Stark effects on bound polarons in polar cylindrical quantum wires with finite confining potential

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The electric field effects on bound polarons in polar quantum wires with a finite confining potential are studied by a variational method. Both the confined bulk longitudinal optical phonons and the interface optical phonons are taken into account in considering the electron-phonon as well as the impurity-ion phonon couplings. The binding energies are calculated as functions of the transverse dimension of the quantum wire, and the donor-impurity position for different electric fields. The numerical results for the GaAs quantum wire are given and discussed as an example. A peak of the binding energy is found at a certain radius and shift toward a larger radius with applying an electric field. The calculated results confirm that the electron-phonon interaction reduces both the binding energies of impurity states and the Stark shifts and cannot be neglected. © 2009 American Institute of Physics. [DOI: 10.1063/1.3095509]

I. INTRODUCTION

A great deal of interest has been devoted to the study of the properties of the quantum well wires (QWWs) and dots of semiconductors. The impurity states in the systems is one of interest problems. Considering the discontinuity of the band gas, Bryant and Brown and Spector calculated the binding energies of the impurity states in QWWs with cylindrical and rectangular cross sections, respectively. Hsieh studied the off-center donor-impurity states in the multilayered quantum wires with circle cross section. A method of dividing the space into a one dimensional subspace and a two dimensional (2D) subspace was employed by Chuu et al. to solve the impurity states energy for the quantum wire.

It is well known that electron-optical phonon couplings play an important role in the physical properties of polar semiconductors. Many researches have studied the electron-phonon (e-p) interaction in QWWs and derived Fröhlich-like e-p Hamiltonians for cylindrical and rectangular quantum wires, respectively. The polaronic effects on impurity states in cylindrical and rectangular quantum wires have also been investigated theoretically.

The effect of the applied electric field on the impurity states in quantum confined systems, i.e., the quantum confinement technique. However, only the bulklike longitudinal optical (LO) phonon coupling with the electron has been considered in the e-p interaction. Therefore the detailed investigations on the QCSE of bound polarons in cylindrical quantum wires need to be done.

In this paper we study donor-impurity states in cylindrical quantum wires of polar semiconductors with a finite barrier in presence of an electric field by taking both the confined bulk LO phonons and the interface optical (IO) phonons into account in considering the e-p as well as the impurity-ion phonon couplings. The binding energies and Stark effects of bound polarons will be calculated and discussed.

II. VARIATIONAL CALCULATION

Let us consider a polar semiconductor QWW with a circular cross section of radius $R$ and surrounded by nonpolar material, whose wire axis is along the $z$-direction and section on the $x$-$y$ plane. An electron is bound to a hydrogenic donor-impurity center in the wire. A uniform electric field is exerted perpendicularly to the wire axis. The effective mass and the continuous medium approximation will be adopted in the calculation.

The Hamiltonian of the bound e-p system in the external electric field can be expressed as

$$H = H_e + H_{ph} + H_{e-ph}. \quad (1)$$

In Eq. (1) $H_e$ is the Hamiltonian of the bound electron without phonons and is written in cylindrical coordinate system,

$$H_e = -\frac{\hbar^2}{2m_e} \left( \frac{\partial^2}{\partial r^2} + \frac{1}{r} \frac{\partial}{\partial r} + \frac{1}{r^2} \frac{\partial^2}{\partial \varphi^2} \right) - \frac{\hbar^2}{2m_e} \frac{\partial^2}{\partial z^2}$$

$$- \left( e^2 \right) \frac{1}{e^2 + \left( r - R_0 \right)^2} + V(r) + |e|Fz \cos (\varphi - \theta). \quad (2)$$

Here the pole axis is set along the direction of the 2D-position-vector $\mathbf{r}_i$ of the impurity center in the cross section. $F$ is the strength of electric field applied along the direction making an angle $\theta$ with polar axis, and $\varphi$ is the pole angle of the 2D projection $\mathbf{\tilde{r}}$ of the electron position-vector in the...
cross section. $e_{\infty}$ is the high-frequency dielectric constant and $m^*$ is the electron-band effective mass. The confining potential $V(r)$ of the wire is given by (see Fig. 1)

$$V(r) = \begin{cases} 0, & r \leq R \\ V_0, & r > R. \end{cases}$$

$H_{ph}$ is the Hamiltonian of the free phonon field of confined LO and IO phonons,

$$H_{ph} = \sum_{mlkz} \hbar \omega_{LO} a_{mlkz}^\dagger a_{mlkz} + \sum_{mqz} \hbar \omega_{TO} b_{mqz}^\dagger b_{mqz},$$

where $\hbar \omega_{LO}$ and $\hbar \omega_{TO}$ are the LO and IO phonon energies, respectively. $a_{mlkz}^\dagger$ ($a_{mlkz}$) and $b_{mqz}^\dagger$ ($b_{mqz}$) are the creation (annihilation) operators for LO and IO phonons with the wave vectors $k_z$ and $q_z$, respectively.

The last term in Eq. (1) describe the couplings of the phonon field with both the electron and impurity ion and is written as

$$H_{e-ph} = \sum_{mlkz} \{ [V_{LO}^*(r)e^{imqZe^{ik_zr}} - V_{LO}^*(r)] a_{mlkz}^\dagger + H.c. \}$$

$$+ \sum_{mqz} \{ [V_{TO}^*(r)e^{imqZe^{ik_zr}} - V_{TO}^*(r)] b_{mqz}^\dagger + H.c. \}.$$  

Here the impurity ion is assumed to be rest (with a zero momentum) and contribute $-V_{LO}^*(r)$ and $-V_{TO}^*(r)$ terms to $H_{e-ph}$, similar to the treatment used by Platzman for the bulk materials.  

The coupling parameter in Eq. (5) is expressed as

$$V_{LO}^*(\rho) = \Gamma_{LO}^m(k_z) J_m \left( \frac{\rho}{R} \right), \quad \rho < R,$$

$$V_{TO}^*(\rho) = \left\{ \begin{array}{ll} \Gamma_{TO}^m(q_z) K_m(q_z R) I_m(q_z \rho), & \rho \leq R \\ \Gamma_{TO}^m(q_z) J_m(q_z R) K_m(q_z \rho), & \rho > R, \end{array} \right.$$
laron Hamiltonian. The tried wave function is chosen as
\[ |\Phi\rangle = \Psi(\vec{r})U_0U_1U_2U_3|0\rangle, \]
where \(|0\rangle\) is the phonon vacuum state and \(\Psi(\vec{r})\) the impurity states wave function chosen as
\[ \Psi(\vec{r}) = N \exp(-\lambda \sqrt{z^2 + |\vec{r} - \vec{r}|^2}) \exp(-\beta \cos(\varphi - \theta)/R) \]
\[ \times \begin{cases} J_0(\alpha r), & r < R \\ J_0(\alpha R)K_0(\beta r), & r \geq R, \end{cases} \]
where \(\beta\) and \(\lambda\) are the variational parameters and \(N\) is the normalization constant of \(\Psi(\vec{r})\). \(a\) and \(b\) in Eq. (15) are determined by
\[ \frac{\hbar^2 a^2}{2m^*} = V_b - \frac{\hbar^2 b^2}{2m^*}, \]
and the boundary conditions on the wave function is
\[ a \frac{dJ_0(\alpha r)}{d(\alpha r)} \bigg|_{r=R} = b \left. \frac{J_0(\alpha R)K_0(\beta r) - J_0(\alpha R)K_0(\beta r)}{K_0(\beta R)d(\beta r)} \right|_{r=R}. \]
Minimizing \(\langle \Phi | H | \Phi \rangle\) with respect to \(f_{m}(k_z)\) and \(g_{m}(q_z)\), one can obtain
\[ f_{m}(k_z) = - \frac{\hbar^2}{\hbar \omega_{LO} + \frac{\hbar^2}{2m^*} \langle \Psi | \hat{k}_z^2 + \frac{m^*}{\hbar^2} \rangle \Psi} - \frac{\hbar k z P}{m^* (1 - \eta)}, \]
\[ g_{m}(q_z) = - \frac{\hbar^2}{\hbar \omega_{LO} + \frac{\hbar^2}{2m^*} \langle \Psi | \hat{q}_z^2 + \frac{m^*}{\hbar^2} \rangle \Psi} - \frac{\hbar q z P}{m^* (1 - \eta)} \]
The variational energy of the ground state of the impurity is then calculated by
\[ \langle \Phi | H | \Phi \rangle = \langle \Psi | \frac{\hbar^2}{2m^*} | \Psi \rangle + \langle \Psi | \frac{\hbar^2}{2m^*} | \Psi \rangle \]
\[ + \langle \Psi | e \hat{F}_e \cos(\varphi - \theta) | \Psi \rangle \]
\[ - \frac{\hbar^2}{\hbar \omega_{LO} + \frac{\hbar^2}{2m^*} \langle \Psi | \hat{k}_z^2 + \frac{m^*}{\hbar^2} \rangle \Psi} \]
\[ - \sum_{m_lk_z} \frac{\hbar \omega_{LO} + \frac{\hbar^2}{2m^*} \langle \Psi | \hat{q}_z^2 + \frac{m^*}{\hbar^2} \rangle \Psi} \]
\[ - \sum_{m_lk_z} \left\{ \langle \Psi | V_{LO}(r) | \Psi \rangle \frac{e^{i\frac{q_z R}{\hbar}} \cos(\phi - \theta)}{\hbar \omega_{LO} + \frac{\hbar^2}{2m^*} \langle \Psi | \hat{q}_z^2 + \frac{m^*}{\hbar^2} \rangle \Psi} + \text{H.c.} | \Psi \rangle \right\} \]
where \(m^{**}\) is the renormalization mass of the electron in the direction along the wire given by
\[ m^{**} = \frac{m^*}{1 - \eta - \eta'}, \]
with
\[ \eta = \frac{\Delta m_{LO}}{1 + \Delta m_{LO}} \]
and
\[ \eta' = \frac{\Delta m_{IO}}{1 + \Delta m_{IO}}. \]
\(\Delta m_{LO}\) and \(\Delta m_{IO}\) are dimensionless constants and given by
\[ \Delta m_{LO} = \frac{2\hbar^2}{m^* \sum_{m_lk_z}} q_z^2 \left( \langle \Psi | V_{LO}(r) | \Psi \rangle \right)^2 \]
\[ \frac{\hbar \omega_{LO} + \frac{\hbar^2}{2m^*} \langle \Psi | \hat{q}_z^2 + \frac{m^*}{\hbar^2} \rangle \Psi} \]
\[ \Delta m_{IO} = \frac{2\hbar^2}{m^* \sum_{m_lk_z}} q_z^2 \left( \langle \Psi | V_{IO}(r) | \Psi \rangle \right)^2 \]
\[ \frac{\hbar \omega_{IO} + \frac{\hbar^2}{2m^*} \langle \Psi | \hat{q}_z^2 + \frac{m^*}{\hbar^2} \rangle \Psi} \]
The ground state energy of the bound polaron can be calculated by
\[ E_g = \min_{\beta_{ph}} \langle \Phi | H | \Phi \rangle. \]
Denoting the free polaron energy as \(E_0\) in the quantum wire, the binding energy can be calculated as
\[ E_B = E_0 - E_g. \]
The Hamiltonian of the free polaron in this system can be written as
\[ H_{\text{free}} = H_0 + H_{ph} + H_{e-ph} = - \frac{\hbar^2}{2m^*} \left( \frac{\partial^2}{\partial r^2} + \frac{1}{r} \frac{\partial}{\partial r} + \frac{1}{r^2} \frac{\partial^2}{\partial \varphi^2} \right) \]
\[ - \frac{\hbar^2}{2m^*} \frac{\partial^2}{\partial z^2} + V(r) + |e| \hat{F}_e \cos(\varphi - \theta) \]
\[ + \sum_{m_lk_z} \hbar \omega_{LO} q_z a_{m_lk_z} a_{m_lk_z} + \sum_{m_lk_z} \hbar \omega_{IO} b_{m_lk_z} b_{m_lk_z} \]
\[ + \sum_{m_lk_z} \left[ \Gamma_{LO}(k_z) \Gamma_{IO}(k_z) e^{i\frac{q_z R}{\hbar}} e^{i\frac{q_z R}{\hbar}} a_{m_lk_z} + \text{H.c.} \right] \]
\[ + \sum_{m_lk_z} \left[ V_{LO}(r) e^{i\frac{q_z R}{\hbar}} e^{i\frac{q_z R}{\hbar}} b_{m_lk_z} + \text{H.c.} \right]. \]
Using the Lee-Low-Pines (LLP)-like unitary transformations
(11)–(13), the expectation value of $H_{\text{free}}$ can be obtained by using the trial wave function

$$|\Phi_0\rangle = \Psi_0(\vec{r})U_1U_2U_3|0\rangle,$$

where $\Psi_0$ is the wave function of the bare electron in the cylindrical quantum wire under an external electric field

$$\Psi_0(\vec{r}) = N_0 \exp\left(-\beta r \cos(\varphi - \theta)/R\right) \times \begin{cases} J_0(\alpha r), & r < R \\ \frac{J_0(\alpha R)}{K_0(\beta R)}K_0(br), & r \geq R, \end{cases}$$

where $N_0$ is the normalization constant.

The free polaronic energy is then calculated by

$$E_0 = \min_{\beta} \langle \Phi_0 | H_{\text{free}} | \Phi_0 \rangle.$$  

The Stark shifts of the impurity binding energy is determined as

$$\Delta E_B = E_B(F) - E_B(F = 0).$$

III. NUMERICAL RESULTS AND DISCUSSION

The numerical results for the binding energy of a donor impurity in the GaAs cylindrical quantum wire embedded in the dielectric of $\varepsilon_r = 2.5$ with different wire radii and external fields, are shown in Figs. 2–7 as an example. The parameters used in calculations are $\varepsilon_r = 13.18$, $\varepsilon_r = 10.89$, $m^* = 0.067m_0$ ($m_0$ is the free-electron mass), $\hbar \omega_{LO} = 36.25$ meV, $\hbar \omega_{TO} = 33.29$ meV, and $V_0 = 20R_k$ ($R_k = m^*e^2/2\hbar^2\varepsilon_0$ is the effective Rydberg).

Figure 2 illustrates the impurity binding energies as functions of the quantum wire radius with and without phonon contributions for two different electric fields: $F = 0$ and 10 kV/cm. The impurity center is located at the center of the cross section in the calculation. It is evident that the binding energies increase considerably with decreasing the wire radius and reach their maximum values at a radius smaller than the half of the impurity effective Bohr radius in GaAs, and then decreases monotonically. This is the case that thinning the wire compresses the electron wave function and reduces the impurity state radius so that the binding energy is enhanced. However, once the wire radius becomes thin enough, the electron leaks considerably out of the well wire because of the finite barrier, and binding energy is decreased. It is also found that the binding energies with the phonon influence are lower than those without including the e-p coupling since the lattice polarization screens the Coulomb potential between the electron and the impurity center. The curves in Fig. 2 also show that the binding energies of the impurity states are obviously reduced as the electric field is applied due to the fact that the applied field separates the electron and donor ion along the direction of the electric field so that the Coulomb interaction is weakened, specially for the larger

FIG. 2. Impurity binding energies with (solid lines) and without (dashed lines) phonon contributions as functions of the quantum wire radius for two different electric field strengths: $F = 0$ and 10 kV/cm. The impurity is located at the wire center.

FIG. 3. Binding energies of the impurity states involving the e-p coupling effects as functions of the electric field strength with $\theta = 0$, $\pi/2$, $\pi$, and $r_i = R/2$.

FIG. 4. Binding energies of the impurity states with phonon influences as functions of the impurity position $r_i$ for different electric field strengths: $F = 0$, 5, and 10 kV/cm, with $\theta = 0$ and $R = 10$ nm.
radius case. The peak of the binding energy shifts toward a larger radius because the well potential inclined and the electron penetrates into the barrier easier with applying the electric field.

The binding energies of the bound polarons as functions of the electric field strength for the different field directions of $\theta=0$, $\pi/2$, $\pi$ are plotted in Fig. 3, where the impurity is located at $r_i=R/2$. One can see that the influence of electric field direction on the impurity binding energies is significant. Binding energies of the impurity states show different behaviors with the electric field as changing the field direction. The binding energy decreases monotonously with increasing the electric field strength when $\theta=0$. The opposite behavior occurs for the case of $\theta=\pi$, where the binding energy increases with increasing the electric field. Otherwise, the binding energy decreases slightly as the direction of electric field is set perpendicular to the polar axes ($\theta=\pi/2$). It is understood that the project of the electric field on the polar axes decreases with increasing $\theta$ so that the field force driving the electron to leave the impurity center is reduced and then binding energy strengthened.

The binding energies of the impurity states as function of the impurity position are illustrated in Fig. 4 for the different electric field strengths: $F=0$, 5, and 10 kV/cm. The radius of the quantum wires is chosen as 10 nm, and the angle between the polar axis and the electric field is taken to be zero in the calculation. It is found from the figure that the impurity binding energies decrease monotonously with moving the impurity away from the center. This is due to the fact that the electronic wave function loses its symmetry as impurity departs from the center, and the probability density of the electron near the impurity center is reduced. It is also seen that the field effect on the impurity binding energy is rather small when the impurity is located at the center of the cross section ($r_i=0$) because of the symmetric quantum confinement. The field effect becomes obvious with increasing $r_i$ since breaking the system symmetry makes it easier for the applied field to displace the charge distribution toward the direction opposite to the impurity moving.

To understand clearly the dependence of the field effect on the impurity position, we also plot the Stark shifts of the impurity binding energies as functions of the impurity position for the fields of $F=5$ and 10 kV/cm and $\theta=0$ in Fig. 5. It is seen that the energy shifts increase while moving the impurity away from the center, and reach their maximum at around $r_i=R/2$ then decrease. This is due to the fact of competition between the confined potential and the electric field. The electric fields push the electron toward the edge of the wire, but the quantum confinement repulses the electron and prevents it from getting close to the edge. As above-mentioned, the system loses its symmetry and the Stark shifts increase once the impurity center moves away from the center. However, the confinement becomes more important

![FIG. 6. Binding energies of the impurity states with (solid lines) and without (dotted lines) phonon contributions as functions of the electric field strength in the GaAs quantum wire for $r_i=0$ and $R=7$ and 15 nm.](image)

![FIG. 7. Stark shifts with (solid lines) and without (dotted lines) phonon contributions as functions of the electric field strength in the GaAs quantum wire for $r_i=0$ and $R=7$ and 15 nm.](image)
so that the field effects decrease with the impurity being far from the center and near the well edge \( r_i > R/2 \).

In Fig. 6 we plot the binding energies with and without phonon contributions in the GaAs quantum wires as functions of the electric field strength for two different radii. The impurity is located at the center and the direction of the electric field is along the polar axis in the calculation. It is found that for the smaller wire radius (7 nm), the binding energies vary slowly with the field since the quantum confinement restricts the field effect. While in the larger wire radius (15 nm) case, the binding energies of the impurity states decrease rapidly while increasing the field.

The phonon influence on the Stark effect can be read from Fig. 7, where the Stark shifts of ground state energies of the impurity with and without phonons as functions of the electric field for the GaAs quantum wires of \( R = 7 \) and 15 nm are plotted. It is found that the energy shift increase with the electric field as well as the wire radius. The phonon field polarization reduces obviously the Stark shifts. The figure shows that the phonon effect on the Stark shift can be up to 17% for finite GaAs quantum wire at \( F = 30 \text{ kV/cm} \) and cannot be neglected.

In conclusion, we have investigated the phonon effects on impurity binding energies in the GaAs cylindrical quantum wire in the presence of an applied electric field perpendicular to the wire axis. The Stark shift of the impurity state depends obviously on the wire radius, impurity position and the field direction. A peak of the binding energy versus the radius is found and shifts toward a larger radius while applying an electric field. The e-p interaction reduces the Stark energy shift of the impurity states as well as the binding energy, and cannot be neglected.

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