The influence of polar optical phonon confinement on the binding energy of a hydrogenic impurity in quantum wires in the perpendicular electric and magnetic fields

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Abstract. The hydrogenic impurity binding energy in cylindrical quantum well wire with a finite confining potential including both barriers of finite height and an applied electric and magnetic fields are studied. The polaron effect on the ground-state binding energy are investigated by means of Landau-Pekar variation technique. The results for the binding energy as well as polaronic correction with taking into account polar optical phonon confinement effect are obtained as a function of the applied fields for different position of the impurity. Our calculations are compared with previous results in quantum wires of comparable dimensions.

1. Introduction
The coupling between electronic and vibrational excitations plays a central role in the physics of nanoscale semiconductor structures. In these systems the presence of an interface necessarily alters the phonon modes and their interaction with electronic excitations is also modified [1-2]. In particular, it is well known that the impurity bound states and excitons are strongly affected by the electron coupling with the polar optical phonons. These effects become more pronounced in the presence of external electric and magnetic fields [3-8].

In this paper we study the both effects of electric and magnetic fields on the bound polaron ground state energy in a polar cylindrical quantum wire (QW) with a finite height barrier for various positions of the impurity by taking into account polar optical (PO) phonon confinement effect. The coupling of phonons with the impurity-ion as well as the electron is considered in our calculations by means of Landau-Pekar variation technique [9].

2. Theory
We consider impurity bound polaron problem for the semiconductor QW embedded in a dielectric medium. In the presence of an electric field applied perpendicular to the axis of the wire (z-axis) and a magnetic field applied parallel with the z-axis the basic Hamiltonian for the single
conduction-band electron interacting with both the Coulomb impurity and the longitudinal optical phonon field can be written within the effective-mass approximation as

\[
H = \frac{1}{2m^*} (\mathbf{p} + e \mathbf{A})^2 + V(\mathbf{\rho}) + eF\mathbf{\rho}\cos\phi - \frac{\mathbf{e}^2}{\varepsilon_\infty R} + 
\]

\[
+ \sum_{npqz} \hbar\omega_{np} a_{np}^\dagger(\mathbf{q}_z) a_{np}(\mathbf{q}_z) + \sum_{sqz} \hbar\omega_{sq} a_{sq}^\dagger(\mathbf{q}_z) a_{sq}(\mathbf{q}_z) -
\]

\[
- \sum_{npqz} \left[ \Gamma_{np}^\dagger(\mathbf{q}_z) \phi_{np}^\dagger(\mathbf{\rho}) e^{iq_zz} a_{np}^\dagger(\mathbf{q}_z) + H.c. \right]
\]

\[
- \sum_{sqz} \left[ \Gamma_{sq}^\dagger(\mathbf{q}_z) Q_{sq}(\mathbf{\rho}) e^{iq_zz} a_{sq}^\dagger(\mathbf{q}_z) + H.c. \right],
\]

where

\[
\phi_{np}(\mathbf{\rho}) = \begin{cases} J_{n}\left(\frac{\kappa_{np}}{R}\right), & \mathbf{\rho} \leq \mathbf{R}, \\ 0, & \mathbf{\rho} > \mathbf{R} \end{cases}
\]

\[
Q_{sq}(\mathbf{\rho}) = \begin{cases} K_{s}(qR)I_{s}(q\mathbf{\rho}), & \mathbf{\rho} \leq \mathbf{R} \\ I_{s}(qR)K_{s}(q\mathbf{\rho}), & \mathbf{\rho} > \mathbf{R} \end{cases}
\]

The first line of equation (1) is the Hamiltonian of a system consisting of an electron bound to a Coulomb impurity, inside a cylindrical QW, in the presence of external fields, the second line describes the non-interacting PO phonon system, and the third and the fourth lines represent the electron–confined optical (CO) phonon, electron–interface optical (IO) phonon interactions, respectively [10]. Here, \(m^*\) is the electron’s effective mass, \(\mathbf{p}\) is the momentum operator, \(\mathbf{A}\) is the vector potential of the magnetic field, which is chosen as \(\mathbf{A}=(0, Bx, 0)\) giving \(\mathbf{B}=(0,0,B)\), the confining potential \(V(\mathbf{\rho})=0\) when \(\mathbf{\rho} < \mathbf{R}\), and \(V(\mathbf{\rho})=V_0\), when \(\mathbf{\rho} \geq \mathbf{R}\), \(F\) is the value of the electric field, and \(r=\sqrt{\mathbf{\rho}^2+\mathbf{\phi}^2-2\mathbf{\rho}\mathbf{\phi}\cos(\mathbf{\phi}-\mathbf{\phi})+\mathbf{\epsilon}^2}\) gives distance of the electron from the impurity, \(\mathbf{r}_i=(\mathbf{\rho}_i, \mathbf{\phi}_i, 0)\) is the impurity position, \(a_{np}^\dagger(\mathbf{q}_z)\), \(a_{np}(\mathbf{q}_z)\) and \(a_{sq}^\dagger(\mathbf{q}_z) a_{sq}(\mathbf{q}_z)\) are respectively the creation and annihilation operators of CO and IO phonons with frequency \(\omega_{np}\) and \(\omega_{sq}\), \(\varepsilon_\infty(\varepsilon_0)\) is the optical (static) dielectric constant,

\[
\omega_{CO} = \omega_{LO}, \quad \omega_{IO} = \sqrt{1 + \frac{\varepsilon_0 - \varepsilon_\infty}{\varepsilon_\infty - \varepsilon_0}} \omega_{IO},
\]

\[
\varepsilon(\omega) = -\frac{I_{s}(qR)\left[K_{s+1}(qR) + K_{s+1}(qR)\right]}{K_{s}(qR)\left[I_{s+1}(qR) + I_{s+1}(qR)\right]} \varepsilon_\infty.
\]

\[
\left|\Gamma_{np}^\dagger(\mathbf{q}_z)\right|^2 = \frac{2e^2\hbar\omega_{np}}{LJ_{s+1}^2(\mathbf{\kappa}_{np})}\left(1 - \frac{1}{\varepsilon_\infty^2}\right),
\]

\[
\left|\Gamma_{sq}^\dagger(\mathbf{q}_z)\right|^2 = \frac{2e^2\hbar\omega_{sq}}{LK_{s}(qR)I_{s}(qR)I_{s+1}(qR)I_{s+1}(qR)}\left(1 - \frac{1}{\varepsilon_\infty^2}\right),
\]

\(K_{s}(x)\) and \(I_{s}(x)\) are the first and second kind modified Bessel functions, respectively, \(J_{n}(x)\) is the Bessel function of the \(n\)th order, \(\mathbf{\kappa}_{np}\) is the \(p\)th zero of \(J_{n}(x)\), \(\varepsilon_\infty\) is the dielectric constant of the embedding medium, and \(R\) is the QW radius[11,12].
In the presence of a hydrogenic impurity and applied fields, the electron ground-state variational wave function can be written as

$$\Psi_0(r, \beta, \lambda) = \begin{cases} 
N_0 F_1(-a_{01}; 1; \frac{1}{2} R^2) e^{\frac{1}{2} \gamma R^2} e^{-\beta \rho} e^{-\lambda z}, & 0 \leq \rho < R \\
N_0 U(-d_{01}; 1; \frac{1}{2} R^2) U(-a_{01}; 1; \frac{1}{2} R^2) e^{-\beta \rho} e^{-\lambda z}, & \rho \geq R 
\end{cases}$$

(8)

where $F_i$ and $U$ are the general forms of confluent hypergeometric functions and $a_{01}$ and $d_{01}$ are the eigenvalues of the ground state for inside and outside of the wire, respectively, $\beta$ and $\lambda$ are the variational parameters. Notice that the variational parameters $\beta$ and $\lambda$ taken into account simultaneously the anisotropy of the hydrogen-like wave function in the presence of an electric field.

To obtain the polaron’s ground state binding energy (BE), we used the Landau–Pekar theory [9].

As a result, the bound polaron’s ground-state energy is obtained as

$$E^{\text{el-ph}}(\beta, \lambda) = -\sum_{q叙, \omega叙, \omega叙叙} \frac{1}{\hbar \omega叙叙叙叙} \left[ \left| \left\langle q叙, \omega叙, \omega叙叙, \omega叙叙叙, \lambda \right| \Psi_0(r, \beta, \lambda) \right| \phi叙叙叙叙(q叙) e^{i \omega叙叙叙叙 \rho} \left| \left\langle q叙, \omega叙, \omega叙叙, \omega叙叙叙, \lambda \right| \Psi_0(r, \beta, \lambda) \right| \right]^2$$

$$- \sum_{q叙, \omega叙} \frac{1}{\hbar \omega叙} \left[ \left| \left\langle q叙, \omega叙, \beta, \lambda \right| Q叙(\rho) e^{-i \omega叙 \rho} \left| \left\langle q叙, \omega叙, \beta, \lambda \right| \Psi_0(r, \beta, \lambda) \right| \right|^2 + E(\beta, \lambda) \right].$$

(9)

The energy of the bound polaron can be found by minimizing $E^{\text{el-ph}}(\beta, \lambda)$ with respect to $\beta$ and $\lambda$. The BE of the bound polaron is determined as the difference between the ground-state energy of the electron confined in the QW in the absence of the impurity and the total energy of the polaron.

3. Numerical results and discussion

In the numerical calculations the parameters of GaAs and Al$_x$Ga$_{1-x}$As have been used. The value of the potential height is determined from the $Al$ concentration $x$, through the expression for the energy-band gap discontinuity $\varepsilon_d$. The finite potential is taken as $V_0 = Q(1.36 \varepsilon_d + 0.22 x^2)(eV)$ where $Q = 0.6$. The $Al$ concentration is taken to be $x = 0.3$, $\alpha_{\text{el-ph}} = 0.0681$, $\varepsilon_0 = 12.7$, $\varepsilon_{\infty} = 10.9$ and $m^* = 0.067m_0$ [13,14].

Figure 1(a),(b) shows the BE of a hydrogenic impurity in a QW as a function of applied electric field for different positions of the impurity, corresponding to magnetic fields $B = 0$, and $B = 15T$. The

![Figure 1](image-url)
dashed and dotted lines in Figure 1(a),(b) represent the BE with and without electron-bulk PO phonon interaction respectively. Solid lines represent the sum of the contributions due to CO and IO phonon modes. It is clearly seen from the Figure 1(a),(b) that the BE for impurity positions (0,0), (0.5R,0) and (R,0) decreases with the increase of electric field, since electric field shifts the maximum of the electronic probability density far from mentioned positions of impurity. On the contrary, for impurity positions (-0.5R,0) and (-R,0) electric field pushes the maximum of the electronic probability density toward impurity positions, consequently, BE increases with increase of electric field, and when the locations of maximum of electronic charge density coincides with the positions of impurity, curves reach to the peaks values. It should be noted that in the presence of magnetic field the maximum of the curves occur for larger values of electric field.

The appropriate polaronic shift of BE due to confined (Figure 2 (a),(b)) and interface (Figure 2 (c),(d)) phonons for magnetic fields \(B = 0\), \(B = 0\) and \(B=15T\) is presented as a function of applied electric field. The solid (dashed) lines correspond to the finite (infinite [15]) confinement potential case. In the finite confinement potential model, the penetration of the bound electron into the barriers is appreciable, which gives a reduction of the electron confinement and impurity BE. Also one may observe that the electric field dependence of the CO phonon caused polaronic shift in case of finite confinement potential has similar qualitative features as BE. In the case of infinite confinement potential the BE polaronic shift decreases for all positions of impurity (Figure 2 (a),(b)). In the model of finite confinement potential the polaronic shift of BE caused by electron-IO phonon coupling increases with increasing electric field whereas in the infinite potential model it decreases for impurity positions (0,0), (0.5R,0), (R,0), and increases for impurity positions (-0.5R,0) and (-R,0).

![Figure 2](image-url)

**Figure 2.** Reduced polaronic shift of the BE as a function of the electric field for different impurity positions and for various values of the magnetic field (\(B = 0, B = 15T\)). The solid and dashed lines represent the finite and infinite confinement potential cases, respectively.

The contribution of the electron-LO bulk phonon interaction in the impurity BE in magnetic field \(B=15T\) in the model of finite (infinite) confining potential increases from 4.3% (6.06%) to 9% (15.6%,) and from 14.28% (10%) to 7.2% (12%) for impurity positions (0,0) and (-R,0).
respectively, when the electric field increases from $F = 0$ to $F = 100\text{ kV/cm}$. In the same conditions, the total contribution due to CO and IO phonon modes increases from 8% (16%) to 14.24% (22.4%), and from 19.1% (21.7%) to 7.3% (26.5%) for impurity positions (0,0) and (-R,0), respectively.

![Graph](image1)

**Figure 3.** Reduced BE for the impurity ground state with (soled and dashed lines) and without electron PO phonon interaction (dotted lines) a function of the magnetic field for different impurity positions and for various values of the electric field ($F = 0$, $F = 25\text{kV/cm}$, $F = 50\text{kV/cm}$). The solid lines represent the sum of the contributions due to confined and interface PO phonon modes. Dashed lines represent contributions bulk PO phonon modes.

The dependencies of the impurity BE on the magnetic field are shown in Figure 3 for two impurity positions ((0,0) and (-R,0)) at electric fields $F = 0$, $F = 25\text{kV/cm}$, and $F = 50\text{kV/cm}$. It is clearly seen
from the Figure 3(a) that, the BE of the on-center impurity increases with the increase of magnetic
field and decreases with increasing of electric field. It is a direct consequence of condensation and
therefore of strengthened localization of electronic charge in the ground state around the axis of the
cylinder on which the impurity is located. For electric field $F = 0$ the sum of the contributions due to
CO and IO phonon modes is less than bulk phonon case and with increasing of electric it increases
and become more than bulk phonon contribution at $F = 50kV/cm$. The curves in Figure 3(b) show that for
impurity position (-R,0) when electric field is $F = 0$ and $F = 25kV/cm$, the binding energy decreases
with increasing of magnetic field and increases at $F = 50kV/cm$. In Figure 4 we present the
appropriate polaronic shift of BE due to confined (Figure 4 (a),(b)) and interface (Figure 4 (c),(d))
phonons for the impurity positions (0,0) and (-R,0). The solid (dashed) lines correspond to the finite
(infinite [15]) confinement potential case. As we can see, the magnetic field dependence of the CO
phonon caused polaronic shift in case of finite confinement potential has similar qualitative features as
BE and for infinite confinement potential it decreases for all impurity positions (Figure 2 (a),(b)). In
the model of finite confinement potential the polaronic shift of BE caused by electron-IO phonon
coupling increases with increasing magnetic field whereas in the infinite potential model it decreases
for impurity positions (0,0), (0.5R,0), (R,0), and increases for impurity positions (-0.5R,0) and (-R,0).

4. Conclusion
We have presented study of the ground state BE of a hydrogenic impurity in cylindrical quantum wire
with a finite confining potential subjected to external electric and magnetic fields and electron PO
phonon interaction with tacking into account phonon confinement effect. We have employed the
Landau-Pekar variational method to obtain the polaronic corrections to the ground state binding
energy. We have shown that the polar optical phonon confinement leads to a considerable
enhancement of the polaron effect. The results of the polaronic effects on the binding energy are
obtained as a function of the applied electric and magnetic fields for different positions of the
impurity.

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