Phonon confinement effect on the polaron basic parameters in nanowires in the presence of external fields

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Abstract. The effect of electric and magnetic fields on the basic parameters of confined and interface polarons in cylindrical nanowires embedded in a non-polar matrix are studied theoretically for the first time. The analytical expressions for the quasi-one-dimensional Fröhlich polaron self-energy and effective mass are obtained as functions of the wire radius and the strength of the external fields; this can be used in the interpretation of optical phenomena related to polaron motion in cylindrical nanowire when the effect of applied fields competes with the spatial quantum confinement.

1. Introduction
Recent precise absolute far-infra-red magneto-transmission experiments performed in ultra-high magnetic fields on a low dimensional systems reveal new singular features related to expected polaronic effects [1-4]. Since the materials commonly used in the fabrication of the low dimensional systems are ionic semiconductors, the polaronic effects may strongly affect their physical properties. Peeters and co-workers [5] have studied the polarons in \( n \)-dimensional crystals and have found that the reduction of dimensionality leads to the enhancement of polaronic effects. Since then, a lot of attention has been paid to the various aspects of the polaronic process in quasi-one dimensional quantum wire systems (see e.g. [6-10]). Polarons in nanowires (NW’s) are markedly different from those in bulk materials, due to the presence of wire potential, which confines the motion of the carriers in the plane transverse to the wire axis and due to the occurrence of confined and either surface or interface optical phonon modes when the confined structure is free standing or embedded in another material, respectively [11]. Polaron effects become more interesting in the presence of external electric and magnetic fields.

By using the Lee-Low-Pines (LLP) variational method [12], Lu et al. have studied the polaron energy shift due to the electron-phonon interaction [13] and polaron effective mass [14] in a rectangular GaAs quantum wire in the presence of a uniform strong magnetic field. In the calculations they have ignored the influence of the interface phonons. A complete theory of the quasiparticle properties, i.e., energy-momentum relation, damping, renormalization factor, and effective mass, for interacting electrons in lower-dimensional nanostructures using many-particle Green’s function technique has been developed in [15]. Applying this theory to the Q1D magnetopolaron problem, an expression for the electron matrix self-energy in the subband space in the framework of a modified Hartree-Fock approximation has been derived. The free moving Fröhlich polaron properties in a rectangular quantum wire in the presence of an external electric field are studied in [16,17], where the...
analytical expressions for the polaron self-energy, the effective mass, and the average number of virtual phonons are obtained without including the effect of phonon confinement. In [18] the influence of phonon confinement as well as of an electric field applied perpendicular to the cylindrical NW axis on the polaron basic parameters has been investigated.

Till now, the problem of the effects of external electric and magnetic fields on the basic parameters (self-energy and effective mass) of confined and surface polarons in a cylindrical NW’s remains unsolved to the best of our knowledge. In the present paper the influence of phonon confinement as well as that of magnetic and electric fields on the properties of Frohlich polaron confined in a polar CdSe quantum wire (embedded in a non-polar matrix) is studied by using the LLP variational approach. The dependencies of the polaron self-energy and effective mass on wire radius, electric field strength and magnetic field induction are obtained. We expect that the obtained results will be helpful in the interpretation of optical phenomena related to polaron motion in cylindrical NW when the effect of applied fields competes with the structural confinement.

2. Theory

Let us consider an electron moving in a polar cylindrical NW of radius \( R \) with infinite confining barriers. A uniform magnetic field applied parallel to the wire axis and an electric field applied perpendicular to the wire axis (\( z \) axis). The wire is surrounded by a non-polar matrix with dielectric constant \( \varepsilon_{\infty} \) and \( \varepsilon_{0} \). To obtain the polaron basic parameters, we perform the standard LLP variational method [12,16,17]. As a result, the following expressions for polaron self-energy and effective mass are obtained

\[
E_{\text{self}}^{\infty}(F,B,R) = -\sum_{p \neq \ell} \left| \frac{\Gamma_{CO}^{\infty}(q_{z})}{\hbar \omega_{CO}} \right| L_{4}(0,p,F,B,R)^{2} - \sum_{q_{z}} \left| \frac{\Gamma_{IO}^{\infty}(q_{z})}{\hbar \omega_{IO}} \right| L_{2}(0,q_{z},F,B,R)^{2},
\]

\[
m_{p\ell}^{\infty} = m^{*} \left( 1 + \sum_{p \neq \ell} \frac{2 \hbar q_{z}^{2}}{m^{*}} \left| \frac{\Gamma_{CO}^{\infty}(q_{z})}{\hbar \omega_{CO}} \right| L_{4}(0,p,F,B,R)^{2} \right) + \sum_{q_{z}} \frac{2 \hbar q_{z}^{2}}{m^{*}} \left| \frac{\Gamma_{IO}^{\infty}(q_{z})}{\hbar \omega_{IO}} \right| L_{2}(0,q_{z},F,B,R)^{2},
\]

where

\[
\left| \frac{\Gamma_{CO}^{\infty}(q_{z})}{\hbar \omega_{CO}} \right|^{2} = \frac{4 \varepsilon_{\omega}^{2}}{LJ_{1}^{2}(\kappa_{wp}^{2} + R^{2} q_{z}^{2})} \left( \frac{1}{\varepsilon_{\infty}} - \frac{1}{\varepsilon_{0}} \right),
\]

\[
\left| \frac{\Gamma_{IO}^{\infty}(q_{z})}{\hbar \omega_{IO}} \right|^{2} = \frac{4 \varepsilon_{\omega}^{2}}{LJ_{1}^{2}(\kappa_{wp}^{2} + R^{2} q_{z}^{2})} \left( \frac{1}{\varepsilon_{\infty}} - \frac{1}{\varepsilon_{0}} \right),
\]

\[
L_{4}(n,p,F,B,R) = \langle \Phi| J_{4}^{\text{(conf)}}(x) | \Phi \rangle, \quad L_{2}(s,q_{z},F,B,R) = \langle \Phi| K_{2}(q_{z},R) | \Phi \rangle,
\]

\[
m^{*} \text{ is the electron’s effective mass, } L \text{ is the length of the wire, } q_{z} \text{ is the phonon wave vector along wire direction, } B \text{ is the magnetic field induction, } F \text{ is the electric field strength, } \varepsilon_{\omega}(\varepsilon_{0}) \text{ is the optical (static) dielectric constant, } K_{n}(x) \text{ and } I_{n}(x) \text{ are the } n \text{th order first and second kind modified Bessel functions, respectively, } J_{n}(x) \text{ is the Bessel function of the } n \text{th order, } \kappa_{wp} \text{ is the } p \text{th zero of } J_{n}(x). \]

We have used dispersionless LO phonons in the description of confined (CO) phonon modes for simplicity, but retained the wave-vector dependence in the case of interface (IO) modes

\[
\omega_{CO} = \omega_{IO}, \quad \omega_{IO} = 1 + \frac{\varepsilon_{0} - \varepsilon_{\infty}}{\varepsilon_{\infty} - \varepsilon},
\]
\[ \varepsilon(\omega) = -\frac{I_s(qR)\left[K_{s+1}(qR) + K_{s+1}(qR)\right]}{I_s(qR)\left[I_{s+1}(qR) + I_{s+1}(qR)\right]} \varepsilon_d. \]  

(7)  

For the trial wave function of an electron moving along the wire axis with momentum \( \hbar k_z \), we have chosen a form \( \Phi(\rho, \varphi, z) = N_F(-a, 1; \rho^2 / 2 \alpha_c^2) \exp[-\rho^2 / 4 \alpha_c^2] \exp[-\beta \rho \cos \varphi] \exp(ik_z z) \) [19], where \( N \) is the normalization constant, \( F(\rho, 1; \rho^2 / 2 \alpha_c^2) \) is the confluent hypergeometric function, \( \beta \) is the variational parameter which takes into account the application of an external electric field, \( \alpha_c = \hbar / m^* \alpha_c^2 \) is the cyclotron frequency, \( \alpha_c = (\hbar e B / m^*)^{1/2} \) is the cyclotron radius. The value of \( a \) is determined by the boundary condition that the wave function vanishes at the surface (\( \rho = R \)) of the NW. CO and IO phonon subsystems become independent and can be considered separately, therefore (1) and (2) allow us to investigate electron-CO phonon and electron-IO phonon interactions and calculate the total contributions in polaron self-energy and effective mass by simply adding up the two parts.

3. Numerical results and discussion

To provide a clear picture of the polaron effect in the cylindrical NW system in the presence of external fields, a numerical calculation is carried on a CdSe with a relatively high electron-phonon coupling constant (\( \alpha = 0.46 \)). The medium outside the NW is vacuum, the material parameters are: \( \varepsilon_0 = 9.56, \varepsilon_\infty = 6.23, \hbar \omega_{LO} = 26.46 \text{meV}, m^* = 0.13m_e, \varepsilon_d = 1 \) [20].

Figures 1a and 1b are respectively the plots of the polaron self-energy and effective mass versus wire radius in a magnetic field \( B = 1T \) and at various values of an electric field (\( F = 10kV/cm, F = 50kV/cm, F = 100kV/cm \)). It can be clearly seen that the polaron self-energy monotonically decreases with the increase of \( R \) due to electron coupling with the IO and CO phonon modes. As a result, the total polaron self-energy, which incorporates the contributions of electron interaction both IO and CO phonons, also decreases. The same behavior is observed for the quasi-1D polaron effective mass (figure 1b).

![Figure 1](image-url)  

Figure 1. The polaron self-energy (a) and the effective mass (b) as a function of CdSe wire radius (expressed in terms of the Bohr radius: \( a_B = \hbar^2 \varepsilon_0 / m^* \varepsilon^2 \approx 39 \AA \)) for several values of the electric field and with a fixed magnetic field value \( B = 1T \).
It should be noted that for the shown region of the wire radius the IO phonon contribution in the polaron self-energy dominates over the contribution of CO phonons and strongly depends on the NW radius. A similar result in the absence of external fields has been reported for narrow NW in [21]. In the polaron effective mass, starting with some value of $R$, CO phonon contribution becomes predominant. The IO phonon contributions (in percentage terms) at above mentioned values of external fields are given in table 1. As can be seen from the table with the increase of the electric field the contribution of IO phonons increases.

|                  | $F = 10kV/cm$ | $F = 50kV/cm$ | $F = 100kV/cm$ |
|------------------|---------------|---------------|---------------|
| **Self-energy**  |               |               |               |
| $R = 0.5a_B$     | 67.8%         | 67.8%         | 67.8%         |
| $R = 2a_B$       | 58.9%         | 60.7%         | 64.1%         |
| **Effective mass** |              |               |               |
| $R = 0.5a_B$     | 73.7%         | 73.7%         | 73.7%         |
| $R = 2a_B$       | 45.4%         | 47.6%         | 51.5%         |

In figures 1a and 1b, the values of self-energy and effective mass of three-dimensional polaron are indicated by arrows. In the regime of weak electron-LO phonon interaction, these values are: $E_{3D}^{Self} = -\alpha h \omega_{LO}$, $m_{3D}^{*} = m(1 + \alpha/6)$ [12]. We notice that for small wire radius the total polaron self-energy as well as the effective mass may be several times greater than the 3D values of considered quantities and the presented curves converge to the 3D limits, when $R$ increases.

Figure 2 shows the polaron self-energy and the effective mass as a function of the electric field applied perpendicular to the NW axis in case of $R = 2a_B$ and $B = 1T$. In the considered region of the electric field the polaron self-energy (effective mass), due to electron interaction with the IO phonons, increases slowly with the increase of the electric field, while the CO part of the self-energy (effective mass) is reduces significantly. Therefore the total self-energy and the effective mass of the polaron

Figure 2. The polaron self-energy (a) and the effective mass (b) as a function of electric field for CdSe wire with radius $R = 2a_B$ and magnetic field $B = 1T$. Dashed (dotted) lines show the CO (IO) phonon contribution. Inset shows the total (CO and IO) contribution.
decreases, which can be seen more clearly in the insets to figures 2a and 2b. The electric field dependences of the IO as well as CO phonon caused polaron self-energy and effective mass can be explained by the fact that the maximum of the electronic charge distribution with increasing electric field displaces from the wire axis towards the barrier region. As a result, the role of IO phonons increases, while the role of CO phonons decreases. The figure 2 shows that the change in polaron self-energy and effective mass is about 8% and 10%, respectively, when the electric field increases up to 120 kV/cm.

In figure 3 the magnetic field dependences of the polaron basic parameters are presented when the electric field strength is \( F = 10 \text{kV/cm} \) (figures 3a, 3b) and \( F = 100 \text{kV/cm} \) (figures 3c, 3d). The results presented in figure 3 clearly show that the IO phonon contributions in polaron basic parameters are decrease with the increase of magnetic field while the opposite behavior occurs for the CO phonons. This is caused by the electron localization close to the wire axis when the magnetic field is applied parallel to that axis. It can be seen from figures 3b and 3d that the relative arrangement of the curves, which represent CO and IO parts of polaron effective mass, changes when the electric field...
increases from $10 \text{ kV/cm}$ to $100 \text{ kV/cm}$. This indicates that the influence of electric field on the CO and IO parts of polaron effective mass appears in a variety of ways, which could be seen also in figure 2. It should be noted that for the relatively high values of the magnetic field and small values of the electric field the decreasing CO phonon caused part of the polaron self energy increases when the wire radius becomes larger. Particularly, at $B = 30 \text{T}$ and $F = 10 \text{kV/cm}$ the change of the behavior occurs at $R \approx 4.2 \alpha_d$. This could be explained by the competition between three factors: spatial confinement, Stark effect and magnetic confinement effect.

4. Conclusion
In conclusion, we have presented a systematic study of the Fröhlich polaron basic parameters in a cylindrical NW in the presence of external fields taking into account the confinement effect on the polar optical phonons. The numerical results on the CdSe material show that the polaron basic parameters strongly depend on the wire radius and the IO phonon modes play a major role in the phonon contributions, especially when the radius is relatively small. Two opposite behaviors of polaron self-energy (effective mass) due to electron interaction with different phonon modes are obtained depending on whether a magnetic or an electric field is applied. As far as we know, there are no experimental data available to compare with our theoretical results; we believe these results will be of importance in the understanding of future experiments in this subject.

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