraint. For $\theta = 0°$ (x-polarization) we found that the probability of finding the electron inside the wire increases with a_0, which agrees with the increase of the binding energy. For $\theta = 90°$, the confinement in the quantum structure is reduced as a_0 increases and the barrier penetration effect becomes predominant.

We remark that for large R values, as $\boldsymbol{\rho}_i$ increases and the wave function of the electron shifts its amplitude toward the barrier, the binding energy is only slightly influenced by the laser field. For a R=200 Å QWW, E_b of an on-edge donor is completely insensitive to the increase of a_0 parameter.

The behavior of the donor binding energy as the impurity position changes along the wire radial direction is shown in figure 3 for several values of the laser-field parameter.

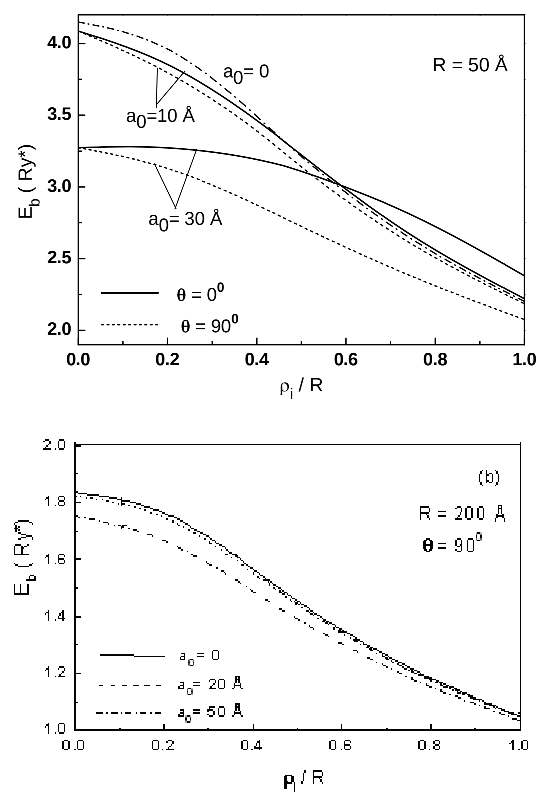

Fig. **3**. Donor binding energies as functions of the impurity position for different values of the laser field parameter

For the used values of the laser field intensity, 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 [21]. This effect is clearly pronounced for $\theta = 90°$ (*y*-polarization of LFR), when the leakage of the wave function into the barrier region becomes more important (Fig. 3(a)). Since for the large wire dimensions the binding energy is relatively insensitive to the polarization of LFR, in Fig. 3(b) we plotted the variation of E_b with the donor position ρ_i, in a R=200 Å QWW, only for $\theta = 90°$. In the case of on-edge donors and in the limit of large wire radius, the binding energy is independent of the laser field.

In fig. 3(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. Thus, the confinement effects in QWWs in intense laser field leads to a large spreading of impurity levels, which depends very much not only upon the impurity position but also upon the polarization direction of LFR.

4. Conclusions

We studied the influence of the intense laser field on the binding energy of an off-center donor impurity in cylindrical GaAs-GaAlAs QWWs. We used the effective-mass approximation within a variational scheme. The study on the effects of a 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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