Polaron effects on the impurity binding energy in quantum wires

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We report a calculation of the electron-phonon interaction effects on donor impurity binding energy in a semiconductor quantum wire of rectangular cross section and finite barrier potential. The results for the binding energy are obtained as a function of the size of the wire for different positions of the impurity and for several values of the potential confining barrier height. It is found that the presence of phonons changes significantly the values of the impurity binding energies of the system.

I. INTRODUCTION

Recently, there has been a growing interest on the study of the properties of electrons confined in quasi-one-dimensional semiconductor quantum wires. In these structures, the motion of the electrons along the length of the wire is almost free but it is quantized in the two directions perpendicular to the wire.

One of the crucial problems in the physics of semiconductors is the presence of ionized impurities, which play an important role in transport mechanisms at low temperatures. In semiconductor heterostructure of reduced dimensionality, the effective Coulomb interaction is greatly enhanced due to the electron confinement and, as a consequence, the impurity binding energy of the ground state is considerably larger in lower dimensions. This fact has stimulated many authors to study the hydrogenic impurity states in semiconductor quantum wire (QW) structures.

First, Lee and Spector[1] have calculated the binding energy of donors in cylindrical QW with infinite confining potential barrier height. They showed that the energy of the lowest state is greatly enhanced over the two- and three-dimensional values by the reduction of the radius of the wire. The binding energies of an impurity placed at the center of a cylindrical QW with finite height for the confining potential barrier was calculated by Bryant.[2] In contrast to the previous results, he found that for very thin wires the electrons leak out and behave as three-dimensional electrons in the barrier-acting material. In a subsequent work, Bryant[3] has observed that in the case of wires with different geometries, but with the same transversal area, the impurity binding energies were nearly the same.

For realistic QW rectangular cross section, Osório, Degani, and Hipólito[4] calculated the impurity binding energies as a function of the size of the wire for several values of the height of the confining potential barrier and different impurity positions. They observed that the binding energies depend dramatically on the size of the wire. Its qualitative behavior, as a function of one confining dimension, with the other fixed, is the same as that obtained previously for the two-dimensional systems.

More recently, extensive theoretical work on hydrogenic impurity states in cylindrical and rectangular QW have been reported. Thoai[5] included the effects of the image charges in the calculations of the ground-state binding energy for an impurity in a cylindrical QW with finite potential barrier height. Branis, Li, and Bajaj[6] studied the effects of a magnetic field on the binding energies of a hydrogenic impurity located at the axis of a quantum wire. The geometric effects on the electric polarizability of a shallow donor was investigated by Narayani and Sukumar[7] for rectangular and square wires with infinite confining potential barrier. The polaronic effects on the binding energy of a donor impurity in a rectangular QW with infinite potential barrier height has also been recently investigated.[8]

The purpose of the present paper is to report a calculation of the ground-state binding energy of a hydrogenic impurity in a realistic rectangular QW of GaAs-$Al_xGa_{1-x}As$. We use a variational method in which a separable trial wave function is taken into account. The electron-longitudinal optical (LO) phonon interaction is included via Lee-Low-Pines variational method. The geometric effects for a realistic QW are considered primarily by comparing our results for square wires with Bryant's result for cylindrical wires with the same cross-section areas.

In this model, we will take into account the non-screened interaction of the electron with the bulk longitudinal optical phonons, not including the interface phonon modes and the nonparabolicity of the conduction band.[9]

The calculation of the binding energies are performed for the case of asymmetric potential barrier height and for several positions of the impurity inside the wire, with and without the polaronic effects. This paper is organized as follows. In Sec. II, we present the theory for calculating the binding energies. The results and discussions

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are presented in Sec. III. The conclusions are finally presented in Sec. IV.

II. THEORY

Let us consider a system consisting of an electron bound to a donor impurity located inside of a rectangular QW of GaAs surrounded by $Al_xGa_{1-x}As$. The confining potential well $V(x,y)$ is defined to be

$$V(x,y)=\begin{cases}0, & |x|<L_x/2, |y|<L_y/2\\ V_{0x}, & |x|>L_x/2, |y|<L_y/2\\ V_{0y}, & |y|>L_y/2,\end{cases} \tag{1}$$

where V_{0x} and V_{0y} denote the discontinuity in the conduction-band edge, and L_x and L_y are the well widths. The values of the potential heights are determined from the Al concentration x, through the expression for the energy-band-gap discontinuity $\Delta E_g, \Delta E_g = 1040x + 470x^2$ meV. The values of V_{0x} and V_{0y} are taken to be 60% of ΔE_g.

Within the framework of the effective mass approximation, the Hamiltonian describing a bound polaron in this system can be written as

$$H = H_0 + H_{\rm ph} + H_{e\text{-ph}} , \tag{2}$$

where H_0 is the Hamiltonian of an electron confined in the QW and interacting with the donor impurity placed at $\mathbf{r}_i=(x_i,y_i,0)$,

$$H_0 = \frac{P^2}{2m_b} + V(x,y) - \frac{e^2}{\varepsilon_0|\mathbf{r}-\mathbf{r}_i|} , \tag{3}$$

where m_b is the effective electron mass, which is different in the two materials, $m_b=0.667m$ in GaAs and $m_b=(0.067+0.083x)m$ in the $Al_xGa_{1-x}As$, m is the free electron mass, and ε_0 is the static dielectric constant of GaAs material inside the wire.

$H_{\rm ph}$ is the free-LO phonon Hamiltonian, which is given by

$$H_{\rm ph} = \sum_{\mathbf{k}} \hbar\omega_{\rm LO}(a_{\mathbf{k}}^{\dagger}a_{\mathbf{k}} + 1/2) , \tag{4}$$

where $a_{\mathbf{k}}^{\dagger}(a_{\mathbf{k}})$ is the creation (annihilation) operator of the longitudinal optical bulk phonon with wave vector $\mathbf{k}$ and frequency $\omega_{\rm LO}$.

The electron-LO phonon interaction is given by

$$H_{e\text{-ph}} = \sum_{\mathbf{k}} (V_{\mathbf{k}} a_{\mathbf{k}} e^{i\mathbf{k}\cdot\mathbf{r}} + \text{H.c.}) , \tag{5a}$$

with

$$V_{\mathbf{k}} = -\frac{i\hbar\omega_{\rm LO}}{|\mathbf{k}|}\left[\frac{2\pi e^2}{\hbar\omega_{\rm LO}\Omega}\left(\frac{1}{\varepsilon_\infty}-\frac{1}{\varepsilon_0}\right)\right]^{1/2} \tag{5b}$$

as the Fourier coefficient of the electron-phonon interaction, Ω is the volume, and ε_∞ is the optical dielectric constant.

In order to calculate the ground-state energy, we choose a trial wave function in the form

$$\psi(\mathbf{r}) = N\phi(x)\phi(y)e^{-\lambda|z|/2}U|0\rangle = \phi(x,y,z)U|0\rangle , \tag{6}$$

where N is the normalization constant, λ is the variational parameter, and $\phi(x)[\phi(y)]$ is the wave function of an electron confined in the one-dimensional quantum well along the $x(y)$ direction with finite confining potential barrier height, and

$$U = \sum_{\mathbf{k}} (f_{\mathbf{k}} a_{\mathbf{k}} + f_{\mathbf{k}}^{*} a_{\mathbf{k}}^{\dagger}) \tag{6a}$$

is the unitary transformation, which displaces the phonon coordinates and $|0\rangle$ represents the state with no phonon present, i.e., the vacuum state. The variational function $f_{\mathbf{k}}$ and the parameter λ are to be determined by minimizing the expectation value of the Hamiltonian, $E=\langle\psi|H|\psi\rangle$, which an be written in the following form:

$$E = E_{\rm kin} + E_{\rm pot} + E_{\rm Coul} + E_{\rm pol} , \tag{7}$$

where

$$E_{\rm kin} + E_{\rm pot} = \langle\psi(\mathbf{r})|\frac{-\hbar^2}{2m_b}\nabla^2 + V(x,y)|\psi(\mathbf{r})\rangle \tag{7a}$$

and

$$E_{\rm Coul} = -\frac{2e^2\lambda^2}{\pi\varepsilon_0}\int_0^{\infty}\frac{F(q)dq}{\lambda^2+q^2} . \tag{7b}$$

$F(q)$ is the form factor associated with the impurity, and it is given by

$$F(q) = \int dx \int dy\, |\phi(x)|^2 \times |\phi(y)|^2 K_0(q[(x-x_i)^2+(y-y_i)^2]) , \tag{8}$$

where $K_0(x)$ is the modified Bessel function of zero order.

Since the electron-LO phonon coupling for GaAs is too small, the calculation of the polaronic contribution to the energy can be performed by using the Lee-Low-Pines variational approach, such as

$$E_{\rm pol} = \langle\psi(\mathbf{r})|\sum_{\mathbf{k}}(a_{\mathbf{k}}^{\dagger}a_{\mathbf{k}} + 1/2) + \sum_{\mathbf{k}}[V_{\mathbf{k}}a_{\mathbf{k}}e^{i\mathbf{k}\cdot\mathbf{r}} + \text{H.c.}]|\psi(\mathbf{r})\rangle . \tag{9}$$

Defining

$$\tilde{V}_{\mathbf{k}} = \langle\psi(\mathbf{r})|V_{\mathbf{k}}e^{i\mathbf{k}\cdot\mathbf{r}}|\psi(\mathbf{r})\rangle \tag{10}$$

and substituting it in the above expression for the polaronic energy, we get

$$E_{\rm pol} = \hbar\omega_{\rm LO}\sum_{\mathbf{k}}|f_{\mathbf{k}}|^2 + \sum_{\mathbf{k}}(\tilde{V}_{\mathbf{k}}^{*}f_{\mathbf{k}}^{*} + \tilde{V}_{\mathbf{k}}f_{\mathbf{k}}) . \tag{11}$$

Minimizing this expression with respect to the function $f_{\mathbf{k}}$, we find the lower bound of the polaronic contribution to be

$$E_{\rm pol} = \frac{e^2\lambda^4}{\pi}\left(\frac{1}{\varepsilon_0}-\frac{1}{\varepsilon_\infty}\right)\int_0^{\infty}\frac{F^{\rm Q1D}(k)dk}{(\lambda^2+k^2)^2} , \tag{12}$$

where $F^{\rm Q1D}(k)$ is the form factor for the quasi-one-dimensional confinement of electrons, which is given by

$$F^{\rm Q1D}(k) = \int dx \int dy\, |\phi(x)|^2|\phi(y)|^2 \int dx' \times \int dy'|\phi(x')|^2|\phi(y')|^2 \times K_0(q[(x-x')^2+(y-y')^2]) . \tag{13}$$

The binding energy of the hydrogenic impurity is then obtained as the difference between the ground-state energy of the system in the absence of the impurity donor term and the value of the ground-state energy minimized in the presence of the Coulomb term.

III. RESULTS AND DISCUSSIONS

We have numerically calculated the values of the binding energy of a donor impurity in GaAs-$Al_xGa_{1-x}As$ quantum wire with and without the presence of the electron-LO phonon interaction as a function of the size of the wire for several concentrations of aluminum and different positions of the impurity inside the wire.

In Fig. 1 we plot the ground-state binding energy as a function of L_x for two values of L_y (50 Å and 100 Å), when the impurity is located at the center of the wire. The solid and the dashed lines represent the results without and with the polaronic contribution, respectively. The concentration of aluminum in the material of both barriers is the same, $x=0.3$. As it can be seen, for a given value of L_y, the binding energy increases with increasing the size of the wire, it then reaches a maximum value and finally decreases monotonically for wider well wires. This qualitative behavior is similar to that previously obtained for quasi-two-dimensional quantum wells. This behavior can be understood in the following way: by decreasing the size of the well, the electron wave function becomes compressed leading to the enhancement of the binding energy. Below a certain value of the size of the wire, the wave function starts to leak into the barrier region and the binding energy decreases until a value characteristic of the barrier material for zero thickness. We also note from Fig. 1 that for fixed value of L_y, the polaronic contribution enhances the binding energy by about 10% of its value without the presence of phonons.

The numerical results for the binding energy, for two different positions of the impurity inside the wire (at the center of the wire and at the center of one boundary) as a function of L_x, for fixed $L_y=50$ Å, are shown in Fig. 2. The barrier heights are all the same and correspond to the aluminum concentration $x=0.3$. The contribution of the polaronic effect on the binding energies is larger in the case where the impurity is located at the center of the QW than it is for the impurity dislocated out to the interfaces. This effect may also be observed in Fig. 3, where we display the binding energy versus impurity positions $(x_i=y_i)$ on the diagonal of a square wire of size 200×200 $Å^2$ for two different barrier heights.

From these results we note that when the impurity is near the center of the wire the binding energies for wires with infinite confining potential are higher than those in the case of wires with finite barrier height. However, when the impurity moves out to the interfaces at larger distances from the center of the wire the situation changes, and the binding energies for wires with the lowest barrier height become higher. This is due to the fact that the contribution of the wave function at the boundary becomes more significant as the potential bar-

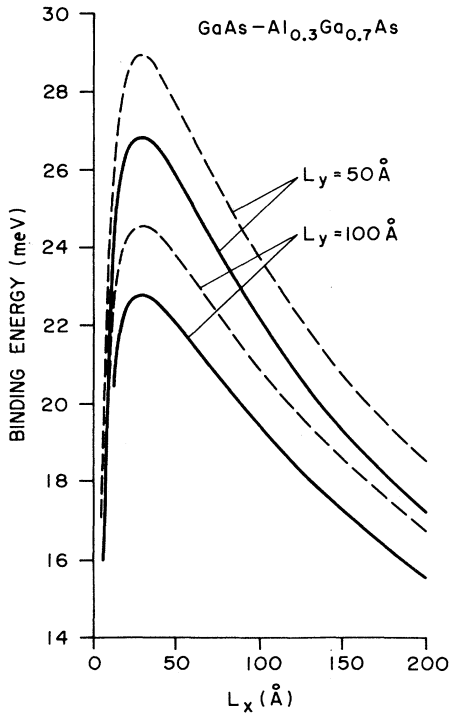

FIG. 1. Binding energy of a donor impurity located at the center of a GaAs-$Al_{0.3}Ga_{0.7}As$ quantum well wire. The solid and the dashed lines represent the binding energies without and with the polaronic contribution, respectively. The barrier heights are the same in the two directions and correspond to $x=0.3$ for the aluminum concentration.

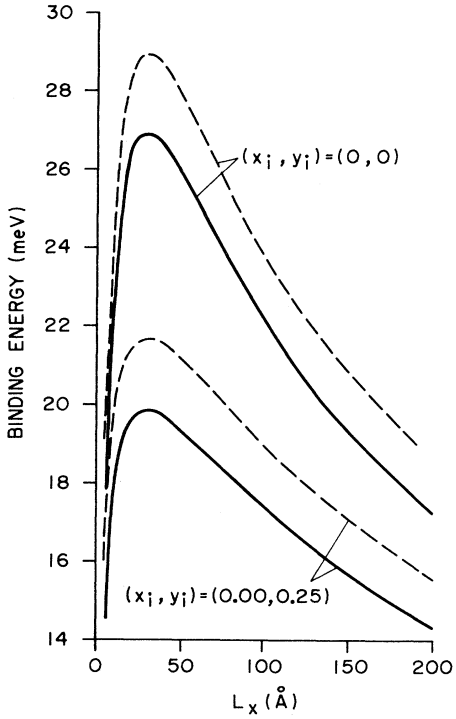

FIG. 2. Binding energy for a QW with aluminum concentration $x=0.3$ in both directions. $L_y=50$ Å for two different positions (x_i,y_i) of the impurity inside the wire. The solid and the dashed lines represent the binding energies without and with the polaronic contribution, respectively.

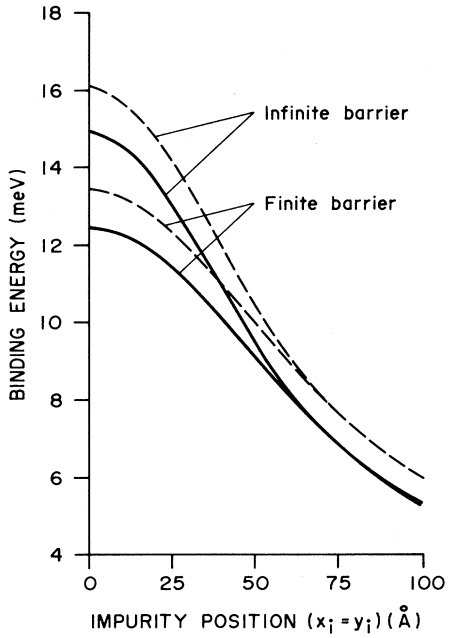

FIG. 3. Binding energy as a function of the impurity position (x_i,y_i) along the diagonal of a square QW (200×200 Å^2) for infinite and finite potential barrier height. The finite barrier is asymmetric and corresponds to aluminum concentrations 0.3 and 0.1 in each direction. The solid and dashed lines represent the binding energy without and with the polaronic contribution respectively.

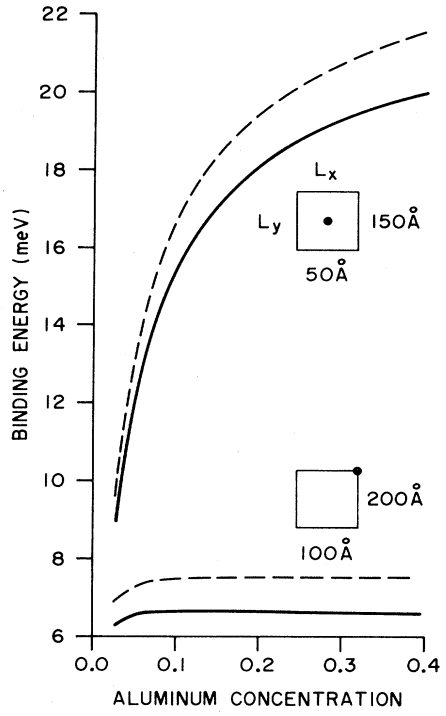

FIG. 4. Binding energy, with (dashed line) and without (solid line) the electron-LO phonon interaction, as a function of the aluminum concentration for two wires with different sizes and impurity positions.

rier height decreases.

In Fig. 4 we plot the values of the binding energy as a function of the confining potential barrier height for two different QW's with different impurity positions. The size of one wire is $L_x = 50$ Å and $L_y = 150$ Å, and the other one is $L_x = 100$ Å and $L_y = 200$ Å. The impurity positions in these wires are at the center and at the corner, respectively. The binding energy and the polaronic contribution increase with increasing potential-barrier height.

In comparing our numerical results, without the polaronic contribution to the binding energy, with Bryant's results, for cylindrical QW,[2] both with the same cross-sectional area and the donor placed at the center of the wire, we observe the same behavior that was related before to wires with infinite confinement potential.[3] However, in the present case, the differences in the binding energies for wires with the same cross-sectional area are between 4% and 9% for wires with radius between 25 Å and 140 Å. This result is an indication that the simplest form for the trial wave function we have used in the calculations is better for QW's of smaller size. For larger QW's, other more elaborated trial wave functions must be chosen. This is a subject to be discussed in detail in a future work.

IV. CONCLUSIONS

In conclusion we have calculated the ground-state binding energy of a hydrogenic impurity placed inside a rectangular GaAs-$Al_xGa_{1-x}As$ quantum wire by taking into account the polaronic contribution. We have shown that the polaronic effect is to enhance significantly the binding energy. Using a variational formalism, the calculation has been performed as a function of the size of the wire for different positions of the impurity as well as for different heights of the barriers. For wires with the same cross-sectional area but with different geometries, we have noted that the binding energies remain almost the same.

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