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Q1D–Polarons in Rigid Boundary Cylindrical Wires: "Mixed–Coupling Approximation"

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Abstract

We consider the interaction of a confined electron with bulk polar-optical phonons in a cylindrical quantum well wire with infinite boundary potential. Expressions for the polaron self energy and mass are derived within a composite variational scheme consisting of a strong-coupling characterization imposed in the lateral directions and a weak-coupling LLP-counterpart structured along the length of the wire. The formulation is seen to be rather commendable and yields a sensible description of the Q1D-polaron in thin wires of weak or intermediate electron-phonon coupling strengths.

1. Introduction

Continuous progress in epitaxial growth techniques has resulted in the fabrication of quasi-one-dimensional semiconductor structures with sharp interfaces [1]. Within this context there has appeared a numerous amount of publications focused to the study of the interaction of one dimensionally confined electrons with the bulk LO phonon modes [2-11]. As one would expect, the common finding in the relevant papers is that the electron couples to the phonon field very effectively and consequently, certain polaron quantities (e.g., the binding energy, polaron mass or the mean phonon density clothing the electron) scale to considerably pronounced values over that in the unconstrained three dimensional case. This follows essentially from that, in thin wires, the polaron cloud becomes squeezed towards the wire axis in the transverse directions resulting in a very high degree of localization of the polaron. Hence, even in weak polar materials the effective electron-phonon coupling shows up a strong-coupling aspect brought about by confinement effects. We therefore think that, even for a weak electron-phonon coupling

strength, the lattice may acquire a relaxed static deformation clothing the entire extent of the rapidly fluctuating electron in the directions transverse to the axis of a thin wire. Still, however, the ions may respond to the instantaneous position of the electron longitudinally along the length of the wire. Consequently, one has the adiabatic (strong-coupling) condition obtained along the two transverse axes, and weak-coupling along the third (z) direction. We refer to this situation as *mixed coupling*. The content of this article is therefore aimed at this particular situation where we review the ground state polaron properties in thin wires of weak polar materials.

In what follows we refer to the case of an electron confined laterally within a free-stand tubular geometry with infinite boundary potential at radius R. For the present we take the confined electron as interacting with the bulk phonon modes only, and refrain from including any modifications such as those due to phonon confinement, the polaron-induced band non-parabolicity or the loss of validity of both the effective–mass approximation and the Fröhlich continuum Hamiltonian in thin microstructures. We also ignore the screening effects and leave out the contributions from the interface phonon modes. In view of these simplifying assumptions and adopting the so called *bulk phonon approximation* we treat the quasi-1D polaron within the framework of a composite "mixed-coupling" approximation and devote almost all emphasis to the formal aspect of the problem.

2. Theory

2.1. Hamiltonian and Wavefunction

Using units for which $2m^* = \hbar = \omega_{LO} = 1$, the Hamiltonian describing an electron coupled to bulk LO-phonons is given by

$$H = H_{\rm e} + \sum_Q a_Q^\dagger a_Q + H_{\rm e-ph} \tag{1}$$

where

$$H_{\rm e} = -\frac{1}{\rho}\frac{\partial}{\partial\rho}\left(\rho\frac{\partial}{\partial\rho}\right) - \frac{\partial^2}{\partial z^2} \tag{2}$$

is the electron part, and

$$H_{\rm e-ph} = \sum_Q \Gamma_Q [a_Q \exp(i\vec{q}\cdot\vec{\rho} + iq_z z) + hc] \tag{3}$$

is the Fröhlich interaction in which the coordinates $\vec{\rho}$ and z give the electron position. The interaction amplitude is related to the electron-phonon coupling constant α and the phonon wavevector $\vec{Q} = (\vec{q}, q_z)$ through $\Gamma_Q = \sqrt{4\pi\alpha}/Q$.

To account for the cylindrical confinement with zero potential inside, and infinitely rigid boundary at $\rho = R$, we shall impose the lateral wavefunction of the electron to be

given in the product form

$$\Phi_{\rm e}(\rho) = N\,{\rm J}_0(\kappa\rho)\,\exp(-\frac{1}{2}\mu^2\rho^2) \tag{4}$$

where the constant N serves for normalization. Clearly, ${\rm J}_0$, the zeroth order cylindrical Bessel function of the first kind, takes care of the geometric confinement, and the further confinement induced by phonon coupling is governed by the Gaussian counterpart through parameter μ. In the above, $\kappa = j_{0,1}/R$, where $j_{0,1}$ is the first zero of ${\rm J}_0$.

2.2. Canonical Transformations

The Hamiltonian, Eq.(1), is invariant to translations of the electron together with its concomitant lattice distortion, and the total momentum along the wire axis is conserved, i.e., H commutes with

$$\mathsf{P}_z = -i\frac{\partial}{\partial z} + \Pi_z \tag{5}$$

in which

$$\Pi_z = \sum_Q q_z a_Q^\dagger a_Q \tag{6}$$

refers to the phonon momentum. Therefore, it is possible to transform to a representation in which the relevant coordinate of the electron is totally eliminated and the total momentum P_z becomes a c-number. On this purpose, applying the LLP – unitary transformation [12]

$$\mathsf{U}_1 = \exp\left\{i(\mathsf{P}_z - \Pi_z)\,z\right\}\,, \tag{7}$$

the Hamiltonian conforms to

$$\begin{aligned} H' &= \mathsf{U}_1^{-1} H \mathsf{U}_1 \\ &= -\frac{1}{\rho}\frac{\partial}{\partial\rho}\left(\rho\frac{\partial}{\partial\rho}\right) + (\mathsf{P}_z - \Pi_z)^2 \\ &+ \sum_Q a_Q^\dagger a_Q + \sum_Q \Gamma_Q(a_Q e^{i\vec{q}\cdot\vec{\rho}} + hc)\,. \end{aligned} \tag{8}$$

With the above form achieved for the polaron Hamiltonian, the problem reduces to the evaluation of the ground state energy for a given momentum P_z. The functional form, $E_{\rm g}(\mathsf{P}_z)$, thus obtained can then be expanded in a power series to second order in the momentum, i.e.,

$$E_{\rm g}(\mathsf{P}_z) \simeq E_{\rm g}(0) + c\,\mathsf{P}_z^2\,,$$

where the reciprocal of the factor multiplying P_z^2 is identified as the polaron mass (in units of the band mass, m^*) along the length of the wire.

For the calculation of $E_{\rm g}$ a variational approach is adopted, and the polaron ground state is postulated in a product ansatz consisting of the electron and lattice parts, i.e.,

$$\Psi_{\rm g} = \Phi_{\rm e}\, \mathsf{U}_2|0\rangle, \tag{9}$$

where $|0\rangle$ is the phonon vacuum state, and

$$\mathsf{U}_2 = \exp \sum_Q u_Q(\Phi_{\rm e})\,[a_Q - a_Q^\dagger], \tag{10}$$

is the the second LLP canonical (displaced oscillator) transformation in which the function $u_Q(\Phi_{\rm e})$ should be determined variationally.

Thus, subjecting the Hamiltonian further to the transformation

$$H' \rightarrow \mathsf{U}_2^{-1} H' \mathsf{U}_2\,,$$

we finally obtain

$$\begin{aligned} H'' &= -\frac{1}{\rho}\frac{\partial}{\partial\rho}\left(\rho\frac{\partial}{\partial\rho}\right) + \sum_Q a_Q^\dagger a_Q + \sum_Q u_Q^2 \\ &- \sum_Q \Gamma_Q u_Q \left(e^{i\vec{q}\cdot\vec{\rho}} + cc\right) + \sum_Q \left\{[\Gamma_Q e^{i\vec{q}\cdot\vec{\rho}} - u_Q]a_Q + hc\right\} \\ &+ \{\mathsf{P}_z - \Pi_z\}^2 + \left\{\mathsf{P}_z - 2\Pi_z^{(0)}\right\}\mathsf{P}_z \\ &+ 2\left\{\mathsf{P}_z - \Pi_z^{(0)}\right\}\Pi_z^{(1)} \;+\; \left\{\Pi_z^{(1)} - 2\Pi_z\right\}\Pi_z^{(1)} \end{aligned} \tag{11}$$

where

$$\Pi_z^{(0)} = \sum_Q u_Q^2 q_z\,, \tag{12}$$

$$\Pi_z^{(1)} = \sum_Q u_Q q_z (a_Q + a_Q^\dagger)\,. \tag{13}$$

Before we proceed with our main theme we should remark that, if the first transformation were by-passed (i.e. U_1 were selected as the identity operator), the theory would then diverse to the strong-coupling approximation for which simultaneous optimisations with respect to $\Phi_{\rm e}$ and $u_Q(\Phi_{\rm e})$ correspond to the self-trapping picture of the polaron where the electron distribution and the lattice polarisation influence each other in such a way that a stable relaxed state is eventually attained. The calculations and results pertaining to such a case (with $\alpha \gg 1$) have already been provided in a previous paper [8], and we do not re-derive them here. We shall be content with only noting that in narrow wires the pure-adiabatic theory is capable of yielding a reasonable description of

the polaron even when the electron-phonon interaction is not dominantly strong enough. For completeness, we make a small digression at this point and demonstrate this aspect by comparing the available data obtained previously from the pure strong coupling [10] and the Feynman path integral theories [11] applied to the case of a polaron in a cylindrical wire with parabolic confinement potential, i.e., $V(\rho) \sim \Omega^2\rho^2$. Although the two types of boundary potentials (rigid and parabolic) are qualitatively different in nature, we find it instructive to display the domain of validity of the strong coupling theory. An immediate glance at the family of curves in Figure 1 reveals that the point where the pure adiabatic theory starts to lie deviated below the path integral approximation shifts down to smaller values of α as the degree of confinement is increased (i.e., as Ω is tuned to large values); and it is this salient feature which leads us be motivated to treat the free direction with the more suitable LLP transformation, but still retain the strong-coupling characterization of the polaron in the lateral directions. We therefore reasonably use an admixture of the strong and intermediate coupling approximations to shed a better insight into the ground state polaron properties in highly anisotropic Q1D structures of weak polar materials.

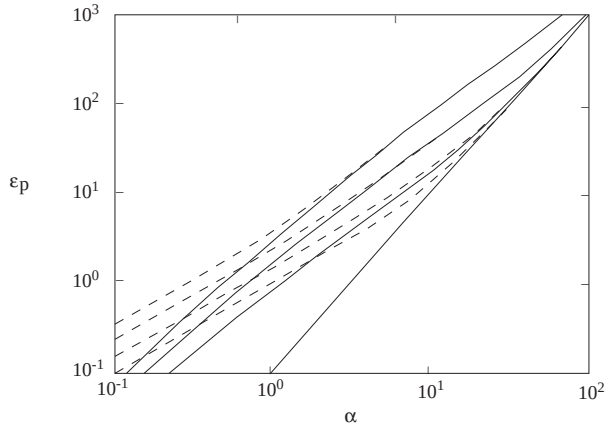

Figure 1. The polaron binding energy $\mathcal{E}_\mathrm{p} = \Omega - E_g$ as a function of α in a parabolic boundary wire. The solid and dashed curves refer respectively to the strong coupling [10] and path integral [11] theories. The set of curves, from bottom to top, are for $\Omega = 0$, 10, 10^2 and 10^3.

2.3. Variational Calculation

In the following, we adopt the case of a stationary polaron, i.e. take

$$\langle 0|\langle\Phi_\mathrm{e}|\mathsf{U}_2^{-1}\mathsf{U}_1^{-1}\mathsf{P}_z\mathsf{U}_1\mathsf{U}_2|\Phi_\mathrm{e}\rangle|0\rangle = 0\,,$$

and thus regard P_z as a virtual momentum which we retain to keep track of the effective mass of the coupled electron-phonon complex.

Calculating the expectation value of H'' (11) in the state $\Phi_{\rm e}|0\rangle$, we obtain the ground state energy, given by

$$\begin{aligned} E_{\rm g} &= \epsilon_k + \mathsf{P}_z^2 - 2\mathsf{P}_z\Pi_z + [\Pi_z^{(0)}]^2 \\ &+ \sum_Q u_Q^2(1+q_z^2) - 2\sum_Q \Gamma_Q u_Q s_q \end{aligned} \tag{14}$$

where

$$\epsilon_k = \langle\Phi_{\rm e}\,| -\frac{1}{\rho}\frac{\partial}{\partial\rho}\left(\rho\frac{\partial}{\partial\rho}\right)|\,\Phi_{\rm e}\rangle\,, \tag{15}$$

$$s_q = \langle\Phi_{\rm e}\,|e^{\pm i\vec{q}\cdot\vec{\rho}}|\,\Phi_{\rm e}\rangle \tag{16}$$

Defining, for notational convenience,

$$\sigma^{(n)}_{mm'}(x) = \int_0^{j_{0,1}} dt\; t^n \mathrm{J}_m(t)\,\mathrm{J}_{m'}(t)\,\mathrm{J}_0(xt)\exp(-\frac{\mu^2}{\kappa^2}t^2)\,, \tag{17}$$

and adopting the form (4) for the electron wavefunction, we obtain ϵ_k and s_q, equations (15) and (16), to be expressible in the following concise forms

$$\epsilon_k = \kappa^2 + \mu^2\left\{2 - \frac{2\sigma^{(2)}_{10}(0) - (\mu/\kappa)^2\sigma^{(3)}_{00}(0)}{\sigma^{(1)}_{00}(0)}\right\}\,, \tag{18}$$

and

$$s_q = \frac{\sigma^{(1)}_{00}(q/\kappa)}{\sigma^{(1)}_{00}(0)}\;. \tag{19}$$

The variational function $u_Q(\Phi_{\rm e})$ minimizing Eq.(14) is found to be given by the following nonlinear equation

$$\left\{1 - 2(\mathsf{P}_z - \Pi_z^{(0)})q_z + q_z^2\right\}u_Q - \Gamma_Q s_q = 0\,, \tag{20}$$

which can easily be handled with the consideration that, from symmetry arguments, the term $\Pi_z^{(0)}$ (12) can only differ from the total momentum by a scalar factor. Hence, setting

$$\Pi_z^{(0)} = \eta\mathsf{P}_z\;, \tag{21}$$

the optimal-fit condition (20) for $u_Q(\Phi_{\rm e})$ conforms to a convenient expression. We obtain

$$u_Q = \frac{\Gamma_Q s_q}{1 - 2(1-\eta)\mathsf{P}_z q_z + q_z^2} \tag{22}$$

in which the unknown scalar, η, is determined by the transcendental equation

$$\eta \mathsf{P}_z = \sum_Q \frac{\Gamma_Q^2 s_q^2 q_z}{\left[1 - 2(1-\eta)\mathsf{P}_z q_z + q_z^2\right]^2} \ . \tag{23}$$

In complete form, with the optimal fit for $u_Q(\Phi_{\rm e})$ substituted in, and the wavevector sums involving powers of first and second order in P_z projected out, equation (14) takes the form

$$E_{\rm g} = \epsilon_k - \sum_Q \Gamma_Q^2 \, s_q^2 \, \frac{1}{1+q_z^2} + (1-\eta)\mathsf{P}_z^2 \ , \tag{24}$$

from which we identify the effective polaron mass as

$$m_{\rm p} = \frac{1}{1-\eta} \ . \tag{25}$$

For a virtual translation ($\mathsf{P}_z \simeq 0$), Eq.(23) can be expanded in powers of P_z to yield

$$\eta = 4(1-\eta) \sum_Q \Gamma_Q^2 \, s_q^2 \, \frac{q_z^2}{(1+q_z^2)^3} + \mathcal{O}(\mathsf{P}_z^2) \ , \tag{26}$$

which, upon solving for η and substituting in the mass expression (25), we obtain

$$m_{\rm p} = 1 + 4 \sum_Q \Gamma_Q^2 \, s_q^2 \, \frac{q_z^2}{(1+q_z^2)^3} \ . \tag{27}$$

Projecting out the $\vec{Q}$-summations in equations (24) and (27), we finally arrive at the following integral - expressions for the ground state energy and the longitudinal mass

$$E_{\rm g} = \epsilon_k - \alpha \int_0^\infty dq \, \frac{1}{1+q} \, s_q^2 \, , \tag{28}$$

$$m_{\rm p} = 1 + \frac{\alpha}{2} \int_0^\infty dq \, q \, \frac{q+3}{(1+q)^3} \, s_q^2 \ . \tag{29}$$

3. Results and Conclusions

The energy expression (28) depends on the variational parameter μ in a complicated manner through the set of equations (17-19). The optimal fit to μ which minimizes $E_{\rm g}$ can therefore be performed by numerical techniques. In the following we give our results in terms of the binding energy of the polaron, $\mathcal{E}_{\rm p} = (j_{0,1}/R)^2 - E_{\rm g}$ (relative to the subband).

It should be re-emphasized that the theory we have used in this work constrains the validity of our results to narrow wires and to electron-phonon coupling strengths that

are not too strong. Clearly, for a small α one requires correspondingly a high degree of lateral confinement to compensate for weak phonon coupling and make the polaron go over to a "pseudo-strong" coupling characterization in the lateral plane achieved by the radially inward localization towards the wire axis. In the meantime, however, the effective phonon coupling in the longitudinal direction will be assumed to remain weak or at least, to grow not too powerful to violate the LLP - weak-coupling condition that we have undertaken for the polaron behaviour along the z axis. Within the framework of the "mixed-coupling" description thus constructed, one obtains a means of studying the ground state polaron properties in thin wires of weak polar materials.

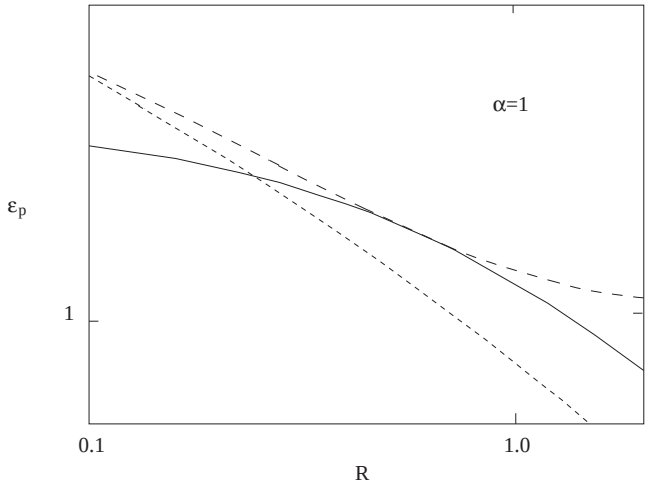

Figure 2. The binding energy $\mathcal{E}_{\rm p}$ as a function of the wire radius for $\alpha = 1$. The solid and dashed curves display the results of the mixed-coupling and path-integral [11] theories, respectively. The dotted curve refers to the results derived within the pure strong-coupling approach [8].

Selecting $\alpha = 1$, an intermediate coupling strength for which the LLP-theory proves to work rather well, we display the results of the present theory as a function of the wire radius for $R \leq 2$. In Figure 2 we also supply the energy values of the pure strong-coupling treatment of the same problem where the canonical transformation (7) is by-passed and the electron wavefunction (4) is extended to include a gaussian spread along the wire axis, i.e., $\Phi_{\rm e}(\rho) \rightarrow \Phi_{\rm e}(\rho)\exp(-\frac{1}{2}\lambda^2 z^2)$ [8]. A comparison of the two theories reveals that the strong coupling binding energy values lie deviated below the present results except for very small values of R simply because, for an intermediate coupling strength like $\alpha = 1$, the pure adiabatic approach can be convenient at only very high degrees of confinement where the pseudo-enhancement in α is dominantly realized. In this extreme, with α scaled to effective values considerably larger than 1, the pure strong-coupling treatment becomes even superior to the LLP-framework and

yields better results since now the effective interaction along the length of the wire should be characterized with a projection more on the strong-coupling side as the wire is made thinner. On the contrary, as the geometric confinement is released allowing the polaron to expand and relax itself laterally, the strong-coupling theory starts to become inadequate and rapidly loses its validity due to that in a comparatively delocalized configuration the effective phonon coupling strength falls far below to sustain the adiabatic condition. With the LLP - canonical transformation U_1 turned on, however, the deficiency encountered for comparatively large R ($R > 0.4$) gets removed and the strong-coupling approach becomes refined by a great extent yielding considerably improved energy upper bounds. To see this we also make reference to the available data from a similar problem treated under the Feynman path integral formulation applied to the case of a wire with parabolic boundary potential, $V(\rho) = \frac{1}{2}\Omega^2\rho^2$ (cf. Ref[11]). Even though the nature of the problem treated therein is qualitatively different from that for the rigid-boundary potential, we find it useful to generate a plot of the path integral results (cf. dashed curve in Figure 2) to shed some insight into the applicability of the present formalism. We correlate the two theories by comparing the relevant subband energies, and simply use $R = j_{0,1}/\sqrt{2\Omega}$ as the corresponding effective radius. We clearly see that within the range $0.4 < R < 0.8$, the present and the path integral theories are in fairly close agreement. Beyond this range, with increasing wire radius, the present theory is seen to display an increasingly large digression from the Feynman results due to that a delocalized nature of the electron in the lateral directions violates the pseudo-adiabatic condition which we have imposed apriori in this problem.

The basic qualitative features practiced for $\alpha = 1$ are seen to be retained for smaller values of α as well. It is observed that, in spite of a coupling constant smaller by an order of magnitude or even more, a sufficiently high degree of localization can still compensate for weak phonon coupling and lead the theory to show up a strong-coupling aspect in the transverse directions perpendicular to the wire axis. As reference to weak electron-phonon coupling, we select CdTe ($\alpha \approx 0.40$) and GaAs ($\alpha \approx 0.07$) based wires, which are of particular interest as typical examples of II-VI and III-V compound semiconductors. In Figure 3 we provide plots of the binding energy $\mathcal{E}_{\rm p}$ and the longitudinal mass $m_{\rm p}$ in these materials as a function of the wire radius.

In the energy plot for $\alpha = 0.40$ we inspect rather prominently that the LLP transformation employed along the z axis enhances the results considerably in good quality over to the values achieved within the pure strong-coupling treatment of the problem. For $\alpha = 0.07$, the digression in the adiabatic approximation is even much greater, and the corresponding strong-coupling binding energy values (not shown in the figure) lie drastically deviated, by almost an order of magnitude, below the present results. The overall feature displayed by the succession of curves calculated within the mixed-coupling approximation used in this work and the Feynman path integral theory is that the range of validity of the present results is limited, from above and below, to not too broad and not too thin wires, yet however, the relevant values within this range ($0.3 < R < 0.9$) are found to be commendable and are in somewhat close agreement with the corresponding

path integral results (cf. Figure 4).

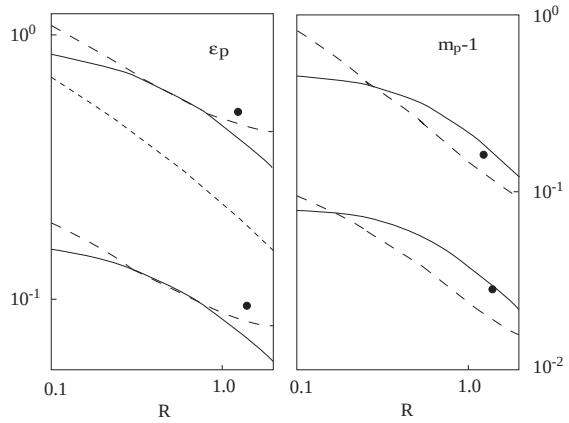

Figure 3. The binding energy $\mathcal{E}_{\rm p}$ and the effective polaron mass $m_{\rm p}$ as a function of the wire radius. The upper (lower) set of curves are for CdTe (GaAs) where $\alpha = 0.40\,(0.07)$. The solid and dashed curves display the results of the mixed-coupling and path-integral [11] theories, respectively. The dotted curve refers to the pure strong-coupling approach [8] performed for $\alpha = 0.07$. The heavy dots, included for further comparison, represent the available data obtained for a square cross section wire under perturbation theory [3] where we have correlated the side length L to R through $R = (j_{0,1}/\sqrt{2}\pi)L$. In the plots, the energy and length units correspond, respectively, to 35 (18) meV and 40 (44) $\mathring{A}$, for GaAs (CdTe).

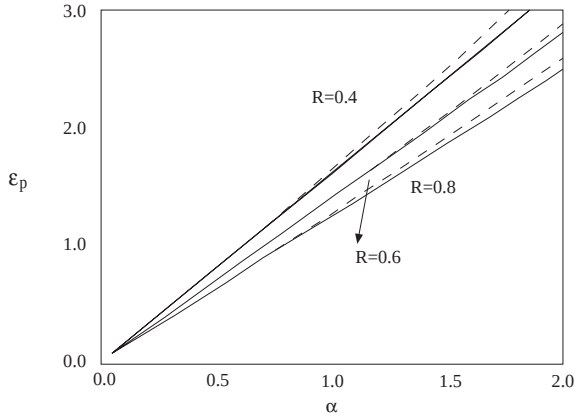

Figure 4. The binding energy $\mathcal{E}_{\rm p}$ as a function of α in the weak/intermediate coupling regime. The set of curves from top to bottom are for $R = 0.4,\ 0.6$ and 0.8. The solid and dashed curves display the results of the mixed-coupling and path-integral [11] theories, respectively.

For large and small values of R lying beyond this range, the mixed-coupling approach fails to yield a satisfying description due to that, for not thin enough wires, the strong-coupling requirement which we have imposed in the lateral directions is not adequately satisfied, or else, in very thin wires, the LLP - weak-coupling approximation employed along the length of the wire becomes violated as a consequence of the pseudo-enhancement in the overall effective phonon coupling strength. Nevertheless, in spite of these drawbacks, we feel that the mixed-coupling theory employed in this work can be regarded as capable of reflecting a sensible characterization of the Q1D-polaron within a reasonable range of the wire diameter lying within $30 - 80$ Angström units in GaAs and CdTe based wires.

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