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The Optical Polaron in Quantum-Well-Type Systems

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Contents

List of Figures

Dedication

To my

Parents,

My sisters and brothers,

and to my Supervisor Dr. Bassam Saqqa.

Zher Fuad Samak

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Abstract

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The polaron problem in a quasi 1D cylindrical quantum wire with infinite boundary potential is investigated using the strong-coupling theory and the mixed-coupling approximation. It is observed that a decrease in the radius of wire produces a pseudo-strong coupling aspect to the problem in spite of weak values of (α). A modification to the mixed-coupling theory is proposed to interpolate between the strong- and the weak-coupling aspects of the problem for all the degrees of confinements. This modified mixed-coupling approach is applied to the problem in a spherically box-type and in a slab like confinements. The same approach is applied to study the ground-state energy of the polaron as a function of the effective dimensionality. It is shown that the problem transforms from the strong-coupling to the weak-coupling limits in a smooth way.

Arabic Abstract

Chapter 1

Introduction

1.1 The Concept of Polaron

To explain the concept of polaron, first we begin with the description of crystals. The structure of all crystals can be described in term of a lattice (A lattice is a regular periodic array of points in space) with a group of atoms attached to every lattice point. The group of atoms is called basis, when repeated periodically in space it forms the crystal structure. At room temperature, the atoms are not fixed, but they vibrates around their equilibrium positions (the lattice points). The vibrations of atoms will form a vector field called the displacement field, which can be quantized, the quanta of the displacement field are called phonons [1]. The ionic polarization in the crystal occurs by the electric field of conduction electron in which the electric field of the electron displaces the positive and negative ions with respect to one another (attracts the positive ions and repels the negative ions according to coulomb forces), this displacement can be described as waves or cloud of phonons. A conduction electron or (hole) together with its self-induced polarization in a polar semiconductor or an ionic crystal forms (***Polaron***).

As a result of formation of polaron, the electron polarizes the lattice producing a potential well around itself in which it becomes trapped. The self-trapping is considered in ionic (polar) materials, so the notation (polaron) is due to this fact.

This concept was first introduced by Landau in (1933) [2].

The polaron concept is of interest, because it describes the particular physical properties of an electron in polar crystals and ionic semiconductors and it is an interesting theoretical model consisting of a fermion interacting with a boson field.

The polaron is characterized by a parameter such as, its binding or (self-)energy, effective mass and its response to the external electric and magnetic field. Also, the number of phonons in the polaron cloud, and the polaron radius are important parameters. Besides, the coupling-constant (α) that describes the strength of the electron-phonon interaction.

The polaron can be classified according to its size to [large and small] and according to the frequency of the phonons which interact with electron to [optical and acoustical polaron].

When the phonons interact with two electrons (or two holes) in the crystal it will form a bipolaron which is spinless although the polaron has a spin [3].

Large polaron [Fröhlich polaron]

It is formed when the displacement of the ion is larger than the lattice constant and the deformation of the lattice will be large. The large polarons are governed by the long-range interaction, and the self-trapped carrier of a large polaron generally extends over several sites [4], [5].

Besides, in a large polaron regime the lattice can be replaced by a continuum medium which is not appropriate for small polaron regime.

Small polaron [Holstein polaron]

It is formed when the displacement of ion is smaller than the lattice constant and the deformation of the lattice will be small. The self-trapped carrier of small polaron is confined to a single site, and the small polarons are governed by the short-range interaction [3], [4].

Optical polaron

This type of polaron is formed in polar materials when a conduction electron interacts with longitudinal optical (LO) modes of the lattice vibrations, which have a high frequency, and easily interact with light.

Acoustical polaron

This polaron is formed in metals when the electron interacts with acoustical phonons which have a low frequency, and correspond to the sound wave in the lattice.
But, it is important to know that, the early work on polarons was devoted to the interaction between a charge carrier (electron, hole) and (LO) phonons.

1.2 Historical Studies and Theories of Polaron

Historically the first studies on polarons is Russian work that described the concept of polaron by Landau (1933) in a paper of a bout one page [2].
In (1937) Fröhlich [5] gave a quantitative discussion of the electron scattering in ionic crystals where he introduced the concept of the field of lattice displacement.
In (1949) Fröhlich derived the so called (Fröhlich Hamiltonian), and solved the problem for the weak-coupling case using perturbation theory [5].
Landau and Pekar (1951) investigated the self-energy and the effective mass of polaron which was shown by Fröhlich (1954) that correspond to the strong-coupling regime [3], [6].
In (1953) Lee, Low and Pines (L.L.P) [7] have derived a variational technique which depends on a series of successive canonical transformations that give good results for intermediate values of the polaronic strength (α)
In (1954) Pekar put the trial wave state for the polaron ψ which is considered as two parts[6], electron wave function ϕ_e, and the field (phonon) wave function ϕ_{ph}, that is,

$$\psi = \phi_e.\phi_{ph} \ , \tag{1.1}$$

which can be written as

$$|\psi\rangle = |\phi_e\rangle|\phi_{ph}\rangle \ . \tag{1.2}$$

In (1955) Feynman studied one of Fröhlich's papers on polarons (Fröhlich, 1954). There, he got the idea to formulate the polaron problem into Lagrangian form of quantum mechanics, he considered that the polaron consists of two classical particles,

and eliminate oscillators (waves). The resulting is Feynman's path integral form [8]. Over the years Feynman model for the polaron has remained in many respects the most successful to the problem of polaron, for the overall range of the coupling constant.

In (1970) Bogolubov applied the well-known method of chronological or T-products. This method appeared to be effective for the theory of the large polarons for all strengths of electron-phonon interaction and also for the derivation of higher terms of the perturbation series in the weak-coupling limit. Like the functional integration formalism, the T-product method has various applications in many fields of quantum physics [9].

Peeters and Devreese (1982) have generalized the Feynman model of the polaron to the case where a static external magnetic field is applied [3], [10], and their calculations are valid for all values of the polaronic strength (α). In this model the free energy of polaron was treated as a path integral [8].

Even though the polaron problem is a rather old subject, it has recently excited renewed interests in the context of low dimensionally confined quantum system, because it represents a theoretical model of a particle interacts with a fluctuating medium, connects the condensed matter physics with the framework of quantum field theory and it is used in the recent developments in a micro-fabrication technology.

Since the Fröhlich Hamiltonian of polaron has no exact solution, many mathematical techniques have been developed to treat the polaron problem.

(1) **The Strong-Coupling Theory** or, **The Adiabatic-Coupling Theory** which developed by Pekar [6]. This theory is valid when the kinetic energy for the electron is much greater than the energy of phonons, because this theory assumes that the wave function of the polaron consists of two wave functions, electron wave function ϕ_e, and the field (phonon) wave function ϕ_{ph} as we explained in [equation (1.1)]. The calculations of this method depends on **the variational method** which supposes a variational parameter in the trial wave state of the polaron, and minimizing the Hamiltonian to find the binding energy of polaron. This method can be used for large values of polaronic

constant (α).

(2) **The Weak-Coupling Theory** which depends on **the perturbation theory**, this theory supposes that the Hamiltonian interaction between electron and phonons as a small perturbed quantity and using the method of the perturbation technique to find the energy of polaron. This method can be used for small values of polaronic constant (α).

(3) **The Mixed-Coupling Approximation**, this method depends on **the variational method** [7], in which two (L.L.P) successive transformations are used. The first transformation is

$$U_1 = \exp[i/\hbar(\mathbf{P} - \sum_Q \hbar\mathbf{Q}a_Q^\dagger a_Q).\mathbf{r}] \,, \tag{1.3}$$

where $\mathbf{P}$ is the total-momentum operator of the polaron, $a_Q^\dagger(a_Q)$ are the creation (and annihilation) operators for (LO) phonons of wave vector ($\overrightarrow{Q}$), $\overrightarrow{r}$ denotes to the position of electron, this transformation eliminates the electron operators from the electron-phonon Hamiltonian part.

The second transformation is

$$U_2 = \exp[\sum_Q u_Q(a_Q^\dagger - a_Q)] \,, \tag{1.4}$$

where u_Q is treated as a variational function. This transformation is called "displaced-oscillator" which related to the phonon operators.

It is important to know that all theories of the polaron depend on using the Fröhlich Hamiltonian (1954) which consists of three parts [7], the Hamiltonian of electron, the Hamiltonian of phonon, and the Hamiltonian of electron-phonon interaction, that is

$$\begin{aligned} H &= H_e + H_{ph} + H_{e-ph} \,, \qquad (1.5) \\ &= H_e + \sum_Q \hbar\omega_{LO} a_Q^\dagger a_Q + \sum_Q V_Q[a_Q \exp i(\overrightarrow{Q}.\overrightarrow{r}) + a_Q^\dagger \exp -i(\overrightarrow{Q}.\overrightarrow{r})] \,, \end{aligned}$$

where H_e represents the electronic Hamiltonian, and V_Q is the amplitude of the electron-phonon interaction which is given as

$$V_Q = -i(\frac{\hbar\omega_{LO}}{Q})(\frac{4\pi\alpha}{V})^{1/2}(\frac{\hbar}{2m\omega_{LO}})^{1/4} , \tag{1.6}$$

where V is the volume of a crystal (which is taken as a unit in most problems of the polaron), ω_{LO} is the frequency of the (LO) phonons, and $\hbar\omega_{LO}$ is the energy of the phonons and α is the standard dimensionless coupling constant of the electron-phonon interaction which is given as

$$\alpha = \frac{e^2}{2\hbar\epsilon_0}\sqrt{\frac{2m}{\hbar\omega_{LO}}}(\frac{\epsilon_0}{\epsilon_\infty} - 1) , \tag{1.7}$$

where $\epsilon_\infty(\epsilon_0)$ is the high frequency (static) dielectric constant of the medium.
By using the previous information, Fröhlich (1954), [5] has provided the first weak-coupling perturbation-theory results

$$\epsilon_p^{3D} = \alpha\hbar\omega_{LO} , \tag{1.8}$$

where $\epsilon_p^{3D}$is the three-dimensional binding energy (3D) of the polaron in the ground-state.
Electron systems in reduced dimensions as in two dimensions like in GaAs-AlGaAs are of great interest. Also the electron-phonon interaction and the polaron effect in such systems receive much attention. For one polaron, confined to two dimensions, but interacting with a (3D) phonon cloud, the Fröhlich Hamiltonian remains of the same form, with a simple modification in the amplitude of the electron-phonon interaction V_Q. The binding energy for a polaron in two-dimensions (2D) for small value of α was first obtained by Sak (1972) [3], and provided us with the result

$$\epsilon_p^{2D} = \frac{\pi}{2}\alpha\hbar\omega_{LO} . \tag{1.9}$$

For large values of α, the strong-coupling corresponding results are [11], [12]

$$\epsilon_p^{3D} = \frac{\alpha^2}{3\pi}\hbar\omega_{LO} , \tag{1.10}$$

$$\epsilon_p^{2D} = \frac{\pi\alpha^2}{8}\hbar\omega_{LO} . \tag{1.11}$$

It is clear that, decreasing dimensions, leads to increase the value of polaron binding energy, from the previous equations, the polaron binding energy is deepened by a factor $\frac{\pi}{2}$ in the weak-coupling regime, and by $\frac{3\pi^2}{8}$ in the strong-coupling regime, that is because the confinements increase the binding energy.
On the other hand, it is important to talk about the effect of the external magnetic field on the polaron problem (***magnetopolaron***), because a large number of experiments and theories [13]-[26] have reported measurements of polaronic effects in semiconductors in the presence and in the absence of a magnetic field.
All studies of magnetopolaron explain the interrelation between the strength of the magnetic field and the coupling strength of the polaron. For the case of magnetopolaron, additional term is added to Fröhlich Hamiltonian that results from the magnetic force so the binding energy becomes large due to the additional degree of localization brought about by the magnetic field.
An important contribution to the theoretical study of polarons in the magnetic fields was made by Larsen [13].

For weak electron-phonon coupling and high magnetic fields, the lattice is thought to be responding only to the overall motion of the faster orbiting electron in its Landau orbit [26]. In this limit the adiabatic approach gives the same result obtained from the second order perturbation theory. This means for small values of α the strong-coupling method gives reasonable results as the strength of the magnetic field increases, that because the strong magnetic field adds another confinement to the polaron problem so the adiabatic theory succeeds in solving the problem of polaron in spite of the weak electron-phonon coupling.
The magnetic field strength and the high degree of confinement lead to the a pseudo-enhancement of α, which increase the polaronic effect. Many studies and researches [25], [26] focused on the quantum confinement systems such as the polaron in (2D), polarons in thin wires, magnetopolaron, and polarons with reduced dimensionality in semiconductors which play an important role in micro-fabrication technology, such as molecular-beam epitaxy. Many theoretical investigations have been made to

study the polaronic properties in lower dimensions [27]-[32]. Recent studies on the electron-phonon interaction in quasi one-dimensional (Q1D) systems have explored a polaronic effect pronounced stronger than in (2D) structures. For this reason, it is important to explain the meaning of the low dimensionally confined quantum system.

When the electron moves through a polar crystal it will generate a distortion which acts back on the electron and for large enough coupling constant the lattice distortion forms a deep potential well that the electron becomes self-trapped in this well. It means that the polarization which is caused by the electron, hinders the movement of electron and decreasing the mobility. Such electron which has a bound state in the potential created by a distorted lattice is considered as (a confined polaron). The meaning of quantum confinement is when the electrons or holes in semiconductors are confined by a potential in 1D (quantum well), 2D (quantum wire) or 3D (quantum dot). Besides, the quantum confinement occurs when one or more of the dimensions of a nanocrystals are made very small, this allow transition from (3D) bulk-like case to (2D) slab-like case, and from (2D) slab-like case to (1D) wire-like case [34], [35].

More studies [33]-[39] about the confined polaron led to the results that, in quantum wires where the electrons are fundamentally (Q1D), the polaronic binding is far much deeper than in two dimensionally confined quantum well systems. It means that, high degrees of confinement (as realized in thin wires) lead to a pseudo-enhancement in the effective electron-phonon coupling, so, in spite of weak-coupling as in GaAs for instance, the polaron problem may show up as a strong-coupling aspect coming from confinement effects [27], [28].

1.3 The Aim of The Work

Despite the long history of polaron study, the interest to the problem does not decrease. Many theoretical investigations have been made to study polaronic effect in low-dimensional structures as ionic crystals and polar semiconductors [18]-[24].

Because of increasing attention on this subject, in our work we focused on studying a confined polaron with reduced dimensionality, starting with Fröhlich Hamiltonian with a parabolic potential.

Reduced dimensionality means that the transition is taken from bulk case (3D) to slab-case (2D) or to wire-case (1D) by decreasing the freedom of movement of polaron or increase the confinement due to the potential.

In our work we attack the following three problems:

(a) **Strong-Coupling Characterization** of the quasi-one dimensional (Q1D) polaron in a cylindrical quantum well wire (QWW), and calculated the binding energy in the strong-coupling range.

(b) Q1D- polarons in rigid boundary cylindrical wires using **"Mixed-Coupling Approximation"**, and we calculated the binding energy for the polaron in the intermediate-coupling range, and compared it with the results obtained using adiabatic (strong) method.

(c) Polaron under a parabolic potential includes calculating the binding energy in both strong- and weak-coupling for 3D and 2D, also polarons with reduced dimensionality, using **"Modified Mixed-Coupling Approximation"** and transition from bulk-like case (3D) to slab-like (2D) and to wire-like case (1D).

In chapter (2), a detailed solution of Q1D-polarons in cylindrical (QWW) using adiabatic approximation which is treated by a variational method. We calculated the binding energy for the polaron, also the relation between the binding energy and the radius of the wire is explained for large values of α, which was calculated before by Erçelebi A. and Senger R. T. [27]. Also we consider the interaction of an electron with bulk optical phonons in a cylindrical (QWW) with infinite boundary potential.

In chapter(3), using the two successive (L.L.P) transformations, we solved the same problem with the "Mixed-Coupling Approximation" and calculated the binding energy for the polaron also, the relation between the binding energy and the radius of the wire and obtained the same results as Erçelebi A. and Senger R. T. [29].

In chapter (4), we solved the problem of polaron under a parabolic potential. With simple modification in the first (L.L.P) transformation [equation (1.3)] we proved that one can obtain the binding energy of the polaron for all range of α,
and the problem was solved with reduced dimensionality (transition from 3D to 2D, and from 3D to 1D).

(a) **In section one**: We calculated the binding energy of the polaron using "Mixed-Coupling Approximation" with adding a variational parameter to the first L.L.P transformation. This modification led to the so-called **"Modified Mixed-Coupling Approximation"** which enabled us to obtain the binding energy for 3D in both weak- and strong-coupling range, which is equal to $(\alpha\hbar\omega_{LO})$ for weak-coupling range, and equal to $(\frac{\alpha^2}{3\pi}\hbar\omega_{LO})$ for strong-coupling range, which was obtained before by Fröhlich and Feynman [5], [8], and others [39], [38].

(b) **In section two**: We calculated the binding energy of the polaron using **"Modified Mixed-Coupling Approximation"** for 2D in both weak- and strong-coupling range, which is equal to $(\frac{\pi}{2}\alpha\hbar\omega_{LO})$ for weak-coupling range, and equal to $(\frac{\pi\alpha^2}{8}\hbar\omega_{LO})$ for strong coupling range, which was obtained before by Fröhlich and Feynman [5], [8], and others [39], [38].

(c) **In section three**: We treated the same problem with reduced dimensionality and transition from bulk-case (3D) to slab-case (2D) and from bulk-case to wire-case (1D) by adding two variational parameters to the first L.L.P transformation.

Chapter 2

Q1D- Polarons in Cylindrical Quantum Well Wires, The Strong-Coupling Regime

In this chapter, we treat the problem of quasi-one dimensional analog of the standard optical polaron relevant to a cylindrical quantum well wire(QWW), using the strong-coupling theory, with infinite boundary potential [27]. In the framework of the adiabatic approximation we start with the Hamiltonian of the electron immersed in the field of bulk (LO) phonons in a cylindrical wire with the radius R, and the units ($2m = \hbar = \omega_{LO} = 1$), where m is the effective mass of the electron.
The Hamiltonian of the polaron is given by

$$H = H_e + H_{ph} + H_{e-ph} \,, \tag{2.1}$$

where H_e is the electronic part of the Hamiltonian, which in cylindrical coordinates, takes the form

$$H_e \;=\; -\frac{1}{\rho}\frac{\partial}{\partial\rho}(\rho\frac{\partial}{\partial\rho}) - \frac{\partial^2}{\partial z^2} \,, \tag{2.2}$$

where $(\overrightarrow{\rho}, z)$ denote the position of the electron in cylindrical coordinates. And the Hamiltonian of phonons is

$$H_{ph} = \sum_Q a_Q^\dagger a_Q \,, \tag{2.3}$$

where $a_Q^\dagger(a_Q)$ is the phonon creation (annihilation) operator, and $\overrightarrow{Q}$ is the wave-vector of the phonons, where $\overrightarrow{Q} = (\overrightarrow{q}, q_z)$,

and

$$H_{e-ph} = \sum_Q V_Q[a_Q \exp(i\overrightarrow{Q}.\overrightarrow{r}) + a_Q^\dagger \exp(-i\overrightarrow{Q}.\overrightarrow{r})] \,, \tag{2.4}$$

is the Hamiltonian representing the electron-phonon interaction, where V_Q is the interaction amplitude which is related to the phonon wave-vector $\overrightarrow{Q}$ through,

$$V_Q = \frac{\sqrt{4\pi\alpha}}{Q} \,. \tag{2.5}$$

To solve the problem of polaronic effect in adiabatic approximation we take the pekar-type [6] trial state as in [equation (1.2)] which is

$$|\psi_g\rangle = |\phi_e\rangle|\phi_{ph}\rangle \,, \tag{2.6}$$

where $|\phi_e\rangle$ is the ground-wave state for the electron, and

$$\phi_{ph} = U_Q|0\rangle \,, \tag{2.7}$$

describes the phonon wave function. The ket $|0\rangle$ is the phonon vacuum state, simply because at low temperature ($KT << \hbar\omega_{LO}$), there will be no effective phonons, (K is Boltzmann's constant and T the absolute temperature) [27].

U_Q is the unitary displacement operator which is given by

$$U_Q = \exp \sum_Q u_Q(a_Q - a_Q^\dagger) \,, \tag{2.8}$$

which produces lattice deformation created at the origin, $u_Q(\phi_e)$ will be considered as a variational function. The electron trial wave function will be taken as

$$\phi_e(\overrightarrow{\rho}, z) = \phi_e(\overrightarrow{\rho})\phi_e(z) \,, \tag{2.9}$$

with

$$\phi_e(\overrightarrow{\rho}) = n_\rho J_0(\kappa\rho) \exp(-\frac{1}{2}\mu^2\rho^2) \,, \tag{2.10}$$

and

$$\phi_e(z) = n_z \exp(-\frac{1}{2}\lambda^2 z^2) \,, \tag{2.11}$$

where μ and λ are two variational parameters accounting for the anisotropic nature of the system.

J_0 is the zeroth order cylindrical Bessel function of the first kind in which $(\kappa = j_{0,1}/R)$ its first zero and $j_{0,1} = 2.4048$, R is the radius of the cylinder.

n_ρ, n_z are the normalization constants of $\phi_e(\overrightarrow{\rho}, z)$ which is normalized function.

Applying the normalization condition $(\int \phi^* \phi dv = 1)$ we will get, $\phi_e(z)$ as

$$\phi_e(z) = (\frac{\lambda^2}{\pi})^{1/4} \exp(-\frac{1}{2}\lambda^2 z^2) \, . \tag{2.12}$$

With the form of [equation (2.10)] adopted for the lateral part of the electron trial state, the Bessel function takes care of the geometric confinement, and the further confinement induced by phonon coupling is governed by the counterpart through the parameter μ.

To calculate the energy of the polaron, return to [equation (2.6)], taken the wave function of polaron as

$$\psi_g = \phi_e U_Q |0\rangle \, , \tag{2.13}$$

the energy can be obtained as

$$\begin{aligned} E_g &= \langle 0|\langle \phi_e|U_Q^{-1} H U_Q|\phi_e\rangle|0\rangle \\ &= \langle 0|\langle \phi_e|H'|\phi_e\rangle|0\rangle \, , \end{aligned} \tag{2.14}$$

where

$$H' \rightarrow U_Q^{-1} H U_Q \, ,$$

By using the identity

$$e^A B e^{-A} = B + \frac{1}{1!}[A,B] + \frac{1}{2!}[A,[A,B]] + \frac{1}{3!}[A,[A,[A,B]]] + ... \tag{2.15}$$

and the [equation (2.8)] which explains the expression of U_Q [27], we obtain the following results:

$$U^{-1} H_e U = H_e \, , \tag{2.16}$$

$$U^{-1} \sum_Q a_Q^\dagger a_Q U = \sum_Q a_Q^\dagger a_Q + \sum_Q u_Q^2 - \sum_Q u_Q (a_Q + a_Q^\dagger) \, , \tag{2.17}$$

and

$$U^{-1}[\sum_Q V_Q(a_Q e^{i\vec{Q}.\vec{r}} + a_Q^\dagger e^{-i\vec{Q}.\vec{r}})]U = -\sum_Q V_Q u_Q(e^{i\vec{Q}.\vec{r}} + e^{-i\vec{Q}.\vec{r}}) + \sum_Q V_Q(a_Q e^{i\vec{Q}.\vec{r}} + a_Q^\dagger e^{-i\vec{Q}.\vec{r}}) . \quad (2.18)$$

The last three equations will form the modified Hamiltonian as

$$H' = H_e + \sum_Q a_Q^\dagger a_Q + \sum_Q u_Q^2 - \sum_Q u_Q(a_Q + a_Q^\dagger) + \sum_Q V_Q(a_Q e^{i\vec{Q}.\vec{r}} + a_Q^\dagger e^{-i\vec{Q}.\vec{r}}) - \sum_Q V_Q u_Q(e^{i\vec{Q}.\vec{r}} + e^{-i\vec{Q}.\vec{r}}) , \quad (2.19)$$

which can be simplified to

$$H' = H_e + \sum_Q a_Q^\dagger a_Q + \sum_Q u_Q^2 - \sum_Q V_Q u_Q[e^{i\vec{Q}.\vec{r}} + e^{-i\vec{Q}.\vec{r}}] + \sum_Q \{[V_Q e^{(i\vec{Q}.\vec{r})} - u_Q]a_Q + [V_Q e^{(-i\vec{Q}.\vec{r})} - u_Q]a_Q^\dagger\} . \quad (2.20)$$

The energy will be then

$$E_g = \langle\phi_e|H_e|\phi_e\rangle + \sum_Q u_Q^2 - \sum_Q V_Q u_Q\langle\phi_e|e^{(i\vec{Q}.\vec{r})}|\phi_e\rangle - \sum_Q V_Q u_Q\langle\phi_e|e^{-(i\vec{Q}.\vec{r})}|\phi_e\rangle . \quad (2.21)$$

Defining

$$\epsilon_\kappa = \langle\phi_e| - \nabla^2|\phi_e\rangle ,$$

and

$$S_Q = \langle\phi_e|e^{\pm(i\vec{Q}.\vec{r})}|\phi_e\rangle .$$

Then E_g, becomes

$$E_g = \epsilon_\kappa + \sum_Q u_Q^2 - 2\sum_Q V_Q u_Q S_Q . \quad (2.22)$$

By minimizing [equation (2.22)] with respect to u_Q, we can obtain u_Q as

$$u_Q = V_Q S_Q . \quad (2.23)$$

Substituting back in [equation (2.22)], for u_Q we obtain

$$E_g = \epsilon_\kappa - \sum_Q V_Q^2 S_Q^2 . \quad (2.24)$$

Using the definitions of ϕ_e given in [equations (2.9)-(2.11)] we obtain

$$\begin{aligned}
\epsilon_\kappa &= \langle\phi_e(\overrightarrow{\rho},z)| - \nabla^2|\phi_e(\overrightarrow{\rho},z)\rangle \\
&= \langle\phi_e(\overrightarrow{\rho})| - \frac{1}{\rho}\frac{\partial}{\partial\rho}(\rho\frac{\partial}{\partial\rho})|\phi_e(\overrightarrow{\rho})\rangle + \langle\phi_e(z)| - \frac{\partial^2}{\partial z^2}|\phi_e(z)\rangle \\
&= \langle\phi_e(\overrightarrow{\rho})| - \frac{1}{\rho}\frac{\partial}{\partial\rho}(\rho\frac{\partial}{\partial\rho})|\phi_e(\overrightarrow{\rho})\rangle + \frac{\lambda^2}{2}\,.
\end{aligned}$$

Defining

$$\sigma^{(n)}_{mm'}(x) = \int_0^{j_{0,1}} dt \quad t^n J_m(t)J_{m'}(t)J_0(xt)\exp(-\frac{\mu^2}{\kappa^2}t^2)\,. \tag{2.25}$$

Finally ϵ_κ can be written as

$$\epsilon_\kappa = \kappa^2 + \mu^2\{2 - \frac{2\sigma^{(2)}_{10}(0) - (\mu/\kappa)^2\sigma^{(3)}_{00}(0)}{\sigma^{(1)}_{00}(0)}\} + \frac{\lambda^2}{2}\,. \tag{2.26}$$

And for S_Q, we have

$$\begin{aligned}
S_Q &= \langle\phi_e(\overrightarrow{\rho})|\langle\phi_e(z)|e^{\pm i\overrightarrow{q}\,.\,\overrightarrow{\rho}}e^{\pm iq_z z}|\phi_e(z)\rangle|\phi_e(\overrightarrow{\rho})\rangle \\
&= \langle\phi_e(\overrightarrow{\rho})|e^{\pm i\overrightarrow{q}\,.\,\overrightarrow{\rho}}|\phi_e(\overrightarrow{\rho})\rangle\ \ \langle\phi_e(z)|e^{\pm iq_z z}|\phi_e(z)\rangle \\
&= r_q\ \ \langle\phi_e(z)|e^{\pm iq_z z}|\phi_e(z)\rangle\,,
\end{aligned}$$

where

$$r_q = \langle\phi_e(\overrightarrow{\rho})|e^{\pm i\overrightarrow{q}\,.\,\overrightarrow{\rho}}|\phi_e(\overrightarrow{\rho})\rangle\,, \tag{2.27}$$

which can be written as

$$r_q = \frac{\sigma^{(1)}_{00}(q/\kappa)}{\sigma^{(1)}_{00}(0)}\,. \tag{2.28}$$

The final form of S_Q is

$$S_Q = r_q\ \ e^{(-q_z^2/4\lambda^2)}\,. \tag{2.29}$$

Projecting out the $\overrightarrow{Q}$-summation in [equation (2.24)] using the transformation

$$\sum_Q = \frac{1}{(2\pi)^3}\int_0^\infty\int_{-\infty}^\infty\int_0^{2\pi} qdq\ \ dq_z\ \ d\phi\,. \tag{2.30}$$

We arrive at the following integral-expression for the ground-state energy:

$$E_g = \epsilon_\kappa - \alpha\int_0^\infty dq\ \ r_q^2\ \ f_q\,, \tag{2.31}$$

where

$$f_q = \exp(\frac{q^2}{2\lambda^2}) \text{ erfc } (\frac{q}{\sqrt{2}\lambda}) \, , \tag{2.32}$$

with (erfc) denoting the complementary error function. In order to obtain the binding energy, we numerically minimize [equation (2.31)] with respect to the variational parameters μ and λ. Then substituting the minimized value of E_g in the relation of binding energy which is defined as

$$\epsilon_p = (j_{0,1}/R)^2 - E_g \, . \tag{2.33}$$

By using Maple Programme **9.5**, we obtain these values that agree with results which was obtained by Erçelebi A. and Senger R. T. [27] such as, for a wire with $\alpha = 3$ and $R = 1$, we obtain $\epsilon_p = 3.34$.

For thinner wires the binding energy gets naturally deeper since the electronic wave function becomes even more localized in all directions perpendicular to the wire axis. We obtain $\epsilon_p = 5.51$ when $R = 0.5$ and $\epsilon_p = 9.98$ when $R = 0.2$.

A comparison of these values with the corresponding three- and two-dimensional values by using [equations (1.10), (1.11)].

We find that $\epsilon_p^{(3D)} = 0.955$, and $\epsilon_p^{(2D)} = 3.534$.

This means that the polaron binding energy is much greater when effective dimensionality is reduced from three to one than when reduced from three to two.

Under the assumption of perfect confinement the ground-state binding energy is given as a function of the wire radius and the electron-phonon interaction strength (α).

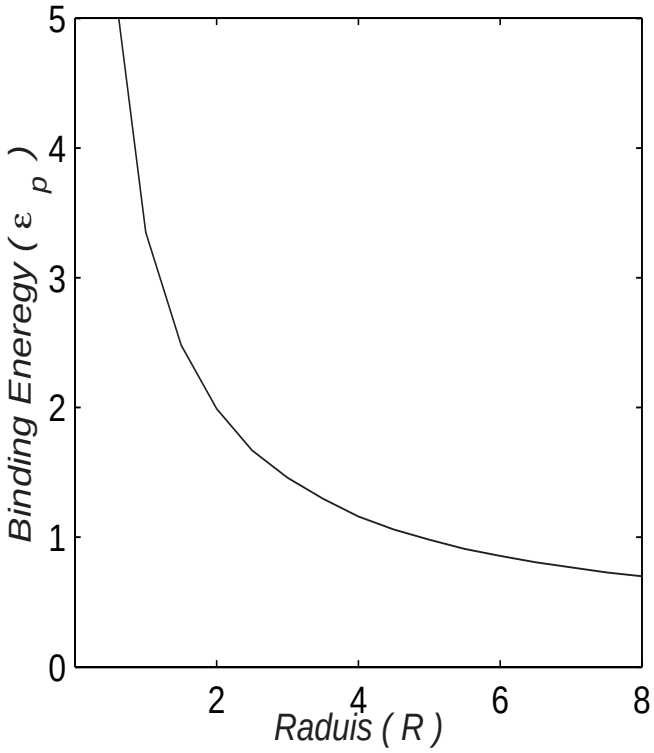

Figure 2.1: The binding energy ϵ_p as a function of the radius of the wire R.

In the Figure (2.1) we plot the binding energy ϵ_p, against the wire radius R. As it is clear from the figure, the binding energy decreases as the radius of the wire becomes larger. It means that small radius leads to large confinement for the polaron so the binding energy becomes larger.

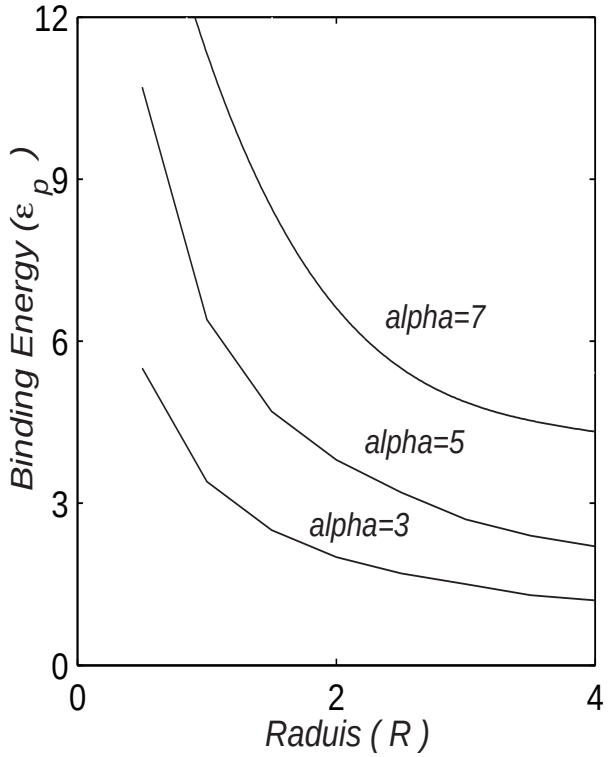

Figure 2.2: The binding energy ϵ_p as a function of the radius of the wire R with different values of α

In the Figure (2.2) we plot the binding energy versus for different values of the polaron coupling constant (α).

As shown in the figure, the growth rates of ϵ_p are moderate for large R, and when R is turned to smaller values, ϵ_p are observed to increase. We have almost an exponential decay of the binding energy as a function of R.

Besides, the binding energy for large value of radius when $\alpha = 7$ is larger than its value when $\alpha = 5, 3$ that because the enhancement of the strength of the coupling constant on the electron-phonon interaction.

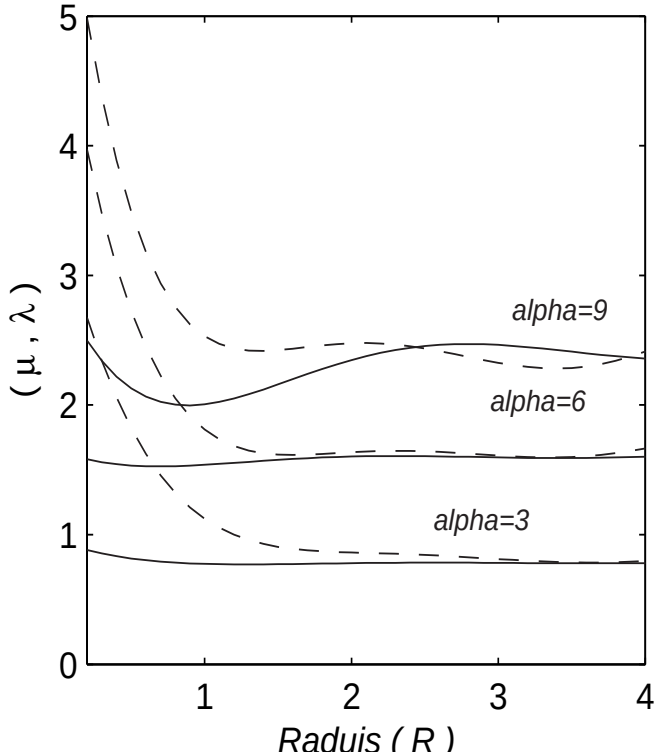

Figure 2.3: The variational parameter μ (solid curve) and λ (dashed curve) as a function of the wire radius R

When we study the relation between the variational parameters μ, λ and the radius of the wire R, we obtain the curves as in the figure (2.3). This family of the curves is plotted for $\alpha = 3, 6$ and 9 respectively.

From the figure, it is clear that for large wire radii the curves for μ and λ both have the same value (nearly). And as R is small, the curves begin to split, depicting the anisotropy due to the confinement imposed by the wire boundary.

The two parameters λ, μ represent the presence of the wave functions of the polaron in all directions of the space (along z-axis, and in the $x - y$ plane).

So from figure (2.3) we note that at large values of R (the case approaches the bulk limit), $\lambda = \mu$, which means that, the wave functions of the polaron are presented in all directions. But for small values of R, it is clear that $\lambda > \mu$ which means that the probability of the presence of the wave function of the polaron along z-axis is larger than in $x - y$ plane. This is due to the confinement of the polaron which is caused

by the rigid boundary of the wire.

For a complementary understanding of the variation of the spatial extent of the polaron in the lateral and longitudinal directions, we also display in [Fig.(2.4)] the measures of localization of the electron coordinates expressed in terms of the corresponding root-mean-square (r.m.s) values which are given by

$$\xi_\rho = \{\langle\phi_e|\rho^2|\phi_e\rangle\}^{(\frac{1}{2})} = \kappa^{-1}\sqrt{\sigma_{00}^{(3)}/\sigma_{00}^{(1)}}\,, \tag{2.34}$$

and

$$\xi_z = \{\langle\phi_e|z^2|\phi_e\rangle\}^{(\frac{1}{2})} = (2\lambda^2)^{-\frac{1}{2}}\,. \tag{2.35}$$

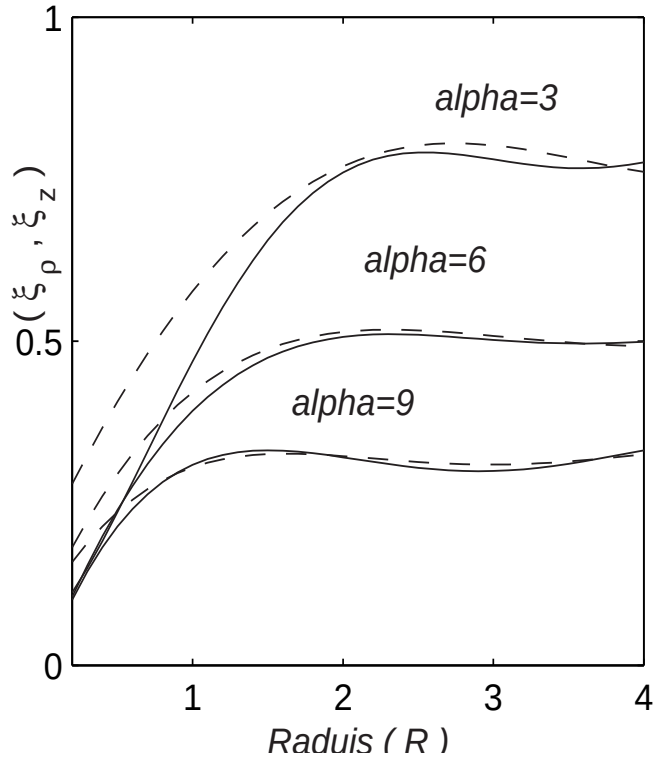

Figure 2.4: The spatial extends ξ_ρ (solid curve) and ξ_z (dashed curve) of the polaron as a function of the wire radius R

We plot the relation between the parameters ξ_ρ, ξ_z as a function of R. Thus the figure includes an implicit coupling between the transverse and longitudinal coordinates of the electron.

When we examine the family of curves for μ and λ and for ξ_ρ and ξ_z, we see that, even though there is no geometric confinement along the wire axis, the axial extent of the polaron shrinks inward contrary to what one might have expected, it means that Figure (2.4) explains the presence of the polaron and its localization in the wire with changing of the radius of the wire. It is clear that, going from the bulk case to the quasi-one dimensional limit (Q1D) there comes about a competitive interrelation between whether the charge distribution (and hence the lattice deformation) will condense onto the origin (the polaron center) or will expand to relax itself in the longitudinal directions along the wire axis.

As we note in this figure the effect of radius on the binding energy is clear when $\alpha = 3$, but when $\alpha = 6, 9$ the effect of radius is not clear, because the dominant is

for α. It means that small value of α and more confinements leads to the so-called pseudo-strong coupling.

Chapter 3

Mixed-Coupling Approximation

3.1 Theory

We consider the interaction of a confined electron with bulk (LO) phonons in cylindrical (QWW) with infinite rigid boundary potential, in which we refer to the case of an electron confined laterally within a free-stand tubular geometry with infinite boundary potential at radius R. In this chapter, we explain the so-called mixed-coupling approximation [29]. As we have seen in chapter (2), in thin wires, the polaron cloud becomes squeezed towards the wire axis from 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 (from the rigid boundary of the wire) [29]. The Mixed-Coupling Approximation, means that, one has adiabatic (strong-coupling) condition obtained in the two transverse axis and weak-coupling along the third direction (z)-axis.

As a result of this we treat the problem using two successive transformations with a variational method consisting of a strong-coupling characterization imposed in the lateral direction ($x-y$) plane, and a weak-coupling LLP-counterpart along the length of the wire.

In our calculations we begin with the Fröhlich Hamiltonian, with the units we used in chapter (2).

We rewrite the Hamiltonian Fröhlich of the problem given in [equation (2.1)] as

$$H = H_e + \sum_Q a_Q^\dagger a_Q + H_{e-ph} \,, \tag{3.1}$$

where

$$H_e = -\frac{1}{\rho}\frac{\partial}{\partial\rho}(\rho\frac{\partial}{\partial\rho}) - \frac{\partial^2}{\partial z^2} \,, \tag{3.2}$$

is the electron part, and

$$H_{e-ph} = \sum_Q V_Q[a_Q \exp(i\overrightarrow{q}.\overrightarrow{\rho} + iq_z z) + a_Q^\dagger \exp(-(i\overrightarrow{q}.\overrightarrow{\rho} + iq_z z))] \,, \tag{3.3}$$

is the Fröhlich interaction in which the coordinates $\overrightarrow{\rho}$ and z give the electron position.

To account for the cylindrical confinement with zero potential inside, and infinitely rigid boundary at $(\rho = R)$, we shall impose the lateral wave function of the electron to be given in the product form

$$\phi_e(\rho) = n_\rho J_0(\kappa\rho)\exp(-\frac{1}{2}\mu^2\rho^2) \,, \tag{3.4}$$

where the constant n_ρ serves for normalization.

The total momentum along the wire axis is given as

$$P_z = -i\frac{\partial}{\partial z} + \Pi_z \,, \tag{3.5}$$

in which

$$\Pi_z = \sum_Q q_z a_Q^\dagger a_Q \,, \tag{3.6}$$

refers to the phonon momentum along the z-axis [29].

Using the LLP-unitary transformation [7], it is possible to transform to a representation in which the relevant coordinate of the electron z is totally eliminated. For this purpose, we apply the fist (L.L.P) transformation that is,

$$U_1 = \exp\{i(P_z - \Pi_z)z\} \tag{3.7}$$

The Hamiltonian [equation(3.1)] will conforms to H' as $H' = U_1^{-1} H U_1$ according to these equations and using the identity [equation(2.15)] we obtain

$$U_1^{-1} p_z U_1 = P_z - \sum_Q q_z a_Q^\dagger a_Q + p_z \,, \tag{3.8}$$

where p_z, and P_z are the momentum of the electron, and the total momentum of the polaron in z-direction, respectively. Also,

$$U_1^{-1} a_Q U_1 = a_Q e^{-iq_z z} \,, \tag{3.9}$$

$$U_1^{-1}(-\frac{1}{\rho}\frac{\partial}{\partial\rho}(\rho\frac{\partial}{\partial\rho}))U_1 = -\frac{1}{\rho}\frac{\partial}{\partial\rho}(\rho\frac{\partial}{\partial\rho}) \,, \tag{3.10}$$

and

$$\begin{aligned} U_1^{-1}(-\frac{\partial^2}{\partial z^2})U_1 &= (P_z - \sum_Q q_z a_Q^\dagger a_Q)^2 \\ &= (P_z - \Pi_z)^2 \,. \end{aligned} \tag{3.11}$$

Because of slow electron $p_z \simeq 0$ [7], this will be used to simplify our calculations. The Hamiltonian of phonons will remain without changing as

$$U_1^{-1} \sum_Q a_Q^\dagger a_Q U_1 = \sum_Q a_Q^\dagger a_Q \,, \tag{3.12}$$

and the Hamiltonian of electron-phonon interaction becomes

$$U_1^{-1} \sum_Q V_Q [a_Q e^{i\vec{Q}.\vec{r}} + a_Q^\dagger e^{-i\vec{Q}.\vec{r}}] U_1 = \sum_Q V_Q [a_Q e^{i\vec{q}.\vec{\rho}} + a_Q^\dagger e^{-i\vec{q}.\vec{\rho}}] \,. \tag{3.13}$$

From previous transformation, it is clear that the coordinate of the electron along z-axis is eliminated. So, H of the polaron under the first (L.L.P) transformation will transform to

$$H' = U_1^{-1} H U_1 \,,$$

which equal to,

$$\begin{aligned} H' &= -\frac{1}{\rho}\frac{\partial}{\partial\rho}(\rho\frac{\partial}{\partial\rho}) + (P_z - \Pi_z)^2 \\ &+ \sum_Q a_Q^\dagger a_Q + \sum_Q V_Q [a_Q e^{i\vec{q}.\vec{\rho}} + a_Q^\dagger e^{-i\vec{q}.\vec{\rho}}] \,. \end{aligned} \tag{3.14}$$

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, $E_g(P_z)$, thus obtained can then be expanded in a power series to second order in the momentum, that is,

$$E_g(P_z) \simeq E_g(0) + cP_z^2 \,, \tag{3.15}$$

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_g a variational approach is adopted, and the polaron ground wave state is postulated in a product ansatz consisting of the electron and lattice parts as,

$$\Psi_g = \Phi_e U_2 |0\rangle \,, \tag{3.16}$$

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

$$U_2 = \exp \sum_Q u_Q(\Phi_e)[a_Q - a_Q^\dagger] \,, \tag{3.17}$$

is the second (L.L.P) canonical (displaced oscillator) transformation in which the function $u_Q(\Phi_e)$ will be determined variationally, and $\Phi_e = U_1\phi_e$, where U_1 is given in [equation (3.7)].

Thus, subjecting the Hamiltonian further to the transformation

$$H'' \longrightarrow U_2^{-1} H' U_2 \,,$$

we will obtain the following results:

$$U_2^{-1} - (\frac{1}{\rho}\frac{\partial}{\partial\rho}(\rho\frac{\partial}{\partial\rho}))U_2 = -\frac{1}{\rho}\frac{\partial}{\partial\rho}(\rho\frac{\partial}{\partial\rho}) \,, \tag{3.18}$$

$$U_2^{-1} a_Q U_2 = a_Q - \sum_Q u_Q \,,$$

$$U_2^{-1} \sum_Q a_Q^\dagger a_Q U_2 = \sum_Q a_Q^\dagger a_Q + \sum_Q u_Q^2 - \sum_Q u_Q(a_Q + a_Q^\dagger) \,, \tag{3.19}$$

and

$$\begin{aligned} U_2^{-1}(P_z - \Pi_z)U_2 &= [P_z - \sum_Q q_z(a_Q^\dagger - u_Q)(a_Q - u_Q)] \\ &= [P_z - \sum_Q q_z a_Q^\dagger a_Q + \sum_Q q_z u_Q(a_Q^\dagger + a_Q) - \sum_Q q_z u_Q^2] \\ &= [P_z - \Pi_z + \Pi_z^{(1)} - \Pi_z^{(0)}] \,. \end{aligned} \tag{3.20}$$

Then

$$U_2^{-1}(P_z-\Pi_z)^2U_2 = (P_z-\Pi_z)^2-2P_z\Pi_z^{(0)}+2\Pi_z^{(0)}\Pi_z+[\Pi_z^{(0)}]^2 \quad (3.21)$$
$$+ (\Pi_z^{(1)}-2\Pi_z)\Pi_z^{(1)}+2(P_z-\Pi_z^{(0)})\Pi_z^{(1)}\,,$$

where Π_z is given in [equation (3.6)], and

$$\Pi_z^{(1)} = \sum_Q q_z u_Q(a_Q^\dagger+a_Q)\,, \quad (3.22)$$

$$\Pi_z^{(0)} = \sum_Q q_z u_Q^2\,, \quad (3.23)$$

Also,

$$U_2^{-1}(\sum_Q V_Q(a_Q e^{i\vec{q}\cdot\vec{\rho}}+a_Q^\dagger e^{-i\vec{q}\cdot\vec{\rho}}))U_2 = -\sum_Q V_Q u_Q(e^{i\vec{q}\cdot\vec{\rho}}+e^{-i\vec{q}\cdot\vec{\rho}}) \quad (3.24)$$
$$+ \sum_Q V_Q(a_Q e^{i\vec{q}\cdot\vec{\rho}}+a_Q^\dagger e^{-i\vec{q}\cdot\vec{\rho}})\,.$$

The last equations will form the modified Hamiltonian as

$$H'' = -\frac{1}{\rho}\frac{\partial}{\partial\rho}(\rho\frac{\partial}{\partial\rho})+(P_z-\Pi_z)^2-2P_z\Pi_z^{(0)}+2\Pi_z^{(0)}\Pi_z+[\Pi_z^{(0)}]^2 \quad (3.25)$$
$$+ (\Pi_z^{(1)}-2\Pi_z)\Pi_z^{(1)}+2(P_z-\Pi_z^{(0)})\Pi_z^{(1)}-\sum_Q u_Q(a_Q+a_Q^\dagger)+\sum_Q u_Q^2$$
$$+ \sum_Q a_Q^\dagger a_Q+\sum_Q V_Q(a_Q e^{i\vec{q}\cdot\vec{\rho}}+a_Q^\dagger e^{-i\vec{q}\cdot\vec{\rho}})-\sum_Q V_Q u_Q[e^{i\vec{q}\cdot\vec{\rho}}+e^{-i\vec{q}\cdot\vec{\rho}}]\,.$$

The Hamiltonian then is simplified to

$$H'' = -\frac{1}{\rho}\frac{\partial}{\partial\rho}(\rho\frac{\partial}{\partial\rho})+(P_z-\Pi_z)^2+[\Pi_z^{(0)}]^2+\sum_Q a_Q^\dagger a_Q \quad (3.26)$$
$$+ \sum_Q u_Q^2+(\Pi_z^{(1)}-2\Pi_z)\Pi_z^{(1)}+2(P_z-\Pi_z^{(0)})\Pi_z^{(1)}+2\Pi_z^{(0)}\Pi_z-2P_z\Pi_z^{(0)}$$
$$- \sum_Q V_Q u_Q[e^{i\vec{q}\cdot\vec{\rho}}+e^{-i\vec{q}\cdot\vec{\rho}}]+\sum_Q[V_Q e^{i\vec{q}\cdot\vec{\rho}}-u_Q]a_Q+\sum_Q[V_Q e^{-i\vec{q}\cdot\vec{\rho}}-u_Q]a_Q^\dagger\,.$$

Now the ground-state energy of the polaron is given by

$$E_g = \langle\Psi_g|H|\Psi_g\rangle \quad (3.27)$$
$$= \langle 0|\langle\phi_e|U_2^{-1}U_1^{-1}HU_1U_2|\phi_e\rangle|0\rangle$$
$$= \langle 0|\langle\phi_e|U_2^{-1}H'U_2|\phi_e\rangle|0\rangle$$
$$= \langle 0|\langle\phi_e|H''|\phi_e\rangle|0\rangle\,,$$

where

$$\Psi_g = \Phi_e U_2|0\rangle = U_1 U_2 \phi_e|0\rangle \ .$$

In which Φ_e is defined as $U_1\phi_e$, U_1 is the first (L.L.P) transformation, and ϕ_e is the wave function of electron which is given in [equation (3.4)]. Using [equations (3.26), (3.27)] we get

$$\begin{aligned} E_g &= \langle\phi_e| - \frac{1}{\rho}\frac{\partial}{\partial\rho}(\rho\frac{\partial}{\partial\rho})|\phi_e\rangle + P_z^2 - 2P_z\Pi_z^{(0)} + [\Pi_z^{(0)}]^2 \\ &+ \sum_Q u_Q^2(1+q_z^2) - \sum_Q V_Q u_Q \langle\phi_e|e^{i\vec{q}\,.\,\vec{\rho}}|\phi_e\rangle - \sum_Q V_Q u_Q \langle\phi_e|e^{-i\vec{q}\,.\,\vec{\rho}}|\phi_e\rangle \ . \end{aligned} \tag{3.28}$$

Defining

$$\epsilon_\kappa = \langle\phi_e| - \frac{1}{\rho}\frac{\partial}{\partial\rho}(\rho\frac{\partial}{\partial\rho})|\phi_e\rangle \ , \tag{3.29}$$

and

$$S_q = \langle\phi_e|e^{\pm i\vec{q}\,.\,\vec{\rho}}|\phi_e\rangle \ , \tag{3.30}$$

we obtain

$$\begin{aligned} E_g &= \epsilon_\kappa + P_z^2 - 2P_z\Pi_z^{(0)} + [\Pi_z^{(0)}]^2 \\ &+ \sum_Q u_Q^2(1+q_z^2) - 2\sum_Q V_Q u_Q S_q \ . \end{aligned} \tag{3.31}$$

The variational function u_Q minimizing E_g [equation(3.31)] is found by the following non-linear equation:

$$[1 - 2(P_z - \Pi_z^{(0)})q_z + q_z^2]u_Q - V_Q S_q = 0 \ , \tag{3.32}$$

which can easily be handled with the consideration that, from symmetry arguments, the term $\Pi_z^{(0)}$ in [equation(3.23)] can only differ from the total momentum by a scalar factor. So we can write

$$\Pi_z^{(0)} = \eta P_z \ . \tag{3.33}$$

Substituting back in [equation (3.32)], for $\Pi_z^{(0)}$. We can obtain u_Q as

$$u_Q = \frac{V_Q S_q}{1 - 2(1-\eta)P_z q_z + q_z^2} \ , \tag{3.34}$$

$$\begin{aligned} \Pi_z^{(0)} &= \sum_Q q_z u_Q^2 \,, \\ \eta P_z &= \frac{V_Q^2 S_q^2 q_z}{[1-2(1-\eta)P_z q_z + q_z^2]^2} \,. \end{aligned} \tag{3.35}$$

The ground-state energy of the polaron becomes

$$E_g = \epsilon_\kappa - \sum_Q V_Q^2 S_q^2 \frac{1}{1+q_z^2} + (1-\eta)^2 P_z^2 \,. \tag{3.36}$$

Comparing between [equation (3.15)] and [equation (3.36)], we can find $E_g(0)$ as

$$E_g = \epsilon_\kappa - \sum_Q V_Q^2 S_q^2 \frac{1}{1+q_z^2} \,, \tag{3.37}$$

from which we identity the effective mass of polaron as

$$m_p = \frac{1}{(1-\eta)^2} \,. \tag{3.38}$$

Projecting out the $\overrightarrow{Q}$-summation in [equation (3.37)], and using [equation (2.30)] we finally arrive at the following integral-expressions for the ground-state energy of the polaron as:

$$E_g = \epsilon_\kappa - \alpha \int_0^\infty dq \frac{1}{1+q} S_q^2 \,, \tag{3.39}$$

where

$$\epsilon_\kappa = \kappa^2 + \mu^2 \{ 2 - \frac{2\sigma_{10}^{(2)}(0) - (\mu/\kappa)^2 \sigma_{00}^{(3)}(0)}{\sigma_{00}^{(1)}(0)} \} \,, \tag{3.40}$$

and

$$S_q = \frac{\sigma_{00}^{(1)}(q/\kappa)}{\sigma_{00}^{(1)}(0)} \,, \tag{3.41}$$

where the expression of $\sigma_{mm'}^{(n)}(x)$ is given in [equation (2.25)]. The binding energy of the polaron is again given by

$$\epsilon_p = (j_{0,1}/R)^2 - E_g \,. \tag{3.42}$$

3.2 Results

Before we proceed with our main theme we should remark that, if the first transformation were by-passed (U_1 were selected as the identity operator), the theory would

then diverse to the strong-coupling approximation for which simultaneous optimizations with respect to Φ_e and $u_Q(\Phi_e)$ correspond to the self-trapping picture of the polaron where the electron distribution and the lattice polarization influence each other in such a way that a stable relaxed state is eventually attained.

The variational parameter μ which minimizes E_g can be performed by numerical techniques. In the following we give our results in terms of binding energy of the polaron, [equation (3.42)].

It should be noted 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 confinement in the lateral direction resulting in a "pseudo-strong" coupling characterization in the lateral plane [29].

However, the effective phonon coupling in the longitudinal direction will be assumed to remain weak, this because the (L.L.P) weak-coupling condition that we have undertaken for the polaron behavior 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 [29].

Selecting $\alpha = 1$, an intermediate coupling strength for which the (L.L.P) theory proves to work rather well, we display the results of the the present theory as a function of the wire radius for $R \leq 2$.

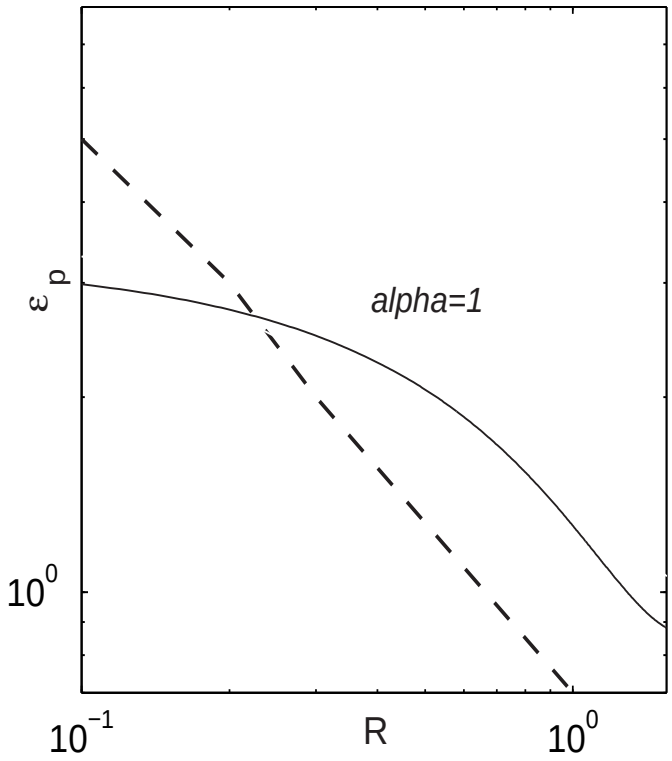

Figure 3.1: The binding energy as a function of the wire radius for $\alpha = 1$. The solid and dashed curves display the results of the mixed-coupling and pure strong-coupling theories, respectively.

In Figure (3.1) we also supply the energy values of the pure strong-coupling treatment of the same problem where the canonical transformation [equation(3.7)] is by-passed and the electron wave function [equation(3.4)] is extended to include a gaussian spread along the wire axis as

$$\phi_e(\rho) \rightarrow \phi_e(\rho) \exp(-\frac{1}{2}\lambda^2 z^2) \ ,$$

as we treated in chapter (2), using strong-coupling theory.
In this Figure, we plot the relation between the binding energy and the radius for the mixed-coupling and the strong-coupling.
A comparison of the two theories explains that the strong coupling binding energy values lie below the present results except for very small values of R simply because, for an intermediate coupling strength like $\alpha = 1$, the pure strong approach can be convenient at only very high degrees of confinement where the pseudo-enhancement

in α is dominantly realized [27].

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 [29], 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.

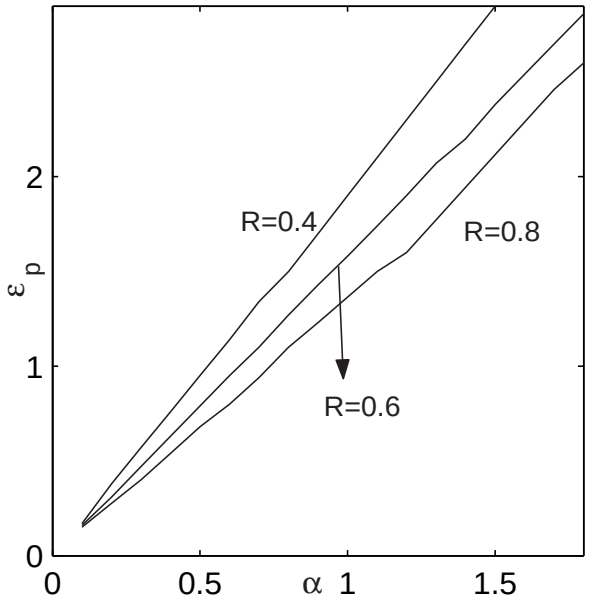

Figure 3.2: The binding energy ϵ_p as a function of α in the weak/intermediate coupling regime. The set of curves from top to bottom are for $R = 0.4$, 0.6 and 0.8

In Figure (3.2) we plot the relation between the binding energy and the coupling-constant (α) for different radius values. It is clear that, when the coupling-constant (α) increases, the binding energy increases because the strong interaction between electron and phonon which becomes important for small value of R.
Small values of radius, increase the confinement of the polaron which makes more enhancement of the interaction between electron-phonon so the binding energy becomes larger.

Chapter 4

The Optical Polaron in a Quantum Well with Tunable Barrier Potential

4.1 The Optical Polaron in a Spherically Box-Type Confinement

The usual Fröhlich polaron Hamiltonian in a symmetric dot with a parabolic potential $V(r)$ is

$$H = p^2 + \frac{1}{4}\omega^2 r^2 + \sum_Q a_Q^\dagger a_Q + \sum_Q V_Q[a_Q e^{(i\vec{Q}.\vec{r})} + a_Q^\dagger e^{(-i\vec{Q}.\vec{r})}] \,, \tag{4.1}$$

where $\mathbf{p}, \mathbf{r}$ represent the momentum and the position of the electron respectively, and ω represents the strength of the quantum dot potential that serves for the measure of the degree of confinement of the electrons, which is given by

$$\omega = (k/m\omega_{LO}^2)^{1/2} \,,$$

in which k denotes the force constant, and $(2m = \omega_{LO} = 1)$ [in Fröhlich units].
For the mixed-coupling approximation to be adopted for such a problem we propose a modification to the first LLP-transformation. The proposed U_1 is

$$U_1 = \exp[i(\mathbf{P} - \Pi).b\mathbf{r}] \,, \tag{4.2}$$

where b is inserted as another variational parameter. This parameter is supposed to trace the problem from the strong-coupling limit ($b = 0$) to the weak-coupling limit ($b = 1$).

Using the modified LLP-transformations defined in [equation (4.2)], and the Hamiltonian in [equation (4.1)] we obtain

$$\begin{aligned} H' &= U_1^{-1} H U_1 \\ &= b^2(P-\Pi)^2 + p^2 + 2bp(P-\Pi) + \frac{1}{4}\omega^2 r^2 + \sum_Q a_Q^\dagger a_Q \\ &+ \sum_Q V_Q [a_Q e^{i(1-b)\overrightarrow{Q}.\overrightarrow{r}} + a_Q^\dagger e^{-i(1-b)\overrightarrow{Q}.\overrightarrow{r}}] \,. \end{aligned} \tag{4.3}$$

From [equation (4.3)] it is clear that when $b = 1$, the terms $e^{\pm i\overrightarrow{Q}.\overrightarrow{r}}$ will be eliminated, leading to the weak-coupling approach. Now applying the second LLP-transformation U_2 of [equation (3.17)], the Hamiltonian of [equation (4.3)] transforms as

$$H'' \rightarrow U_2^{-1} H' U_2 \,.$$

Explicitly

$$\begin{aligned} H'' &= U_2^{-1} H' U_2 \\ &= p^2 + \frac{1}{4}\omega^2 r^2 + b^2(P-\Pi)^2 + b^2[\Pi^{(0)}]^2 + \sum_Q a_Q^\dagger a_Q \\ &+ \sum_Q u_Q^2 + b^2(\Pi^{(1)} - 2\Pi)\Pi^{(1)} + 2b^2(P - \Pi^{(0)})\Pi^{(1)} + 2b^2\Pi^{(0)}\Pi - 2b^2 P\Pi^{(0)} \\ &- \sum_Q V_Q u_Q [e^{i(1-b)\overrightarrow{Q}.\overrightarrow{r}} + e^{-i(1-b)\overrightarrow{Q}.\overrightarrow{r}}] + 2bp(P - \Pi + \Pi^{(1)} - \Pi^{(0)}) \\ &+ \sum_Q [V_Q e^{i(1-b)\overrightarrow{Q}.\overrightarrow{r}} - u_Q] a_Q + \sum_Q [V_Q e^{-i(1-b)\overrightarrow{Q}.\overrightarrow{r}} - u_Q] a_Q^\dagger \,, \end{aligned} \tag{4.4}$$

The ground-state energy can be obtained as

$$\begin{aligned} E_g &= \langle 0_e|p^2|0_e\rangle + \langle 0_e|\frac{1}{4}\omega^2 r^2|0_e\rangle + b^2 P^2 - 2b^2 P\Pi^{(0)} \\ &+ b^2[\Pi^{(0)}]^2 + \sum_Q u_Q^2(1 + b^2 Q^2) + \langle 0_e|\langle 0_{ph}|2bp(P - \Pi + \Pi^{(1)} - \Pi^{(0)})|0_{ph}\rangle|0_e\rangle \\ &- \sum_Q V_Q u_Q \langle 0_e|e^{-i(1-b)\overrightarrow{Q}.\overrightarrow{r}}|0_e\rangle - \sum_Q V_Q u_Q \langle 0_e|e^{i(1-b)\overrightarrow{Q}.\overrightarrow{r}}|0_e\rangle \,. \end{aligned} \tag{4.5}$$

Expressing the coordinates and momenta of the electron as

$$p_\mu = \lambda_1^{\frac{1}{2}}(\sigma_\mu + \sigma_\mu^\dagger) , \tag{4.6}$$

$$x_\mu = i/\lambda_1^{-\frac{1}{2}}(\sigma_\mu - \sigma_\mu^\dagger) , \tag{4.7}$$

$$p_z = \lambda_2^{\frac{1}{2}}(\sigma_z + \sigma_z^\dagger) , \tag{4.8}$$

$$z = i/\lambda_2^{-\frac{1}{2}}(\sigma_z - \sigma_z^\dagger) , \tag{4.9}$$

where the index μ refers to the x and y directions, λ_1, λ_2 are variational parameters, and $\sigma^\dagger, (\sigma)$ are the creation (and annihilation) operators for electron.
Defining the ground-state $|0\rangle$ by

$$\begin{aligned} \sigma_\mu|0_e\rangle &= \sigma_z|0_e\rangle = 0 , \\ a_Q|0_{ph}\rangle &= 0 , \\ \langle 0|0\rangle &= 1 , \end{aligned}$$

and after performing straightforward calculation we obtain the ground-state energy of the polaron as

$$\begin{aligned} E_g &= \frac{\lambda_1}{2} + \frac{\omega^2}{2\lambda_1} + \frac{\lambda_2}{4} + \frac{\omega^2}{4\lambda_2} + b^2P^2 - 2b^2P\Pi^{(0)} \\ &+ b^2[\Pi^{(0)}]^2 + \sum_Q u_Q^2(1 + b^2Q^2) - 2\sum_Q V_Q u_Q S_Q , \end{aligned} \tag{4.10}$$

where

$$S_Q = \langle 0_e|e^{\pm i(1-b)\overrightarrow{Q}.\overrightarrow{r}}|0_e\rangle , \tag{4.11}$$

which is found to be

$$S_Q = e^{-(1-b)^2q^2/2\lambda_1}e^{-(1-b)^2q_z^2/2\lambda_2} . \tag{4.12}$$

The variational function u_Q minimizing [equation (4.10)] is found to be given by the following equation:

$$[1 + b^2Q^2]u_Q - V_Q S_Q = 0 . \tag{4.13}$$

The momentum $\Pi^{(0)}$ differs from the total momentum by a scalar factor as

$$\Pi^{(0)} = \eta\mathbf{P} . \tag{4.14}$$

So we can write u_Q as

$$u_Q = \frac{V_Q S_Q}{1 + b^2 Q^2} \,. \tag{4.15}$$

In which the unknown scalar, η is determined by the equation

$$\begin{aligned} \Pi^{(0)} &= \sum_Q \mathbf{Q} u_Q^2 \,, \\ \eta \mathbf{P} &= \frac{\mathbf{Q} V_Q^2 S_Q^2}{[1 + b^2 Q^2]^2} \,. \end{aligned} \tag{4.16}$$

Substituting back in [equation (4.10)], we obtain the following results:

$$E_g = \frac{\lambda_1}{2} + \frac{\omega^2}{2\lambda_1} + \frac{\lambda_2}{4} + \frac{\omega^2}{4\lambda_2} - \sum_Q \frac{S_Q^2 V_Q^2}{[1 + b^2 Q^2]^2} + b^2 (1 - \eta)^2 P^2 \,. \tag{4.17}$$

But E_g may be well represented by the first two terms of a power series expansion in P^2 as

$$E_g = E_g(0) + \beta P^2/2 + ...O(P^4) + ... \tag{4.18}$$

The effective mass of the polaron is then β^{-1}.

By comparing [equations (4.17) and (4.18)] we give the expression for the ground-state energy of the polaron as

$$E_g(0) = \frac{\lambda_1}{2} + \frac{\omega^2}{2\lambda_1} + \frac{\lambda_2}{4} + \frac{\omega^2}{4\lambda_2} - \sum_Q \frac{V_Q^2 S_Q^2}{[1 + b^2 Q^2]} \,, \tag{4.19}$$

and the mass of the polaron as

$$m_p = \frac{1}{b^2 (1 - \eta)^2} \,. \tag{4.20}$$

Using the expression for S_Q in [equation (4.12)], the ground-state of the energy becomes

$$E_g = \frac{\lambda_1}{2} + \frac{\omega^2}{2\lambda_1} + \frac{\lambda_2}{4} + \frac{\omega^2}{4\lambda_2} - \sum_Q \frac{V_Q^2 e^{-(1-b)^2 q^2/\lambda_1} e^{-(1-b)^2 q_z^2/\lambda_2}}{[1 + b^2 Q^2]} \,. \tag{4.21}$$

Thus [equation (4.21)] explains the general formula for the ground-state of the confined polaron. This formula enables us to find the binding energy of the 3D polaron in both weak- and strong-coupling range.

Before going on in the calculation for all value of α, we want to test the theory for

the extreme limits of the approach. In the limit $b \to 0$, the ground-state energy gives the adiabatic (strong) limit as

$$E_g = \frac{\lambda_1}{2} + \frac{\omega^2}{2\lambda_1} + \frac{\lambda_2}{4} + \frac{\omega^2}{4\lambda_2} - \sum_Q V_Q^2 e^{-q^2/\lambda_1} e^{-q_z^2/\lambda_2} \,. \tag{4.22}$$

Projecting out the $\overrightarrow{Q}$-summation in [equation (4.22)] we obtain

$$E_g = \frac{\lambda_1}{2} + \frac{\omega^2}{2\lambda_1} + \frac{\lambda_2}{4} + \frac{\omega^2}{4\lambda_2} - \frac{\alpha}{\sqrt{\pi}} \sqrt{\frac{\lambda_1 \lambda_2}{\lambda_2 - \lambda_1}} \tan^{-1} \sqrt{\frac{\lambda_2}{\lambda_1} - 1} \,, \tag{4.23}$$

and for the polaron binding energy, we have

$$\epsilon_p = \frac{3}{2}\omega - E_g \,. \tag{4.24}$$

For $\omega = 0$, we obtain numerically that

$$\lambda_1 = \lambda_2 = \frac{4\alpha^2}{9\pi} \,,$$

and

$$\epsilon_p^{(3D)} = \frac{\alpha^2}{3\pi} \,, \tag{4.25}$$

which is the well-known strong-coupling result obtained in [38].

Also, in the limit $b \to 1$, the ground-state energy describes the case of weak-coupling as

$$E_g = \frac{\lambda_1}{2} + \frac{\omega^2}{2\lambda_1} + \frac{\lambda_2}{4} + \frac{\omega^2}{4\lambda_2} - \sum_Q \frac{V_Q^2}{[1 + Q^2]} \,. \tag{4.26}$$

For $\omega = 0$, we obtain $\lambda_1 = \lambda_2 \to 0$, and

$$\epsilon_p^{(3D)} = \alpha \,, \tag{4.27}$$

which is the same results for 3D polaron of Fröhlich [5]. Thus for $0 < b < 1$ we expect that our formula of the ground-state energy will describe an arbitrary coupling, this means that it will give the value of energy for any value of α.

It is important to explain the difference between the meaning of bulk polaron and polaron in spherically-box confinement. Bulk polaron is free from the potential confinement $\omega = 0$, and then the polaron will be in all directions in the space, but polaron in spherically-box confinement means ω is not equal zero ($\omega \neq 0$).

4.2 The Optical Polaron in a Slab-Like Confinement

In this section we derive an analytical expression for the ground-state energy of 2D polaron in both strong- and weak-coupling range using the Modified Mixed-Coupling Approximation. When we talk about slab-like case, we mean the 2D polaron which is free in $x-y$ plane and not free along z-axis due to the potential $(\frac{1}{4}\omega_2^2 z^2)$.

The Hamiltonian describing an electron confined in a slab-like quantum well and interacts with the bulk-optical phonons is

$$H = p_\rho^2 + p_z^2 + \frac{1}{4}\omega_2^2 z^2 + \sum_Q a_Q^\dagger a_Q + \sum_Q V_Q[a_Q e^{(i\overrightarrow{Q}.\overrightarrow{r})} + a_Q^\dagger e^{(-i\overrightarrow{Q}.\overrightarrow{r})}] \,, \tag{4.28}$$

and the potential will be only along z-axis, that is

$$V(\overrightarrow{\rho}, z) = \frac{1}{4}\omega_2^2 z^2 \,. \tag{4.29}$$

The modified first and second LLP-transformations are, respectively

$$U_1 = \exp[i(\mathbf{P}_\rho - \Pi_\rho).b\overrightarrow{\rho}] \,, \tag{4.30}$$

$$U_2 = \exp \sum_Q u_Q(\phi_e)[a_Q - a_Q^\dagger] \,, \tag{4.31}$$

where

$$\mathbf{P}_\rho = \mathbf{p}_\rho + \Pi_\rho \,, \tag{4.32}$$

and $\mathbf{p}_\rho$ represents the momentum of the electron and b is the variational parameter, which was defined in the preceding section plays an important role in changing the problem from strong-coupling approach to weak-coupling approach.

Defining Π_ρ as

$$\Pi_\rho = \sum_Q \mathbf{q} a_Q^\dagger a_Q \,, \tag{4.33}$$

which refers to the phonon momentum in $x-y$ plane.

The Hamiltonian under the first LLP-transformation will be transformed as

$$\begin{aligned} H' &= p_\rho^2 + p_z^2 + b^2(P_\rho - \Pi_\rho)^2 + \frac{1}{4}\omega^2 z^2 + \sum_Q a_Q^\dagger a_Q + 2bp_\rho[P_\rho - \Pi_\rho] \\ &+ \sum_Q V_Q[a_Q^\dagger e^{-i\overrightarrow{Q}.\overrightarrow{r}} e^{ib\overrightarrow{q}.\overrightarrow{\rho}}] + \sum_Q V_Q[a_Q e^{i\overrightarrow{Q}.\overrightarrow{r}} e^{-ib\overrightarrow{q}.\overrightarrow{\rho}}] \,. \end{aligned} \tag{4.34}$$

Which can be written as

$$\begin{aligned} H' &= p_z^2 + p_\rho^2 + b^2(P_\rho - \Pi_\rho)^2 + 2bp_\rho(P_\rho - \Pi_\rho) + \frac{1}{4}\omega_2^2 z^2 \\ &+ \sum_Q a_Q^\dagger a_Q + \sum_Q V_Q[a_Q e^{i(1-b)\overrightarrow{q}.\overrightarrow{\rho}} e^{iq_z z} + a_Q^\dagger e^{-i(1-b)\overrightarrow{q}.\overrightarrow{\rho}} e^{-iq_z z}] \,. \end{aligned} \tag{4.35}$$

Under the second LLP-transformation the Hamiltonian becomes

$$\begin{aligned} H'' &= p_\rho^2 + p_z^2 + \frac{1}{4}\omega^2 z^2 + b^2(P_\rho - \Pi_\rho)^2 + b^2[\Pi_\rho^{(0)}]^2 + \sum_Q a_Q^\dagger a_Q \\ &+ \sum_Q u_Q^2 + b^2(\Pi_\rho^{(1)} - 2\Pi_\rho)\Pi_\rho^{(1)} + 2b^2(P_\rho - \Pi_\rho^{(0)})\Pi_\rho^{(1)} + 2b^2\Pi_\rho^{(0)}\Pi_\rho - 2b^2 P_\rho \Pi_\rho^{(0)} \\ &- \sum_Q V_Q u_Q[e^{i(1-b)\overrightarrow{q}.\overrightarrow{\rho}} e^{iq_z z} + e^{-i(1-b)\overrightarrow{q}.\overrightarrow{\rho}} e^{-iq_z z}] + 2bp_\rho(P_\rho - \Pi_\rho + \Pi_\rho^{(1)} - \Pi_\rho^{(0)}) \\ &+ \sum_Q [V_Q e^{i(1-b)\overrightarrow{q}.\overrightarrow{\rho}} e^{iq_z z} - u_Q] a_Q + \sum_Q [V_Q e^{-i(1-b)\overrightarrow{q}.\overrightarrow{\rho}} e^{-iq_z z} - u_Q] a_Q^\dagger \,. \end{aligned} \tag{4.36}$$

The ground-state energy is the expectation value of H'', that is

$$E_g = \langle 0_e | \langle 0_{ph} | H'' | 0_{ph} \rangle | 0_e \rangle \,. \tag{4.37}$$

Using [equation (4.37)] we get

$$\begin{aligned} E_g &= \langle 0_e | p^2 | 0_e \rangle + \langle 0_e | \frac{1}{4}\omega_2^2 z^2 | 0_e \rangle + b^2 P_\rho^2 - 2b^2 P_\rho \Pi_\rho^{(0)} \\ &+ b^2[\Pi_\rho^{(0)}]^2 + \sum_Q u_Q^2(1 + b^2 q^2) + \langle 0_e | \langle 0_{ph} | 2bp_\rho(P_\rho - \Pi_\rho + \Pi_\rho^{(1)} - \Pi_\rho^{(0)}) | 0_{ph} \rangle | 0_e \rangle \\ &- \sum_Q V_Q u_Q \langle 0_e | e^{-i(1-b)\overrightarrow{q}.\overrightarrow{\rho}} e^{iq_z z} | 0_e \rangle - \sum_Q V_Q u_Q \langle 0_e | e^{i(1-b)\overrightarrow{q}.\overrightarrow{\rho}} e^{-iq_z z} | 0_e \rangle \,, \end{aligned} \tag{4.38}$$

or

$$\begin{aligned} E_g &= \epsilon_k + b^2 P_\rho^2 - 2b^2 P_\rho \Pi_\rho^{(0)} + b^2[\Pi_\rho^{(0)}]^2 \\ &+ \sum_Q u_Q^2(1 + b^2 q^2) - 2\sum_Q V_Q u_Q S_q \,, \end{aligned} \tag{4.39}$$

where ϵ_k is

$$\langle 0_e | p_\rho^2 + p_z^2 + \frac{1}{4}\omega^2 z^2 | 0_e \rangle \,, \tag{4.40}$$

and S_q is

$$\langle 0_e | e^{\pm i(1-b)\overrightarrow{q}.\overrightarrow{\rho}} e^{\pm iq_z z} | 0_e \rangle \,. \tag{4.41}$$

The variational function u_Q minimizing [equation (4.39)] is found to be given by the equation

$$[1 - 2b^2(P_\rho - \Pi_\rho^{(0)})q + b^2q^2]u_Q - V_Q S_q = 0 \,, \tag{4.42}$$

where $\Pi_\rho^{(0)}$ differs from the total momentum by a scalar factor

$$\Pi_\rho^{(0)} = \eta \mathbf{P}_\rho \,. \tag{4.43}$$

So we can write u_Q as

$$u_Q = \frac{S_q V_Q}{1 - 2b^2(1-\eta)qP_\rho + b^2q^2} \,. \tag{4.44}$$

In which the unknown scalar, η is determined by

$$\begin{aligned} \Pi_\rho^{(0)} &= \sum_Q q u_Q^2 \\ \eta P_\rho &= \frac{q S_q^2 V_Q^2}{[1 - 2b^2(1-\eta)qP_\rho + b^2q^2]^2} \,. \end{aligned} \tag{4.45}$$

Substituting back in [equation (4.39)] we obtain the result

$$\begin{aligned} E_g &= \epsilon_k + \sum_Q \frac{S_q^2 V_Q^2 (1 + b^2q^2)}{[1 - 2b^2(1-\eta)qP_\rho + b^2q^2]^2} \\ &- 2\sum_Q \frac{S_q^2 V_Q^2}{[1 - 2b^2(1-\eta)qP_\rho + b^2q^2]} + b^2(1-\eta)^2 P_\rho^2 \,. \end{aligned} \tag{4.46}$$

But E_g may be well represented by the first two terms of a power series expansion in P^2 as

$$E_g(P) = E_g(0) + cP^2/2 + ...O(P^4) + ... \tag{4.47}$$

The effective mass of the polaron is then c^{-1}.

By comparing [equations (4.46) and (4.47)] we give the expression for the ground-state energy as

$$E_g(0) = \epsilon_k - \sum_Q \frac{S_q^2 V_Q^2}{[1 + b^2q^2]} \,, \tag{4.48}$$

and the mass of the polaron is

$$m_p = \frac{1}{b^2(1-\eta)^2} \,. \tag{4.49}$$

To find ϵ_k and S_{qz} we express the coordinate and momentum of the electron by the creation and annihilation operators using the [equations (4.6), (4.7), (4.8), (4.9)].

Then, ϵ_k and S_q are found to be

$$\epsilon_k = \frac{\omega_2^2}{4\lambda_2} + \frac{\lambda_1}{2} + \frac{\lambda_2}{4}\,, \tag{4.50}$$

$$S_q = \exp^{-(1-b)q^2/2\lambda_1} \exp^{-q_z^2/2\lambda_2}\,, \tag{4.51}$$

where λ_1, λ_2 are two variational parameters.

So, E_g can be written as

$$E_g = \frac{\omega_2^2}{4\lambda_2} + \frac{\lambda_1}{2} + \frac{\lambda_2}{4} - \sum_Q V_Q^2 \frac{e^{-(1-b)q^2/\lambda_1} e^{-q_z^2/\lambda_2}}{[1+b^2q^2]}\,. \tag{4.52}$$

The binding energy of 2D polaron is given as

$$\epsilon_p = \frac{\omega_2}{2} - E_g\,. \tag{4.53}$$

This formula of the ground-state energy is used to find the binding energy for 2D polaron in both strong- and weak-coupling range, the calculations depend on the values of b. In the limit $b = 0$ the result will be

$$E_g = \frac{\lambda_1}{2} + \frac{\lambda_2}{4} + \frac{\omega_2^2}{4\lambda_2} - \sum_Q V_Q^2 e^{-q^2/\lambda_1} e^{-q_z^2/\lambda_2}\,. \tag{4.54}$$

In the limit, $\lambda_2 = \omega_2 \to \infty$, λ_1 which minimize E_g can be obtained numerically as

$$\lambda_1 = \frac{\pi\alpha^2}{4}\,,$$

and the binding energy will be

$$\epsilon_p^{(2D)} = \frac{\pi\alpha^2}{8}\,. \tag{4.55}$$

This is the 2D binding energy for strong-coupling range obtained in [38]. In the limit $b \to 1$, the ground-state energy describes the case of weak-coupling as

$$E_g = \frac{\lambda_1}{2} + \frac{\lambda_2}{4} + \frac{\omega_2^2}{4\lambda_2} - \sum_Q \frac{V_Q^2 e^{-q_z^2/\lambda_2}}{[1+q^2]}\,. \tag{4.56}$$

In the strict 2D limit, $\lambda_2 = \omega_2 \to \infty$ and $\lambda_1 \to 0$ the energy will be

$$\epsilon_p^{(2D)} = \sum_Q \frac{V_Q^2}{[1+q^2]} \tag{4.57}$$

Projecting out the $\overrightarrow{Q}$-summation in [equation (4.57)] we finally obtain

$$\epsilon_p^{(2D)} = \frac{\pi}{2}\alpha \, . \tag{4.58}$$

Again this is in exact agreement with the weak-coupling 2D result in [39]. As we have seen in this section, the Modified Mixed-Coupling Approximation succeeded in calculating the 2D polaron binding energy for strong-coupling range, which was calculated before using the adiabatic-theory [6], [12].

Also, the Modified Mixed-Coupling Approximation succeeded in calculating the binding energy for 2D polaron binding energy for weak-coupling range which was calculated before by Fröhlich and others by using perturbation theory [5]. On the other hand, one can obtain the binding energy of the polaron for any value of α when the value of a variational parameter b is between 0 and 1.

4.3 The Ground-State Description of The Optical Polaron versus The Effective Dimensionality in Quantum Well Systems

In this section we display a unifying and comprehensive theoretical model yielding an explicit track of the polaronic effects as a function of the effective dimensionality in the overall range of the coupling-constant strength.

The model we use consists of an electron confined in anisotropic potential box with tunable dimensions immersed in the field of bulk LO-phonon modes.

The Hamiltonian describing such a model is given by

$$H = p^2 + \frac{1}{4}\omega_1^2\rho^2 + \frac{1}{4}\omega_2^2 z^2 + \sum_Q a_Q^\dagger a_Q + \sum_Q V_Q[a_Q e^{(i\vec{Q}.\vec{r})} + a_Q^\dagger e^{(-i\vec{Q}.\vec{r})}] \, . \tag{4.59}$$

With ω_1 and ω_2 stand for the dimensionless measures for the degree of confinement in the $x-y$ plane and z-direction respectively. By tuning ω_1 and/or ω_2 from zero to values much larger than unity, one can trace the transition from the bulk to all possible extremes of the effective dimensionality. The modified first and the second

LLP-transformations are, respectively

$$U_1 = \exp[i(\mathbf{P}_\rho - \Pi_\rho).b_1\overrightarrow{\rho} + i(P_z - \Pi_z)b_2 z] \,, \tag{4.60}$$

$$U_2 = \exp\sum_Q u_Q(\phi_e)[a_Q - a_Q^\dagger] \,, \tag{4.61}$$

where b_1 and b_2 are two variational parameters indicate to the presence of the polaron in $x-y$ plane and z-axis respectively, Π and $\mathbf{P}$ are the total momenta of phonon and polaron. The Hamiltonian under the first LLP-transformation transforms to

$$\begin{aligned} H' &= U_1^{-1} H U_1 \qquad (4.62)\\ &= p^2 + \frac{1}{4}\omega_1^2\rho^2 + \frac{1}{4}\omega_2^2 z^2 + b_1^2(P_\rho - \Pi_\rho)^2 + 2b_1 p_\rho(P_\rho - \Pi_\rho) \\ &+ b_2^2(P_z - \Pi_z)^2 + 2b_2 p_z(P_z - \Pi_z) + \sum_Q a_Q^\dagger a_Q \\ &+ \sum_Q V_Q[a_Q e^{-i(b_1\overrightarrow{q}.\overrightarrow{\rho} + b_2 q_z z)} e^{i\overrightarrow{Q}.\overrightarrow{r}} + a_Q^\dagger e^{i(b_1\overrightarrow{q}.\overrightarrow{\rho} + b_2 q_z z)} e^{-i\overrightarrow{Q}.\overrightarrow{r}}] \,. \end{aligned}$$

Under second LLP-transformation the Hamiltonian becomes

$$\begin{aligned} H'' =& p^2 + \frac{1}{4}\omega_1^2\rho^2 + \frac{1}{4}\omega_2^2 z^2 + b_1^2(P_\rho - \Pi_\rho)^2 + b_1^2[\Pi_\rho^{(0)}]^2 + 2b_1 p_\rho(P_\rho - \Pi_\rho + \Pi_\rho^{(1)} - \Pi_\rho^{(0)}) \qquad (4.63)\\ &+ \sum_Q u_Q^2 + b_1^2(\Pi_\rho^{(1)} - 2\Pi_\rho)\Pi_\rho^{(1)} + 2b_1^2(P_\rho - \Pi_\rho^{(0)})\Pi_\rho^{(1)} + 2b_1^2\Pi_\rho^{(0)}\Pi_\rho - 2b_1^2 P_\rho \Pi_\rho^{(0)} \\ &+ b_2^2(P_z - \Pi_z)^2 + b_2^2[\Pi_z^{(0)}]^2 + \sum_Q a_Q^\dagger a_Q + 2b_2 p_z(P_z - \Pi_z + \Pi_z^{(1)} - \Pi_z^{(0)}) \\ &+ b_2^2(\Pi_z^{(1)} - 2\Pi_z)\Pi_z^{(1)} + 2b_2^2(P_z - \Pi_z^{(0)})\Pi_z^{(1)} + 2b_2^2\Pi_z^{(0)}\Pi_z - 2b_2^2 P_z\Pi_z^{(0)} - \sum_Q u_Q(a_Q + a_Q^\dagger) \\ &+ \sum_Q V_Q e^{-i(b_1\overrightarrow{q}.\overrightarrow{\rho} + b_2 q_z z)} e^{i\overrightarrow{Q}.\overrightarrow{r}}(a_Q - u_Q) + \sum_Q V_Q e^{i(b_1\overrightarrow{q}.\overrightarrow{\rho} + b_2 q_z z)} e^{-i\overrightarrow{Q}.\overrightarrow{r}}(a_Q^\dagger - u_Q) \,, \end{aligned}$$

where

$$\mathbf{P}_\rho = \mathbf{p}_\rho + \Pi_\rho \,, \tag{4.64}$$

$$\Pi_\rho = \sum_Q \mathbf{q} a_Q^\dagger a_Q \,, \tag{4.65}$$

and

$$P_z = p_z + \Pi_z \,. \tag{4.66}$$

$$\Pi_z = \sum_Q q_z a_Q^\dagger a_Q \,, \tag{4.67}$$

which describes the momenta of the polaron and phonon in the $x-y$ plane and along the z-axis, respectively. Also

$$\Pi_\rho^{(1)} = \sum_Q q u_Q (a_Q^\dagger + a_Q) \,, \tag{4.68}$$

$$\Pi_\rho^{(0)} = \sum_Q q u_Q^2 \,, \tag{4.69}$$

and

$$\Pi_z^{(1)} = \sum_Q q_z u_Q (a_Q^\dagger + a_Q) \,, \tag{4.70}$$

$$\Pi_z^{(0)} = \sum_Q q_z u_Q^2 \,. \tag{4.71}$$

The ground-state energy is

$$\begin{aligned} E_g &= \langle 0_e|p^2|0_e\rangle + \langle 0_e|\frac{1}{4}\omega_1^2\rho^2 + \frac{1}{4}\omega_2^2 z^2|0_e\rangle + b_1^2 P_\rho^2 - 2b_1^2 P_\rho \Pi_\rho^{(0)} \\ &+ b_1^2[\Pi_\rho^{(0)}]^2 + \sum_Q u_Q^2(1 + b_1^2 q^2 + b_2^2 q_z^2) + \langle 0_e|\langle 0_{ph}|2b_1 p_\rho (P_\rho - \Pi_\rho + \Pi_\rho^{(1)} - \Pi_\rho^{(0)})|0_{ph}\rangle|0_e\rangle \\ &- \sum_Q V_Q u_Q \langle 0_e|e^{-i(b_1 \overrightarrow{q}.\overrightarrow{\rho} + b_2 q_z z)} e^{i\overrightarrow{Q}.\overrightarrow{r}}|0_e\rangle - \sum_Q V_Q u_Q \langle 0_e|e^{i(b_1 \overrightarrow{q}.\overrightarrow{\rho} + b_2 q_z z)} e^{-i\overrightarrow{Q}.\overrightarrow{r}}|0_e\rangle \\ &+ b_2^2 P_z^2 - 2b_2^2 P_z \Pi_z^{(0)} + b_2^2[\Pi_z^{(0)}]^2 + \langle 0_e|\langle 0_{ph}|2b_2 p_z (P_z - \Pi_z + \Pi_z^{(1)} - \Pi_z^{(0)})|0_{ph}\rangle|0_e\rangle \end{aligned} \tag{4.72}$$

Using the expressions of the momenta and the coordinates of the electron as in [equations (4.6), (4.7), (4.8), (4.9)], we get

$$\begin{aligned} E_g &= \frac{\lambda_1}{2} + \frac{\lambda_2}{4} + \frac{\omega_1^2}{2\lambda_1} + \frac{\omega_2^2}{4\lambda_2} + b_1^2 P_\rho^2 - 2b_1^2 P_\rho \Pi_\rho^{(0)} \\ &+ b_1^2[\Pi_\rho^{(0)}]^2 + b_2^2 P_z^2 - 2b_2^2 P_z \Pi_z^{(0)} + b_2^2[\Pi_z^{(0)}]^2 \\ &+ \sum_Q u_Q^2(1 + b_1^2 q^2 + b_2^2 q_z^2) - 2\sum_Q V_Q u_Q S_Q \,, \end{aligned} \tag{4.73}$$

where

$$S_Q = \langle 0_e|e^{\pm i(b_1 \overrightarrow{q}.\overrightarrow{\rho} + b_2 q_z z)} e^{\pm i\overrightarrow{Q}.\overrightarrow{r}}|0_e\rangle \,, \tag{4.74}$$

which is found to be

$$S_Q = e^{-(1-b_1)^2 q^2/2\lambda_1} e^{-(1-b_2)^2 q_z^2/2\lambda_2} \,. \tag{4.75}$$

The variational function u_Q minimizing [equation (4.73)] is given by the following equation:

$$[1 + b_1^2 q^2 + b_2^2 q_z^2 + 2b_1^2 q\Pi_\rho^{(0)} + 2b_2^2 q_z \Pi_z^{(0)} - 2b_1^2 q P_\rho - 2b_2^2 q_z P_z]u_Q - V_Q S_Q = 0 \,, \quad (4.76)$$

$\Pi^{(0)}$ differs from the total momentum by a scalar factor as

$$\Pi_\rho^{(0)} = \eta P_\rho \,, \quad (4.77)$$

and

$$\Pi_z^{(0)} = \eta P_z \,, \quad (4.78)$$

so we can write u_Q as

$$u_Q = \frac{V_Q S_Q}{1 + b_1^2 q^2 + b_2^2 q_z^2 + 2b_1^2 q\Pi_\rho^{(0)} + 2b_2^2 q_z \Pi_z^{(0)} - 2b_1^2 q P_\rho - 2b_2^2 q_z P_z} \,, \quad (4.79)$$

which can be simplified to

$$u_Q = \frac{V_Q S_Q}{[1 + b_1^2 q^2 + b_2^2 q_z^2 - 2b_1^2 q P_\rho (1-\eta) - 2b_2^2 q_z P_z (1-\eta)]} \,. \quad (4.80)$$

In which the unknown scalar, η is determined by this equation

$$\begin{aligned} \Pi_\rho^{(0)} &= \sum_Q q u_Q^2 \,, \\ \eta P &= \frac{q V_Q^2 S_Q^2}{[1 + b_1^2 q^2 + b_2^2 q_z^2 - 2b_1^2 q P_\rho (1-\eta) - 2b_2^2 q_z P_z (1-\eta)]^2} \,. \end{aligned} \quad (4.81)$$

Substituting back in [equation (4.73)] we obtain

$$\begin{aligned} E_g &= \frac{\lambda_1}{2} + \frac{\lambda_2}{4} + \frac{\omega_1^2}{2\lambda_1} + \frac{\omega_2^2}{4\lambda_2} + b_1^2 P_\rho^2 - 2b_1^2 \eta P_\rho^2 \\ &+ b_1^2 [\eta P_\rho]^2 + b_2^2 P_z^2 - 2\eta b_2^2 P_z^2 + b_2^2 [\eta P_z]^2 \\ &+ \sum_Q u_Q^2 (1 + b_1^2 q^2 + b_2^2 q_z^2) - 2\sum_Q V_Q u_Q S_Q \,, \end{aligned} \quad (4.82)$$

which can be simplified to

$$\begin{aligned} E_g &= \frac{\lambda_1}{2} + \frac{\lambda_2}{4} + \frac{\omega_1^2}{2\lambda_1} + \frac{\omega_2^2}{4\lambda_2} \\ &+ b_1^2 P_\rho^2 (1-\eta)^2 + b_2^2 P_z^2 (1-\eta)^2 \\ &+ \sum_Q u_Q^2 (1 + b_1^2 q^2 + b_2^2 q_z^2) - 2\sum_Q V_Q u_Q S_Q \,. \end{aligned} \quad (4.83)$$

Using [equation (4.80)], the ground-state energy becomes

$$\begin{aligned} E_g &= \frac{\lambda_1}{2}+\frac{\lambda_2}{4}+\frac{\omega_1^2}{2\lambda_1}+\frac{\omega_2^2}{4\lambda_2}+b_1^2P_\rho^2(1-\eta)^2+b_2^2P_z^2(1-\eta)^2 \\ &+ \sum_Q \frac{V_Q^2S_Q^2(1+b_1^2q^2+b_2^2q_z^2)}{[1+b_1^2q^2+b_2^2q_z^2-2b_1^2qP_\rho(1-\eta)-2b_2^2q_zP_z(1-\eta)]^2} \\ &- 2\sum_Q \frac{V_Q^2S_Q^2}{[1+b_1^2q^2+b_2^2q_z^2-2b_1^2qP_\rho(1-\eta)-2b_2^2q_zP_z(1-\eta)]}\,. \end{aligned} \tag{4.84}$$

But $E_g(P)$ may be well represented by the first two terms of a power series expansion in P^2 as

$$E_g(P)=E_g(0)+\beta P^2/2+...O(P^4)+... \tag{4.85}$$

The effective mass of the polaron is then β^{-1}.

By comparing [equations (4.84) and (4.85)], we give the expression for the ground-state energy as

$$E_g = \frac{\lambda_1}{2}+\frac{\lambda_2}{4}+\frac{\omega_1^2}{2\lambda_1}+\frac{\omega_2^2}{4\lambda_2}-\sum_Q \frac{V_Q^2S_Q^2}{[1+b_1^2q^2+b_2^2q_z^2]}\,, \tag{4.86}$$

and the mass of the polaron is

$$m_p=\frac{1}{b_1^2(1-\eta)^2}\,. \tag{4.87}$$

Using the expression of S_Q which is given in [equation (4.75)], the energy becomes

$$E_g=\frac{\lambda_1}{2}+\frac{\lambda_2}{4}+\frac{\omega_1^2}{2\lambda_1}+\frac{\omega_2^2}{4\lambda_2}-\sum_Q \frac{V_Q^2e^{-(1-b_1)^2q^2/\lambda_1}e^{-(1-b_2)^2q_z^2/\lambda_2}}{[1+b_1^2q^2+b_2q_z^2]}\,. \tag{4.88}$$

This is the general formula of the ground-state energy which supposed to be valid for both 3D and 2D polaron in the all values of the polaronic coupling constant. In the limit $b_1=b_2\to 0$ the ground-state energy gives the adiabatic (strong) limit as

$$E_g=\frac{\lambda_1}{2}+\frac{\omega_1^2}{2\lambda_1}+\frac{\lambda_2}{4}+\frac{\omega_2^2}{4\lambda_2}-\sum_Q V_Q^2e^{-q^2/\lambda_1}e^{-q_z^2/\lambda_2} \tag{4.89}$$

Projecting out the $\overrightarrow{Q}$-summation in [equation (4.89)] we obtain

$$E_g=\frac{\lambda_1}{2}+\frac{\omega_1^2}{2\lambda_1}+\frac{\lambda_2}{4}+\frac{\omega_2^2}{4\lambda_2}-\frac{\alpha}{\sqrt{\pi}}\sqrt{\frac{\lambda_1\lambda_2}{\lambda_2-\lambda_1}}\tan^{-1}\sqrt{\frac{\lambda_2}{\lambda_1}-1} \tag{4.90}$$

and for the polaron binding energy, we have

$$\epsilon_p = \omega_1 + \frac{1}{2}\omega_2 - E_g \,, \tag{4.91}$$

For $\omega_1 = \omega_2 = 0$, we obtain numerically

$$\lambda_1 = \lambda_2 = \frac{4\alpha^2}{9\pi} \,,$$

and

$$\epsilon_p^{(3D)} = \frac{\alpha^2}{3\pi} \,. \tag{4.92}$$

Which is the strong-coupling result for the 3D polaron as found in [equation (4.25)]. Also, in the limit $b_1 = b_2 \to 1$, the ground-state energy describes the case of weak-coupling as

$$E_g = \frac{\lambda_1}{2} + \frac{\omega_1^2}{2\lambda_1} + \frac{\lambda_2}{4} + \frac{\omega_2^2}{4\lambda_2} - \sum_Q \frac{V_Q^2}{[1+Q^2]} \tag{4.93}$$

For $\omega_1 = \omega_2 = 0$, we obtain $\lambda_1 = \lambda_2 \to 0$, and

$$\epsilon_p^{(3D)} = \alpha \,. \tag{4.94}$$

Which is the same results of Fröhlich [5] for 3D polaron. To obtain the 2D polaron results for strong-coupling limit we put $b_2 = 0$ and $b_1 = 0$ the result will be

$$E_g = \frac{\lambda_1}{2} + \frac{\lambda_2}{4} + \frac{\omega_1^2}{2\lambda_1} + \frac{\omega_2^2}{4\lambda_2} - \sum_Q V_Q^2 e^{-q^2/\lambda_1} e^{-q_z^2/\lambda_2} \quad . \tag{4.95}$$

In the strict 2D limit, $\lambda_2 = \omega_2 \to \infty$, and λ_1 which minimizes E_g can be obtained numerically as

$$\lambda_1 = \frac{\pi\alpha^2}{4} \,.$$

The binding energy will be

$$\epsilon_p^{(2D)} = \frac{\pi\alpha^2}{8} \,, \tag{4.96}$$

and for the weak-coupling limit we put $b_1 = 1$ and $b_2 = 0$, so the ground-state energy becomes

$$E_g = \frac{\lambda_1}{2} + \frac{\lambda_2}{4} + \frac{\omega_1^2}{2\lambda_1} + \frac{\omega_2^2}{4\lambda_2} - \sum_Q \frac{V_Q^2 e^{-q_z^2/\lambda_2}}{[1+q^2]} \,. \tag{4.97}$$

In the strict 2D limit, $\lambda_2 = \omega_2 \to \infty$ and $\lambda_1 \to 0$ the binding energy will be

$$\epsilon_p^{(2D)} = \sum_Q \frac{V_Q^2}{[1+q^2]} \, . \tag{4.98}$$

Projecting out the $\overrightarrow{Q}$-summation in [equation (4.98)] we finally obtain

$$\epsilon_p^{(2D)} = \frac{\pi}{2}\alpha \, . \tag{4.99}$$

This is the 2D binding energy for weak-coupling range described in [39].

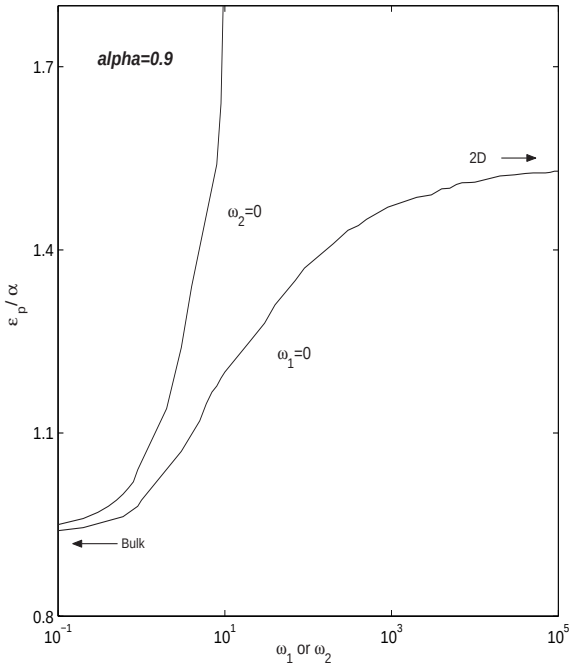

Figure 4.1: The binding energy ϵ_p as a function of the degree of confinement ω_1 or ω_2, for $\alpha = 0.9$

In figure (4.1) we plotted the binding energy as a function of the degree of confinement, (ω_1 or ω_2), respectively for the wire and slab-like configurations for $\alpha = 0.9$ (weak-range).

When we put $\omega_1 = 0$, and increase ω_2 from non zero to ∞ we obtain the binding energy of the slab-case (2D polaron).

Also, when we put $\omega_2 = 0$, and increase ω_1 from non zero to ∞ we obtain the binding energy of the wire-case (1D polaron) as it is clear in the figure.

This figure is comparable to the figure given by T. Yildirim and Erçelebi A. [39], using perturbation theory appropriate only to the weak-coupling limit.

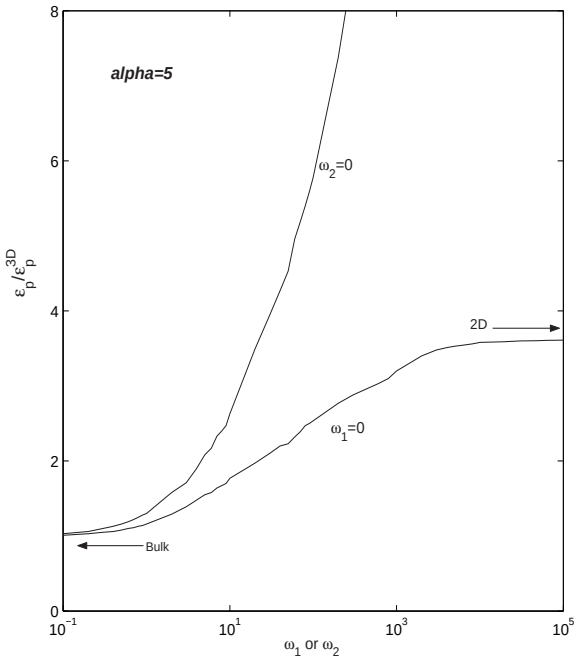

Figure 4.2: The binding energy ϵ_p as a function of the degree of confinement ω_1 or ω_2, for $\alpha = 5$

In figure (4.2) we plotted the binding energy as a function of the degree of confinement, for the wire and slab-like configurations for $\alpha = 5$ which a rather strong value.

Again fixing ω_1 at zero and increasing ω_2 to large values we approach the result of the slab-case. If, however, fixing ω_2 at zero and increasing ω_1 to large values we get the result of the wire-case. Comparing this figure with the strong-coupling calculation of [38] using a variational approach we see that the present calculations give a reasonable results. using variational theory.

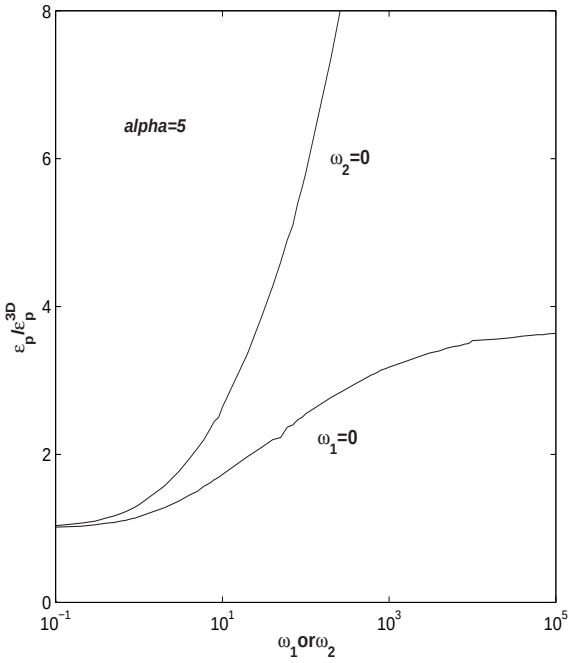

Figure 4.3: The binding energy ϵ_p as a function of the degree of confinement ω_1 or ω_2, for $\alpha = 5$ and $(b_1 = b_2 = 0)$ (pure strong-coupling)

It should be noted that when $(b_1 = b_2 = 0)$ the problem will be turned to the pure strong-coupling regime.
Plotting the binding energy as a function of the degree of confinement in figure (4.3), we obtain the same results as that obtained by T. Yildirim and Erçelebi A. [38]

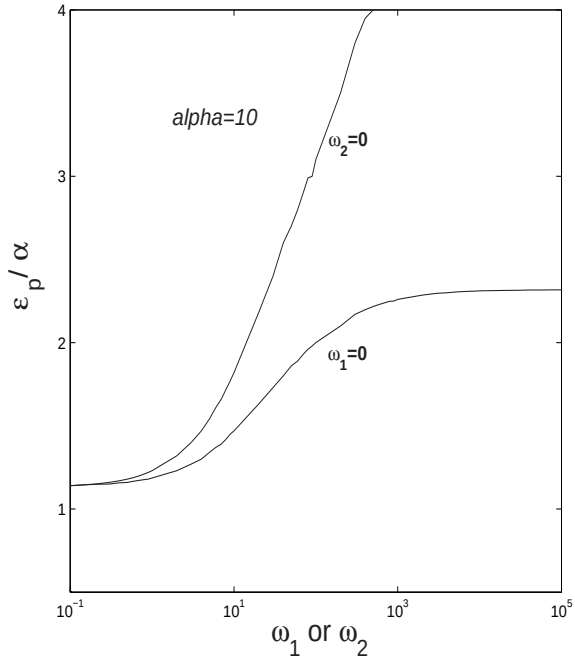

Figure 4.4: The binding energy ϵ_p as a function of the degree of confinement ω_1 or ω_2, for $\alpha = 10$

If we let $b_1 = b_2 = b$ and plotting the binding energy as a function of the degree of confinement ω_1 or ω_2 we obtain the figure (4.4). We note that with increasing barrier slopes of the confining potential, the binding energy for the wire geometry rapidly becomes much larger than in the Q2D-configuration, which follows essentially from the fact that in the wire geometry the polaron cloud is squeezed towards the wire axis in all transverse directions resulting in a much stronger effective electron-phonon coupling than for the slab-like configuration. Because in this chapter we used the modified formula for the first LLP-transformation (by adding the variational parameter b), we will explain the relation between b and α.

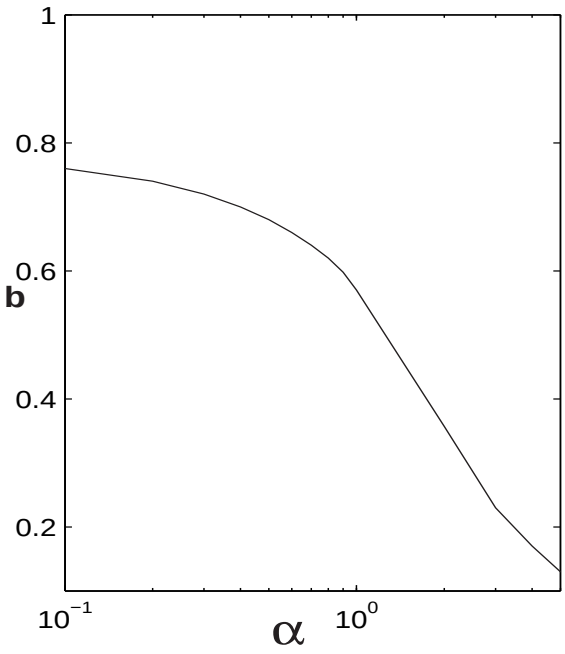

Figure 4.5: The variational parameter (b) versus the coupling constant (α)

In figure (4.5) we plot the variational parameter as a function of the coupling-constant (α). As the figure explains, for small value of α, the variational parameter takes the large value, which makes the problem is similar results as weak-coupling methods. And for large value of α, the variational parameter takes the small value, which makes the problem is similar results as strong-coupling methods. When the variational parameter is between (0, 1) the method we used is correct for intermediate-coupling range. This figure agrees with the results we obtained in section (2), when b is equal nearly (one), the problem and the results are closely to weak-coupling approximation. And when b is equal nearly (zero), the problem and the results are closely to strong-coupling approximation.

Chapter 5

Conclusion

We have investigated the basic features of the Fröhlich polaron in a number of low dimensional systems. Different approximation approaches have been studied.
We begin by applying the strong-coupling approximation to the Q1D-polaron in cylindrical well wire. It is observed that the polaronic coupling constant (α) and the radius of the wire R do not affect the problem independently but take part together in an interrelated way, thus inducing an implicit coupling between the transverse and the longitudinal coordinates of the electron. Starting from the 3D case to the 1D limit, a competitive interrelation between whether the lattice deformation will condense onto the origin or will expand in the longitudinal directions appears. As the radius of the wire decreases the contribution coming from expanding the polaron in the longitudinal direction is compensated by the enhancement of the phonon-coupling due to the localization in the lateral direction.
The same problem is reconsidered using an approach consisting of a strong-coupling aspect imposed in the lateral directions and a weak-coupling LLP-theory along the length of the wire. This approach, the mixed coupling approach, is assumed to be valid for not too strong coupling strength and narrow wires. For small values of α a high degree of confinement in the lateral direction is required to compensate for the weak coupling characterization.
It is observed that the decrease of the radius of the wire produces a pseudo-strong coupling aspect to the problem in spite of the weak values of α.

For small values of α ($\alpha < 1$), it is shown that the LLP-transformation employed to that using the pure strong- coupling approach.

To compensate for the drawbacks encountered in the mixed-coupling approximation a modification is proposed by imposing a further variational parameter intended to interpolate between the strong- and weak-coupling aspects of the problem. The application of this modified mixed-coupling theory to the polaron in a spherically box-type and in a slab-like confinements reveals that this additional variational parameter b enables the problem to go smoothly from the strong-coupling limit ($b = 0$) to the weak-coupling aspect ($b = 1$).

The same modified approach is applied to study the ground-state energy of the polaron versus the effective dimensionality. The theory is intended to display a unifying and comprehensive theoretical presentation giving an explicit track of the electron-phonon interaction for all degrees of confinement and for all possible values of the coupling constant. The formalism is supposed to set up a weighted admixture of the strong- and weak-coupling counterparts of the problem and thus enables the adiabatic results to conform successfully to those attained from perturbation theory.

A common remark from this work is that high degrees of confinements cause an enhancement in the effective phonon coupling. This brings about the phenomena of pseudo-strong-coupling case, In spite of small coupling constant, the problem may have a strong-coupling counterpart coming from the confinement effects.

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