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Shallow Donors in a Quantum Well Wire: Electric Field and Geometrical Effects*

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Abstract

Subband and shallow donor binding energies are calculated. The emphasis is given on the electric field effects for wires of different shapes. It is shown that the donor binding energy is sensitive to the interplay of the electric field and geometrical effects.

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1. Introduction

Sakaki was the first to suggest mobility enhancement in thin semiconducting wires [1]. This has increased considerably the theoretical and experimental studies on quantum well wires [QWW] [2, 3].

Thermopower, carrier mobility and other transport properties have been extensively studied [4-10].

Exciton and shallow donor binding energies have also been investigated [11-15]. However, there has been very limited work on the effects of an external electric field [16-23].

In the present work, we investigate the effects of an external electric field on donor binding energies in QWWs with cylindrical and square cross-sections. We have chosen a system with GaAs quantum well surrounded by $Al_xGa_{1-x}As$ potential barriers in the

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x-y plane. The electron is thus free to move in the z-direction, i.e. along the axis of the QWW in the absence of a Coulomb centre binding the electron. We consider only an infinite potential wall model.

The behaviour of E_B under an electric field is different for QWWs of rectangular and cylindrical wires. While the direction of the electric field is immaterial for cylindrical wires it is very important for wires with rectangular cross-section.

We find that the binding energy of the hydrogenic impurities is a rather sensitive function of the geometry of the wire especially under the influence of an electric field. It is found that the electric field effects on E_B are extremely sensitive to the impurity position in or outside the wire.

2. Theory and Calculations

It is convenient to use the cartesian coordinates for wires of rectangular cross section and cylindrical coordinates for wires of circular cross section. The Hamiltonian for the wire of rectangular cross section, lying along the z-direction, is

$$H_0 = -\frac{\hbar^2}{2m^*}\left(\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}\right)+V(x,y), \tag{1}$$

where

$$V(x,y)=\begin{cases} \infty & |x|\geq \frac{L_x}{2},\ \ |y|\geq \frac{L_y}{2} \\ 0 & \text{elsewhere .} \end{cases} \tag{2}$$

Thus, the electron is free to move along the z-direction, but constrained along x- and y-directions. The subband structure of the wire is obtained by variational method using the following trial wave function:

$$\Psi_0(x,y) = N_0 \cos\left(\frac{\pi x}{L_x}\right)\cos\left(\frac{\pi y}{L_y}\right). \tag{3}$$

Here, N_0 is the normalization constant and subband energy

$$E_0 = \frac{\hbar^2\pi^2}{2m^*}\left(\frac{1}{L_x^2}+\frac{1}{L_y^2}\right),$$

where we have taken the cross section to be a square with sides $L_x = L_y = L$.

Next, we calculate the effect of an electric field on subband energies by using the Hamiltonian

$$H_1 = H_0 + \eta(x\cos\theta + y\sin\theta), \tag{4}$$

where $\eta = |e|F$. F is the field strength and θ is the angle between the electric field and the x-axis. The trial function in this case is modified to be

$$\psi_1(x,y) = N_1\psi_0(x,y)\exp(-\beta(x\cos\theta + y\sin\theta)/L), \tag{5}$$

where N_1 is the normalization constant and β is the variational parameter.

With the impurity at $(x_i, y_i, 0)$ the Hamiltonian becomes,

$$H_2 = H_1 - \frac{\hbar^2}{2m^*}\frac{\partial^2}{\partial z^2} - \frac{e^2}{\epsilon\sqrt{z^2+(x-x_i)^2+(y-y_i)^2}}, \tag{6}$$

where ϵ is the static dielectric constant of the medium in which the electron moves. The trial function for this problem is taken to be

$$\psi_2 = N_2\psi_1(x,y)\exp(-\lambda\sqrt{z^2+(x-x_i)^2+(y-y_i)^2}), \tag{7}$$

where N_2 is the normalization constant and λ is the variational parameter. The binding energy of the electron is written with respect to the subband energy calculated in the presence of an applied electric field. Numerical results are found for the $GaAs/Ga_{1-x}Al_xAs$ system.

For cylindrical wires, the Hamiltonian is

$$H_0 = -\frac{\hbar^2}{2m^*}\left(\frac{\partial^2}{\partial r^2} + \frac{1}{r}\frac{\partial}{\partial r} + \frac{1}{r^2}\frac{\partial^2}{\partial \varphi^2}\right) + V(r,\varphi), \tag{8}$$

where

$$V(r,\varphi) = \begin{cases} 0, & r \le d \\ \infty, & r \ge d. \end{cases} \tag{9}$$

The wave function for the ground state becomes,

$$\psi_0(r,\varphi) = N_0 J_0(r_{10} r) \tag{10}$$

where $r_{10} \approx \frac{2.4}{d^2}$.

With an applied electric field in x-y plane, the Hamiltonian becomes,

$$H_1 = H_0 + \eta r\cos(\varphi - \theta). \tag{11}$$

The trial function in this case is taken to be

$$\psi_1 = N_1\psi_0(r,\varphi)\exp(-\beta r\cos(\varphi-\theta)/d), \tag{12}$$

where N_1 is the normalization constant and β is the variational parameter.

For an impurity at $r = r_i$, the Hamiltonian becomes

$$H_2 = H_1 - \frac{\hbar^2}{2m^*}\left(\frac{\partial^2}{\partial z^2}\right) - \frac{e^2}{\epsilon\sqrt{z^2+(r-r_i)^2}}. \tag{13}$$

The trial function for the bound electron is taken to be

$$\psi_2 = N_2\psi_1(r,\varphi)\exp(-\lambda\sqrt{z^2+(r-r_i)^2}), \tag{14}$$

where λ is the variational parameter.

3. Results and Discussion

We have done a series of calculations and investigated the impurity binding energy as a function of electric field, impurity position and wire dimensions. The parameters used in numerical calculations are $m^* = 0.067m_0$, $\epsilon = 12.5$ which are suitable for $GaAs/Al_xGa_{1-x}As$ well material. The resulting effective Rydberg is $R^* = e^2/(2\epsilon a^*) = 5.83\,\mathrm{MeV}$, and the effective Bohr radius is $a^* = \hbar^2\epsilon/(m^*e^2) = 98.7\mathring{A}$.

Our results are in perfect agreement with previous calculations without the electric field. For example, the binding energies are found to be almost identical for wires of circular and square cross sections if wire dimensions taken to be comparable. As the diameter of the wire tends to zero the binding energy E_B tends to infinity. The work with a finite potential barrier is in progress. In this case, we expect to find smaller and finite binding energies in the limit of very small radius.

The impurity binding energy (E_B) as a function of the length of the square is shown in Figure 1 for three different electric field values.

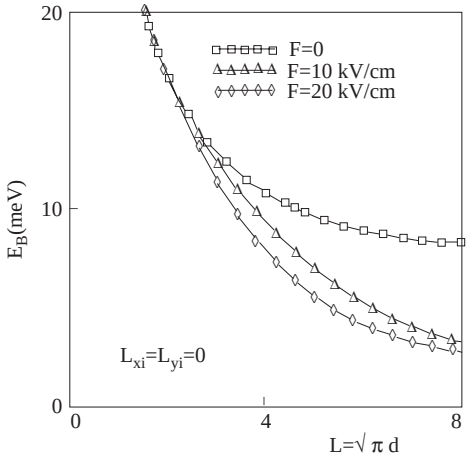

Figure 1. The binding energy as a function of side length of the square wire for different electric fields.

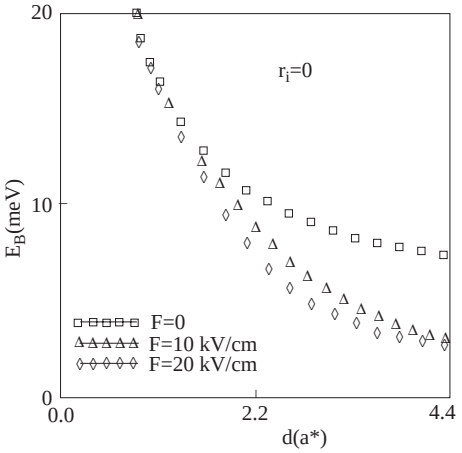

Figure 2. The binding energy as a function of radius for a cylindrical wire under different electric fields.

The impurity is taken to be at the centre of the wire. The electric field is taken to be applied along the positive axis direction with $\theta = 0$. Thus, the electron shifts towards the negative part of the axis.

The impurity position dependence of the binding energy is shown in Figures 3 and 4 for two types of wires. As expected the binding energy becomes smaller for impurities located at the boundary of the wires.

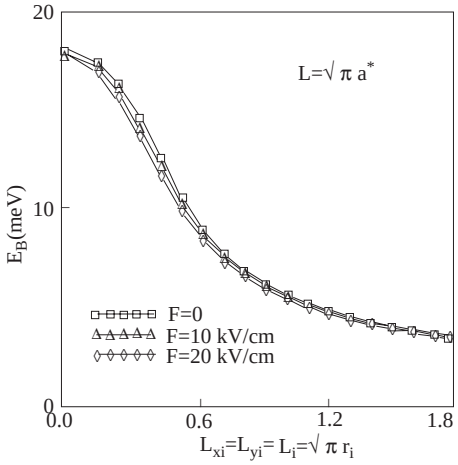

Figure 3. The binding energy as a function of impurity position along the diagonal of a square wire ($L = \sqrt{\pi}a^*$) for different electric fields.

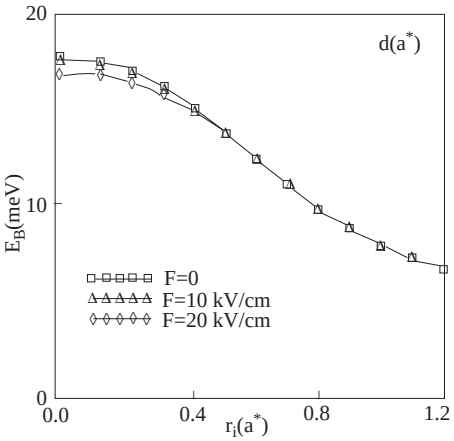

Figure 4. The binding energy as a function of impurity position along the radius of a cylindrical wire ($d = a^*$) for different electric fields.

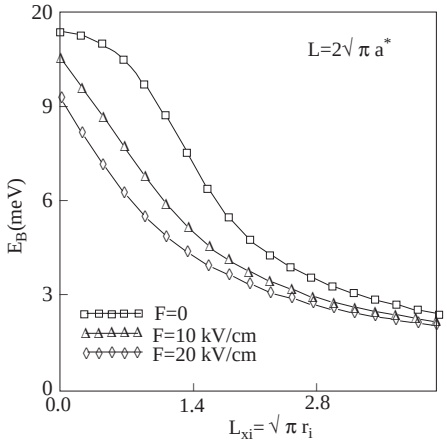

Figure 5. The binding energy as a function of impurity position along the x-axis of a square wire ($L = \sqrt{\pi}2a^*$) for different electric fields.

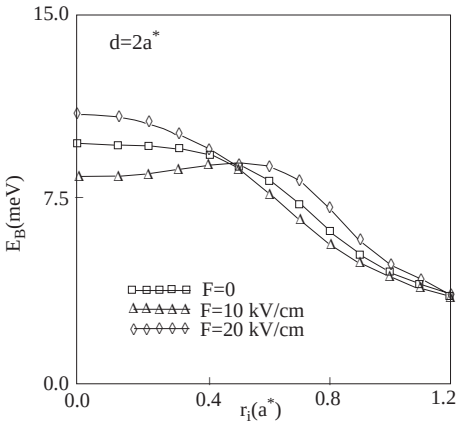

Figure 6. The binding energy as a function of impurity position along the radius of a cylindrical wire ($d = 2a^*$) for different electric fields.

The impurity position dependence of the binding energy is shown in Figures 5 and 6 when we increase the dimensions of the wire. This produces more complex behaviour for wires of circular cross section.

The electric field dependence of E_B is shown in Figure 7, for three different impurity positions in a wire of circular cross section. It is seen from this figure that the binding energy for the impurity at the center of the wire is influenced more from the electric field, as expected.

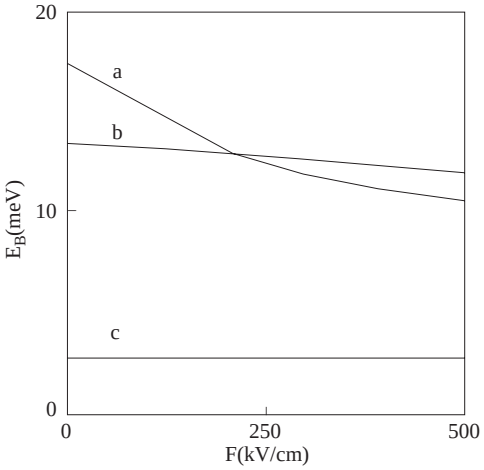

Figure 7. The binding energy as a function of electric field for hydrogenic impurities in a cylindrical wire ($d = a^*$). a, b, and c refer to impurity positions for $r_i = 0, 0.5a^*$ and $3a^*$, respectively.

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