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Effect of electron–phonon interaction on the electronic properties of an axially symmetric polar semiconductor quantum wire with transverse parabolic confinement

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Abstract

A variational calculation based on the Lee–Low–Pines–Huybrechts method is performed to obtain the polaronic binding energies corresponding to the ground state and the first excited state of an electron in a polar quantum wire with parabolic confinement in the transverse direction. It is shown that the polaronic effects are considerably large and size-dependent if the effective radius of the wire is reduced below a certain length scale. It is also shown that even the longitudinal effective mass of the polaron is strongly enhanced by the transverse confinement in a quantum wire.

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Keywords: Quantum wire; Polaron; Binding energy

1. Introduction

Recent years have witnessed a flurry of investigations in the area of mesoscopic systems with the spectacular progress in the microfabrication techniques and material growth at the nanoscale. These low-dimensional systems are highly interesting because they exhibit very many novel physical properties that are quite different from those of their bulk counterparts and have tremendous potential for application in microelectronic semiconductor devices.

Among the several interesting nanomaterials available today, the zero-dimensional quantum dots (see Ref. [1] for references) and quasi-one-dimensional structures such as quantum wires have attracted particular attention [2]. In the present work, we shall be interested in quantum wire structures. In a quantum wire the electron's motion is free along the length of the wire while its motion in the plane normal to the length is confined. Therefore, the energy levels

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corresponding to electron's motion in the plane normal to the length of the wire are highly quantized and because of this quantization quantum wires show pronounced quantum effects. Associated with every sharp and discrete energy level, however, there is a band of quasi-continuous energy levels arising from the motion of the electron along the length of the wire which may be referred to as subbands. Since most of the quantum wire structures available today are made of polar semiconductors, one expects that the electron–longitudinal-optical(LO)-phonon interaction will have pronounced effects on the electronic states of a polar quantum wire and furthermore these effects should be size dependent. Quite a few investigations [3–11] have already been made to study the polaronic effects in quantum wires with different kinds of confinement potential and using different methods. It may be mentioned that a quasi-one-dimensional behaviour can also be obtained by magnetic confinement of a three-dimensional electron through a large magnetic field in which the electron is confined to move along the magnetic field [12].

Degani and Hipólito [3] have calculated the polaronic corrections to the energy and the effective mass of an electron in a quantum wire of GaAs surrounded by $Ga_{1-x}Al_xAs$ using a variational method which is based on the canonical transformation method of Lee, Low and Pines (LLP) [13]. They have found that the polaron mass is dramatically dependent on the wire size and also larger than its values in corresponding two- and three-dimensional structures. Yildirim and Ercelebi [4] have studied the polaronic effects on the ground state electronic energy in a quasi-one-dimensional structure with parabolic confinement using the second-order Rayleigh–Schrödinger perturbation theory (RSPT). They have given a unified overview of the polaronic binding energy interpolating between all possible confinement geometries. Quinghu et al. [5] have been able to give following the method used by Mukhopadhyay and Chatterjee [14] a simple expression for the polaronic correction to the electronic energy in a parabolic quantum wire within the framework of the second-order RSPT. Buonocore et al. [6] have studied the polaronic effects in a cylindrical quantum wire using a generalization of the LLP method and considering both the bulk and the surface phonon modes. Xie [7] has considered a free standing cylindrical quantum wire and obtained the polaronic corrections due to electron–LO-phonon interaction and also electron –surface-optical(SO)-phonon interaction using the second-order perturbation theory and taking into account the contributions from higher energy subbands. Li et al. [8] have studied using the LLP variational method the electron-confined-phonon interaction in a rectangular quantum wire under an additional parabolic potential. All these investigations are, however, valid only for weak and intermediate electron–phonon coupling strengths. Yildirim and Ercelebi [9] have studied the ground state binding energy and the effective mass of an electron–LO-phonon system as a function of the effective dimensionality within the framework of the strong-coupling theory of Landau and Pekar [15,16]. Zhou and Gu [10] have also used the strong-coupling variational theory of Landau and Pekar [15,16] with an additional variational parameter to calculate the polaron binding energies for the ground state and the first excited state. Obviously these investigations give results that are valid for very large values of electron–phonon coupling constant only. Chen et al. [11] have studied the polaron problem in a parabolic quantum wire using theFeynman–Hayken path-integral formalism [17]. The results of this investigation are certainly valid for the entire range of the coupling parameter. In fact, for the quantum dot case, the Feynman–Hayken path-integral method was earlier used by Mukhopadhyay and Chatterjee [18] for the investigation of the polaronic effects. However, as is well known, the Feynman–Hayken approach can be successfully applied only to the ground state and therefore this method also has a limited applicability. Furthermore, it is also not so convenient to calculate the effective mass in this framework. Bound polaron problems have also been studied in quantum wire by several investigators [19]. Hai et al. [20] have studied the effect of screening of the electron–phonon interaction on the polaronic properties in a quasi-one-dimensional

polaron gas using Hatree–Fock and random phase approximations. Shen [21] has investigated the excitonic polaron problem in a quantum wire.

We purport to investigate in the present work the polaronic effects in a quantum wire for the ground state and the first excited state for the entire range of the electron–phonon coupling constant and for arbitrary confinement length. We shall use the Lee–Low–Pines–Huybrechts (LLPH) variational method [18,22] which is a variant of the LLP theory and is known to yield good results for the entire range of the coupling parameter [23]. We shall apply our results to some of the realistic semiconductor quantum wires available today. We shall consider the confining potential to be parabolic which is consistent with the far infra-red spectroscopic measurements on quantum dots [24] and the generalized Kohn's theorem [25].

For the sake of mathematical simplicity we neglect the size quantization of phonons and treat the relevant phonon modes within the framework of the Fröhlich model [16,26]. This approach may not be rigorously valid if the confinement length in the transverse direction is reduced to a very small value, but may still serve as a good enough approximation to capture some of the most important and interesting features of the electron–phonon interaction effects in quantum wires.

2. The model hamiltonian

The hamiltonian for an electron interacting with LO-phonons in an axially symmetric quantum wire structure with a parabolic confinement in the x–y plane and free motion in the z-direction can be written by modifying the Fröhlich hamiltonian [16] as

$$\mathbf{H} = -\frac{\hbar^2}{2m}\vec{\nabla}^2_{\vec{r}'} + \frac{1}{2}m\omega_h^2(x'^2+y'^2) + \hbar\omega_0\sum_{\vec{q}'} b^\dagger_{\vec{q}'}b_{\vec{q}'} + \sum_{\vec{q}'}(\xi'_{q'}e^{-i\vec{q}'\cdot\vec{r}}b^\dagger_{\vec{q}'} + \text{h.c.}), \quad (1)$$

where the first term refers to the kinetic energy of the electron, m being its effective mass and $\vec{r}'(x'y'z')$ its position vector. The second term describes the parabolic confining potential for the electron in the x'–y' plane, ω_h giving the measure of the strength of confinement. The third term is the free phonon hamiltonian where $b^\dagger_{\vec{q}'}(b_{\vec{q}'})$ is the creation (annihilation) operator for an LO-phonon of dispersionless frequency ω_0 and wave vector $\vec{q}'$ and the last term describes the electron–phonon interaction with $\xi'_{q'}$ as the electron–phonon interaction coefficient. We shall use the Feynman units [27] in which the energy is scaled by $\hbar\omega_0$, length by r_0 where $r_0 = q_0^{-1}$, q_0 being an inverse length defined by $\hbar^2q_0^2/m = \hbar\omega_0$, volume by r_0^3 and wave vectors by q_0. Such scalings are equivalent to putting $\hbar = m = \omega_0 = 1$. In these units, hamiltonian (1) reads

$$\mathscr{H} = -\frac{1}{2}\nabla^2_{\vec{r}} + \frac{1}{2}\omega^2\rho^2 + \sum_{\vec{q}'} b^\dagger_{\vec{q}'}b_{\vec{q}'} + \sum(\xi_q e^{-i\vec{q}\cdot\vec{r}}b^\dagger_q + \text{h.c.}), \quad (2)$$

where $\vec{r} \equiv (\vec{\rho}, z) \equiv (x, y, z)$ is the dimensionless position coordinate of the electron in the Feynman units i.e. $\vec{r}(x,y,z) = \vec{r}'(x',y',z')/r_0$, $\rho^2 = (x^2+y^2)$, $\vec{q} = \vec{q}'/q_0$, $\omega = \omega_h/\omega_0$ and ξ is given by

$$|\xi_q|^2 = \left(\frac{2\sqrt{2}\pi}{Vq^2}\right)\alpha, \quad (3)$$

where V is the dimensionless volume of the whole system (in Feynman units) and α is the dimensionless electron–phonon coupling constant. We first note that the total crystal momentum operator $\vec{\mathscr{P}} = -i\vec{\nabla} + \sum_{\vec{q}}\vec{q}b^\dagger_q b_q$ does not commute with hamiltonian (2), though its z-component $\mathscr{P}_z = -i\partial/\partial z + \sum_{\vec{q}} q_z\vec{q}b^\dagger_q b_q$ does i.e. $[\hat{\mathscr{P}}_z, \mathscr{H}] = 0$. Therefore $\hat{\mathscr{P}}_z$ is a conserved quantity. This is, however, not very surprising in view of the inherent axial symmetry present in the geometry of the system for the entire z-direction. Thus, in this case it will make sense to define an effective mass for the polaron along the z-direction, unlike in the usual quantum dot structures. This effective mass may be referred to as the longitudinal effective mass of the polaron.

3. Formulation

We shall use the LLPH method to study the polaron problem described by hamiltonian (2). We first transform the hamiltonian $\mathscr{H}$ with a unitary operator $\mathscr{U}_1 = e^{\mathscr{S}_1}$ with the generator $\mathscr{S}_1$ given by

$$\mathscr{S}_1 = i\sum_{\vec{q}} (a_\rho \vec{q}_\rho . \vec{\rho} + a_z q_z z) b_q^\dagger b_q, \tag{4}$$

where a_ρ and a_z are two variational parameters and $\vec{q} \equiv (\vec{q}_\rho, q_z)$. Then after the second LLP transformation

$$\mathscr{U}_2 = \exp\left[\sum_{\vec{q}} (f_{\vec{q}} b_{\vec{q}}^\dagger - f_{\vec{q}}^* b_{\vec{q}})\right], \tag{5}$$

hamiltonian (2) becomes

$$\begin{aligned}\tilde{\mathscr{H}} = {} & \frac{\hat{\vec{p}}^2}{2} + \sum_{\vec{q}} \left[1 - (a_\rho \vec{p}_\rho \cdot \vec{q}_\rho + a_z p_z q_z) \right. \\ & \left. + \frac{1}{2}(a_\rho^2 q_\rho^2 + a_z^2 q_z^2)\right](b_{\vec{q}}^\dagger + f_{\vec{q}}^*)(b_{\vec{q}} + f_{\vec{q}}) + \frac{1}{2}\omega^2\rho^2 \\ & + \frac{1}{2}\sum_{\vec{q}\vec{q}'} (a_\rho^2 \vec{q}_\rho \cdot \vec{q}'_\rho + a_z^2 q_z q'_z)(b_{\vec{q}}^\dagger + f_{\vec{q}}^*) \\ & \times (b_{\vec{q}'}^\dagger + f_{\vec{q}'}^*)(b_{\vec{q}} + f_{\vec{q}})(b_{\vec{q}'} + f_{\vec{q}'}) \\ & + \sum_{\vec{q}} [\xi_q e^{-i[(1-a_\rho)\vec{q}'_\rho \cdot \vec{\rho} + (1-a_z)q_z z]}(b_{\vec{q}}^\dagger + f_{\vec{q}}^*) \\ & + \text{h.c.}],\end{aligned} \tag{6}$$

where $\hat{\vec{p}}$ is the electron momentum operator and $f_{\vec{q}}$ is to be obtained variationally. When a_ρ and a_z are equal to 1, this procedure reduces to the LLP method, which should provide a good description in the extended state limit, while for a_ρ and a_z equal to zero, this approach is equivalent to the Landau–Pekar method, which is valid in the adiabatic limit and will be a useful approach in the localized state limit. Thus treating a_ρ and a_z as variational parameters in the range $(0, 1)$, one can have a theory encompassing the entire parameter space. The variational energy is now written as

$$\mathbf{E} = \langle \Phi | \langle 0 | \tilde{\mathscr{H}} | 0 \rangle | \Phi \rangle, \tag{7}$$

where $\Phi(\vec{r})$ is the electronic function to be chosen variationally and $|0\rangle = \prod_{\vec{q}} |0_{\vec{q}}\rangle$ is the unperturbed zero-phonon state satisfying $b_{\vec{q}}|0_q\rangle = 0$ for all $\vec{q}$.

4. The ground state

For the ground state (GS) calculation we choose Φ as

$$\Phi_0 = \frac{\mu_0 \sqrt{\mu_0'}}{\pi^{3/4}} e^{-(1/2)\mu_0^2 \rho^2} e^{-(1/2)\mu_0'^2 z^2} e^{-ip_0 z} \tag{8}$$

so that the energy expression (7) is then denoted as E_{GS}. For the GS, we shall define $a_\rho = a_0$, $a_z = a_0'$ and $f_{\vec{q}} = f_{\vec{q}}^{(0)}$. To obtain the variational energy we should minimize $\mathbf{E}$ subject to the constraint that $\hat{P}_z$ is a constant of motion. This can be accomplished by minimizing the functional

$$\mathscr{J}_{GS} = \mathbf{E}_{GS} - u_0 \langle \Phi_0 | \langle 0 | \hat{\tilde{P}}_z | 0 \rangle | \Phi_0 \rangle, \tag{9}$$

where u_0 is a Lagrange multiplier which can be identified as the polaron velocity along the z-direction and

$$\hat{\tilde{P}}_z = \mathscr{U}_2^{-1} \mathscr{U}_1^{-1} \hat{P}_z \mathscr{U}_1 \mathscr{U}_2. \tag{10}$$

In what follows, we shall assume $f_q^{(0)}$ to be symmetric in $\vec{q}_\rho$. Minimizing $\mathscr{J}_{GS}$ with respect to $p_0, f_q^{(0)}$ and $f_q^{*(0)}$ and substituting their values in (7) and expanding the energy in powers of u_0 and retaining terms up to quadratic in u_0 we get the expression for the polaron GS energy and the polaron effective mass corresponding to the motion along the z-direction as

$$\begin{aligned}\mathbf{E}_{GS} = {} & \frac{\mu_0^2}{2} + \frac{\mu_0'^2}{4} + \frac{\omega^2}{2\mu_0^2} \\ & - \sum_{\vec{q}} \frac{|\xi_q|^2 e^{-((1-a_0)^2/2\mu_0^2)q_\rho^2} e^{-((1-a_0')^2/2\mu_0'^2)q_z^2}}{\left[1 + \frac{1}{2}(a_0^2 q_\rho^2 + a_0'^2 q_z^2)\right]},\end{aligned} \tag{11}$$

$$\begin{aligned}m_{GS}^* = {} & 1 + 2\sum_{\vec{q}} \\ & \frac{|\xi_q|^2 q_z^2 e^{-((1-a_0)^2/2\mu_0^2)q_\rho^2} e^{-((1-a_0')^2/2\mu_0'^2)q_z^2}}{\left[1 + \frac{1}{2}(a_0^2 q_\rho^2 + a_0'^2 q_z^2)\right]^3},\end{aligned} \tag{12}$$

where μ_0 and μ_0' have to be obtained by minimizing $\mathbf{E}_{GS}$ with respect to them.

4.1. Limiting results

As expected, we can get from (11) and (12) the well-known analytical results in the limiting cases. For instance, in the weak electron–phonon coupling limit and for not so strong confinement we can put $a_0 = a_0' = 1$. This is the so-called extended state limit. However, even in this case, $\mu_0 \neq \mu_0'$, in general, because of the confinement effect. We then get $\mu_0' = 0$ and the GS energy is given by

$$\mathbf{E}_{\mathrm{GS}} = \omega - \alpha, \tag{13}$$

which in the limit, $\omega \to 0$, gives the well-known weak-coupling bulk result for the GS energy. Similarly in the weak-coupling regime and for weak confinement ($\omega \to 0$), the effective mass can be obtained as

$$m_z^* = 1 + \frac{\alpha}{6}, \tag{14}$$

which is again the well-known bulk result.

In the case of strong electron–phonon coupling and weak confinement we can set $a_0 = a_0' = 0$ and $\mu_0' = \mu_0$. The GS energy then reduces to

$$\mathbf{E}_{\mathrm{GS}} = -\frac{\alpha^2}{3\pi} + \frac{9\pi\omega^2}{4\alpha^2}, \tag{15}$$

which in the bulk-limit ($\omega \to 0$) reduces to the well-known Landau–Pekar result for the GS energy in the gaussian approximation. In the same regime the effective mass expression (12) reduces to the well-known Landau–Pekar effective mass of a bulk polaron in the gaussian approximation.

To obtain the GS energy and the effective mass for the entire range of α and for arbitrary confinement, Eq. (11) is to be minimized numerically. Before we discuss our numerical results, we shall first present in the following section our calculation for the first excited state energy.

5. The first excited state

For the first excited state we take the electronic function as

$$\Phi_1 = \frac{\sqrt{2}\mu_1 {\mu_1'}^{3/2}}{\pi^{3/4}} \mathrm{e}^{-(1/2)\mu_1^2\rho^2} \mathrm{e}^{-(1/2){\mu_1'}^2 z^2} z \mathrm{e}^{-ip_1 z}. \tag{16}$$

The first excited state (ES) energy (E_{ES}) is then given by Eq. (7) with $\Phi = \Phi_1$. For the first ES we shall define $a_\rho = a_1$, $a_z' = a_1'$ and $f_q = f_q^{(1)}$. To get the first ES energy we should minimize $\mathbf{E}_{\mathrm{ES}}$ subject to the constraint that $\tilde{\mathscr{P}}_z$ is a conserved quantity. Thus we have to minimize

$$\mathscr{J}_{\mathrm{ES}} = \mathbf{E}_{\mathrm{ES}} - u_1 \langle \Phi_1 | \langle 0 | \tilde{\tilde{\hat{P}}}_z | 0 \rangle | \Phi_1 \rangle, \tag{17}$$

where again u_1 is the Lagrange multiplier which as before can be identified as the polaron velocity. Minimizing the functional $\mathscr{J}_1$ with respect to p_1 and f_q^* and substituting their optimum values in (7) and expanding it in powers of u_1, we can get the lowest ES energy and the corresponding ES effective mass which read

$$\mathbf{E}_{\mathrm{ES}} = \frac{\mu_1^2}{2} + \frac{3{\mu_1'}^2}{4} + \frac{\omega^2}{2\mu_1^2} - \sum_{\vec{q}} \frac{|\xi_q|^2 \left(1 - \frac{(1-a_1')^2}{2{\mu_1'}^2} q_z^2\right)^2 \mathrm{e}^{-((1-a_1)^2/2\mu_1^2)q_\rho^2} \mathrm{e}^{-((1-a_1')^2/2{\mu_1'}^2)q_z^2}}{[1 + \frac{1}{2}(a_1^2 q_\rho^2 + a_1'^2 q_z^2)]}, \tag{18}$$

$$m_{\mathrm{ES}}^* = 1 + 2\sum_{\vec{q}} \frac{|\xi_q|^2 \left(1 - \frac{(1-a_1')^2}{2{\mu_1'}^2} q_z^2\right)^2 q_z^2 \mathrm{e}^{-((1-a_1)^2/2\mu_1^2)q_\rho^2} \mathrm{e}^{-((1-a_1')^2/2{\mu_1'}^2)q_z^2}}{[1 + \frac{1}{2}(a_1^2 q_\rho^2 + a_1'^2 q_z^2)]^3}, \tag{19}$$

where μ_1, μ_1', a_1 and a_1' are to be finally obtained by minimizing $\mathbf{E}_{\mathrm{ES}}$ with respect to them. For some limiting cases, we can again have the usual analytical results. For example, in the weak electron–phonon coupling limit and for a not so strong confinement, we can again have $a_1 = a_1' = 1$. Then we get $\mu_1' = 0$, the energy $\mathbf{E}_{\mathrm{ES}}$ and the effective mass m_{ES}^* reduce to the same results (13)

and (14) as in the case of GS. In the case of strong electron–phonon coupling and weak confinement, we can take $a_1 = a_1' = 0$ and $\mu_1 = \mu_1'$. Eq. (18) then reduces to

$$\mathbf{E}_{ES} = -\frac{49^2\alpha^2}{18,000\pi} + \frac{150^2\pi\omega^2}{49^2\alpha^2}, \tag{20}$$

which in the bulk limit $\omega \to 0$ gives the Landau–Pekar result for the first ES energy of a bulk polaron in the gaussian approximation. In the same regime the effective mass expression (19) also reduces to the Landau–Pekar result for a bulk polaron.

6. Numerical results

It is often convenient to define a dimensionless confinement length l given by $l = l_0/r_0 = 1/\sqrt{\omega}$, where $l_0 = (\hbar/m\omega_h)^{1/2}$. This is the effective radius of the wire. The GS polaronic correction $\Delta\mathbf{E}_{GS}$ can then be defined as

$$\Delta\mathbf{E}_{GS} = \mathbf{E}_{GS} - \omega = \mathbf{E}_{GS} - \frac{1}{l^2}. \tag{21}$$

One can also define a quantity called the polaron binding energy (BE_{GS}) which is just the negative of $\Delta\mathbf{E}_{GS}$.

In Fig. 1 we plot BE_{GS} as a function of l for three values of α. As expected, the polaronic binding in a quantum wire increases as the confinement in the transverse direction increases. The increase in the polaronic binding becomes quite substantial if the effective radius is made very small. We have also plotted the results of the second-order RSPT for the sake of comparison. The agreement is evidently quite good.

In Fig. 2 we have shown the binding energy as a function of the effective wire radius in the strong coupling regime. We have shown results for $\alpha = 9$ and 10. Again it is clear that the polaronic effects become quite pronounced as the wire is made thinner and thinner. For comparison, we have plotted the Landau–Pekar results of Zhou and Gu and the FH results of Chen et al. [11]. It is clear that our LLPH results are better than the results of Zhou and Gu but inferior to those of FH.

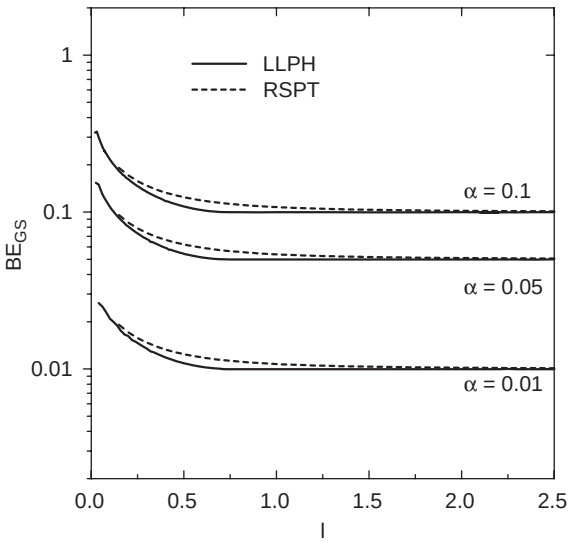

Fig. 1. The polaron binding energy (in Feynman units) of an electron in the GS of an axially symmetric parabolic quantum wire as a function of the effective confinement length l (in Feynman units) in the transverse direction for $\alpha = 0.1, 0.05$ and 0.01. The solid lines refer to the results of our LLPH calculation while the dashed lines correspond to the RSPT results of Quinghu et al. [5].

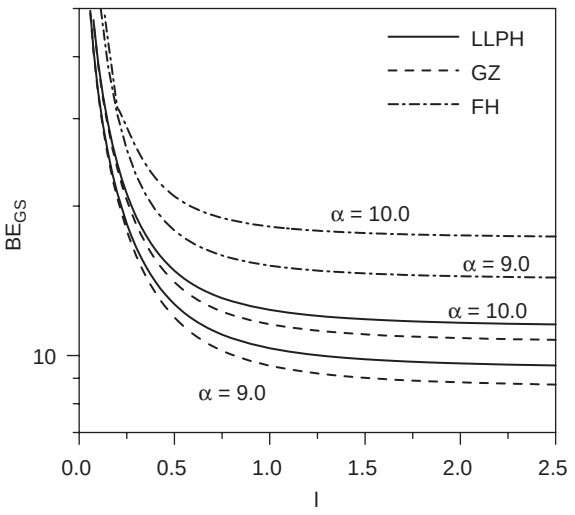

Fig. 2. The polaron binding energy (in Feynman units) of an electron in the GS of an axially symmetric parabolic quantum wire as a function of the effective confinement length l (in Feynman units) in the transverse direction for $\alpha = 9.0$ and 10.0. The solid lines refer to the results of our LLPH calculation, the dashed lines correspond to the strong coupling results of Zhou et al. [10] and the dash-dot curves represent the Feynman–-Hayken results [11].

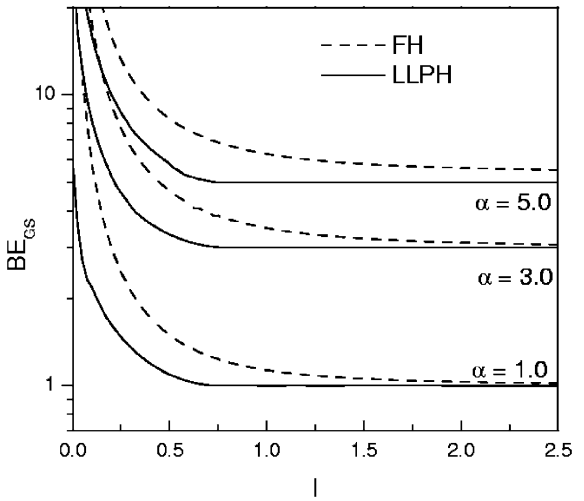

Fig. 3. The polaron binding energy (in Feynman units) of an electron in the GS of an axially symmetric parabolic quantum wire as a function of the effective confinement length l (in Feynman units) in the transverse direction for $\alpha = 1.0, 3.0$ and 5.0. The solid lines refer to the results of our LLPH calculation while the dashed lines correspond to the Feynman–Haken results of Chen et al. [11].

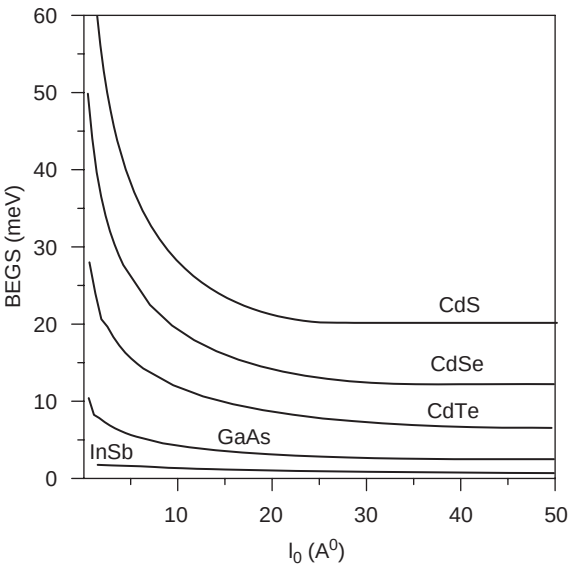

Fig. 4. The polaron binding energy (in meV) for CdS, CdSe, CdTe, GaAs and InSb as a function of confinement length l_0(in angstorms).

In Fig. 3, we have shown the results for the intermediate coupling region. Again the binding energy behaviour is along the expected line. For comparison, we have also plotted the Feynman–Haken results of Chen et al. [11]. Obviously for large values of α and for strong confinement Feynman–Haken results are more accurate than our LLPH results, but the palpable advantage with the LLPH theory is that it can be applied to the ESs unlike the Feynman theory and, furthermore, it is also a convenient method to obtain the effective mass. The Landau–Pekar theory can also be applied to the ESs but the LLPH method provides better results than the Landau–Pekar approach. In the weak-coupling region, the second-order RSPT does give good results for the GS energy, but again the LLPH procedure is more convenient for the effective mass calculation. Furthermore, the calculations of ES energies are often plagued with singularity problems in the second-order RSPT because of the possible instability of the ESs with respect to the emission of a phonon.

It would be interesting to have binding energy values of real semiconductor quantum wires available in the laboratory. In Fig. 4, we have shown the plot of ground state BE as a function of l_0 for systems like GaAs, CdS, CdSe, CdTe and InSb. It is clear that the polaronic effects become significantly strong if the transverse confinement lengths are reduced below a few nanometers.

In Fig. 5, we show the variation of the effective mass of the polaron along the length of the wire as a function of the confinement length in the transverse direction for two values of the coupling constant. As evident from the curves, the effective mass becomes extremely large below a certain radius of the wire. Thus, though the z-component of the total crystal momentum is a conserved quantity, it seems that it is possible to have some kind of a localization of the polaron even along the length of the wire. However as l increases, m^* goes over asymptotically to the bulk value.

One may notice that in the limit $\alpha \to 0$, $\mathbf{E}_{ES}$ reduces to just ω. Therefore, the first ES polaronic correction should also be defined in our model as

$$\Delta\mathbf{E}_{ES} = \mathbf{E}_{ES} - \omega = \mathbf{E}_{ES} - \frac{1}{l^2}. \tag{22}$$

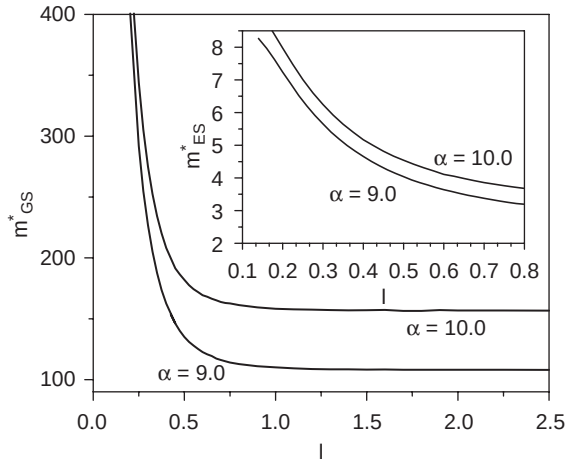

Fig. 5. The longitudinal polaron effective mass (in Feynman units) in the GS subband of an axially symmetric parabolic quantum wire as a function of the effective confinement length l (in Feynman units) in the transverse direction for $\alpha = 9.0$ and 10.0. The inset shows the effective mass for the ES.

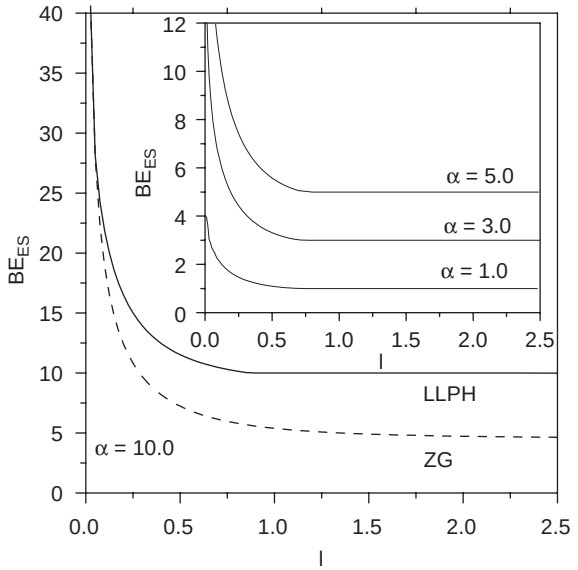

Fig. 6. The polaron binding energy (in Feynman units) of an electron in the first ES of an axially symmetric parabolic quantum wire as a function of the effective confinement length l (in Feynman units) in the transverse direction for $\alpha = 10.0$. The solid line refers to the results of our LLPH calculation while the dashed line corresponds to the strong coupling results of Zhou and Gu [10]. The inset shows the variation for intermediate values of α.

The negative of $\Delta \mathbf{E}_{ES}$ may be referred as the polaron binding energy in its first ES in an axially symmetric parabolic quantum wire.

In Fig. 6 we show the variation of the binding energy of the polaron in the first ES (BE_{ES}) as a function of the effective wire radius l for $\alpha = 10$. Again we find that as l decreases, the polaronic binding increases and below a certain confinement length the polaronic binding becomes very large. However, we find that the polaronic binding effect is less pronounced in the ES than in the GS. For the sake of comparison we have also shown in the same figure the Landau–Pekar results of Zhou and Gu [19]. We are not aware of any other calculation for the ES energy of a polaron in a parabolic quantum wire. As is clearly evident, our LLPH results are better than the Landau–Pekar results of Zhou and Gu which is quite understandable because the LLPH method is an all-coupling method while the Landau–Pekar method is alright in the limit $\alpha \to \infty$.

In the inset we have shown the results for $\alpha = 1, 3, 5$. The results are qualitatively similar. In the inset of Fig. 5, we have shown the variation of the longitudinal effective mass of a polaron in the ES as a function of the confinement length for two values of the coupling constant. The behaviour is

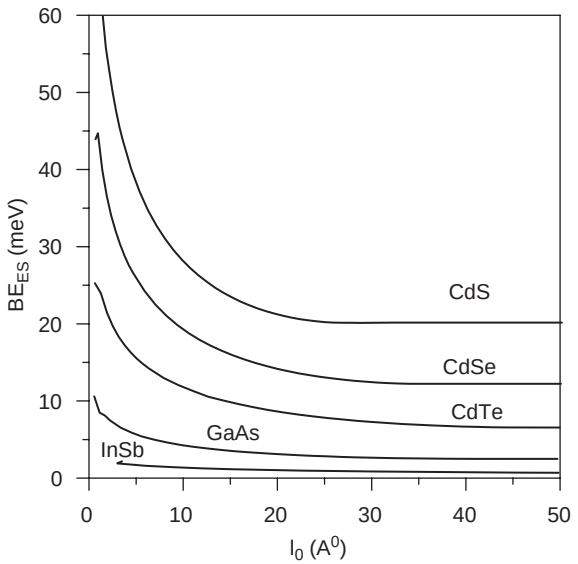

Fig. 7. The ES polaron binding energy (in meV) of an electron in GaAs, CdS, CdSe, CdTe and InSb.

qualitatively similar to that in the GS. Quantitatively however the effective mass is smaller in the ES than in the GS. In Fig. 7 we have shown the ES polaron binding energy results for the quantum wires of GaAs, InSb, CdTe, CdSe and CdS semiconductors. Again we find that significant polaronic effects can be observed if the confinement length is reduced below a few nanometers. One may however notice that for the systems we have considered the GS and the ES polaronic corrections are essentially same. This is however expected because for these materials the electron–phonon coupling constant is very small.

7. Conclusions

In conclusion, we have studied the motion of an electron in an axially symmetric polar semiconductor quantum wire with symmetric parabolic confinement in the transverse direction. We have employed the LLPH variational method to obtain the polaronic corrections to the ground state and the first excited state energies of the electron for the entire range of the electron–phonon coupling constant and for arbitrary confinement length. For the weak electron–phonon coupling we have compared our results with those of second-order RSPT. Agreement is found to be pretty good. Comparison with the Feynman–Haken results for the intermediate coupling regime shows that the LLPH theory can be considered to be fairly accurate in this region. For strong electron–phonon coupling we have compared our results with those of Landau–Pekar theory and it is found that the LLPH theory yields better results. The LLPH method has however some distinct advantages as compared to other methods. For example, the effective mass calculation is quite convenient in this method. Furthermore, the LLPH method can be applied to the excited state quite easily, while the Feynman path-integral method which in general gives better results for the ground state cannot be applied to the excited states at all. We have shown that the polaronic corrections to the ground and the first excited state energies of the quantum wire electron increases with decreasing effective wire radius l. This increase is quite slow if the wire radius is large but becomes quite rapid when the transverse confinement length l is reduced below a certain value. We have observed that the polaronic effects in the first excited state are in general less pronounced than in the ground state. We have also presented the polaronic binding energies for realistic semiconductor quantum wires such as GaAs, InSb, CdTe, CdSe and CdS systems. We have shown that polaronic effects in these systems can indeed be significant if the confinement lengths are reduced below certain values. Furthermore, we have shown that the longitudinal effective mass of the polaron also undergoes a substantial enhancement because of the transverse confinement in the quantum wire.

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