إقرار

أنا الموقع أدناه مقدم الرسالة التي تحمل العنوان:

The Polaronic Effect on Quantum Well-Wires

(التأثير البولاروني على الآبار الكمية)

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The Polaronic Effect on Quantum Well-Wires

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بناءً على موافقة شئون البحث العلمي والدراسات العليا بالجامعة الإسلامية بغزة على تشكيل لجنة الحكم على أطروحة الباحث/ **محمود أسامة محمد المملوك** لنيل درجة الماجستير في **كلية *العلوم*** **قسم الفيزياء** وموضوعها:

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Contents

List of Figures

Dedication

To my

Parents,

My sisters and brothers,

My wife (Bayan),

And to my teachers and friends.

Mahmoud Osama AL Mamlouk

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First of all, I would like to thank Islamic university and Prof. Dr. Bassam Saqqa my Supervisor, for his great help, continuous support and his valuable guidance, and I am indebted to those who have encouraged me along the way and opened the doors for me.

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Abstract

The Polaronic Effect on Quantum Well-Wires

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The polaron problem in a quasi 1D cylindrical quantum well-wire with infinite boundary potential is investigated using the strong-coupling theory. It is observed that a decrease in the radius of wire produce a pseudo strong aspect to the problem in spite of weak values of (α).

The effect of an external magnetic field on the problem is also studied. It is observed the polaronic effect becomes more important for strong values of the magnetic field and large values of the wire radius. As the radius of the wire getting smaller the effect of the magnetic field becomes negligible.

ملخص باللغة العربية

التأثير البولاروني على الآبار الكمية للأسلاك

تحت إشراف

الأستاذ الدكتور / بسّام هاشم السقا

الباحث / محمود أسامه المملوك

لقد تم دراسة مسألة البولارون المحصور في سلك أسطواني لا نهائي الطول وذلك باستخدام الطريقة الادياباتيكية. وتبين أنه ومع تقليل قطر السلك وبالرغم من قيم صغيرة لثابت الاقتران بين الالكترون والفونونات يمكن أن نحصل على حالة تشبه حالة الاقتران القوي سُميِّت الاقتران شبه قوي.

كما تم دراسة تأثير المجال المغناطيسي الخارجي على نفس المسألة، لوحظ أن التأثير البولاروني يزداد أهمية خصوصاً عند زيادة شدة المجال المغناطيسي وزيادة قيم نصف قطر السلك.

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 it 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 displacement field are called phonons [1]. The ionic polarization in the crystal occurs by 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, the electron, interacting with a boson field, The polaron is characterized by many parameters such as: its binding or (self- energy), its effective mass and its response to the external electric and magnetic fields. Also, the number of phonons in the polaron cloud, and the polaron radius are important parameters. 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 acoustic polaron].

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

Small polaron [Holstein polaron]:

It's formed when the displacement of the ion is smaller than the lattice constant and the deformation of the lattice will be small. Because for small polarons the lattice polarization is mostly confined to one unit cell, the atomicity of solid is felt by carrier, which takes into account the detailed local structure of solid, the Fröhlich continuum approximation would not be adequate. Nevertheless, actual small-polaron theories as developed, e.g., by Yamashita and Kurosawa (1958), Holstein (1959) and others are based on analytical approximation as starting point. Thus, the adiabatic eigenstates of an electron placed in a deformable continuum were shown to depend drastically on the character of the electron lattice in interaction as well as on the dimensionality of system. (Emin, Holstein, 1976) The self-trapped carrier of small polaron is confined to a single site, and the small polaron are governed by the short-range interaction [3], [4].

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 large-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.

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.

Acoustic polaron:

This polaron is formed in metals when the electron interacts with acoustic phonons which have a low frequency. 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 [21].

1.2 Historical Studies

Historically, the first studies on polarons is a Russian work that described the concept of polaron by Landau (1933) in a paper of about 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 coupling strength.

In (1954) Pekar put the trial wave state Ψ for the polaron, which is considered as two parts electron wave function φ_e, and the field (phonon) wave function φ_{ph}, that is [6]

$$\Psi = \varphi_e . \varphi_{ph} \, , \tag{1.1}$$

which can be written as

$$|\Psi\rangle = |\varphi_e\rangle\big|\varphi_{ph}\rangle \tag{1.2}$$

In (1955) Feynman studied one of Fröhlich`s papers on polarons (Fröhlich, 1945). There, he got the idea to formulate the polaron problem into Lagrangian form of quantum mechanics. He considered 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 strength.

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-radius 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. In this model the free energy of polaron was treated as a path integral [8]. Even though the polaron problem is 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.

1.3 The Hamiltonian of The Polaron

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

$$H = H_e + H_{ph} + H_{e-ph} \tag{1.5}$$
$$= H_e + \sum_Q \hbar\,\omega_{LO} a_Q^\dagger a_Q + \sum_Q V_Q \left[a_Q\, exp\, i\left(\vec{Q}.\vec{r}\right) + a_Q^\dagger\, exp - i\left(\vec{Q}.\vec{r}\right)\right]$$

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

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

where V is the volume of the crystal (which is taken as a unit in most problem of the polaron), ω_{LO} is the frequency of the (LO) phonons, $\hbar\omega_{LO}$ is the energy of the phonons, and α is the standard dimensionless coupling constant of the electron-phonon interaction which is given as [5]

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

where $\epsilon_\infty(\epsilon_0)$ is high frequency (static) dielectric constant of the medium.

By using the pervious information, Fröhlich (1954), [5] has provided the first weak coupling perturbation-theory results

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

where ϵ_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 (Gallium Arsenic) are of great interest. Also the electron-phonon interaction and the polaron effect in such systems received much attention. For one polaron, confined to two dimensions, but interacting with a (3D) phonon gas, 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 value of (α), the strong-coupling corresponding result are [11], [12]

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

It is clear that, decreasing dimensions, leads to increase in the value of polaron binding energy. the polaron binding energy is depend 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]-[14] 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 that 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 [15]. Many studies explained the combined effect of the external magnetic field and the polaronic interaction and the important result is [14]

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 [16]. 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, more studies and researches focused on the quantum confinement systems, such as the polaron (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 investigation have been made to study the polaronic properties in lower dimensions [17]-[18]. Recent studies on the electron-phonon interaction in quasi one-dimensional (Q1D) system have explored a polaronic effect pronounced strong than in (2D) structures [17].

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

(1) **The Strong-Coupling Theory** or, **The Adiabatic-Coupling Theory**

This theory which developed by Pekar [6] 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 depend on the variational method which supposes a variational parameters in 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 coupling strength.

(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 [5].

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

1.4 The Aim of The Work

The progress in semiconductor nanotechnology has made it possible to fabricate various kinds of semiconductor hetrostructure including low dimension structure. The quantum well wires system is one of these systems. Many theoretical investigations have been made to study polaronic effect in low-dimensional structures as ionic crystals and polar semiconductors. Because of increasing attention on this subject, in our work we focus on studying a confined polaron in a quantum well wire, starting with Fröhlich Hamiltonian with a parabolic potential.

In chapter 2 we retrieve within the strong-coupling theory, the quasi-one dimensional analog of standard optical polaron relevant to a cylindrical quantum well wire. Under the assumption of perfect confinement the ground state binding energy, effective polaronic mass and the phonon-coupling-induced potential well profiles will be studied as a function of the wire radius and the electron-phonon interaction strength.

The effect of the magnetic field on a quantum well is studies in chapter 3. Chapter 4 is devoted to the results and discussion. We observe that the binding energy increases with increasing field intensity and/or decreasing well size, and further that the enhancement in the binding brought about by electron-phonon coupling is rather noticable.

Chapter 2

Theory and Calculation

2.1 The Strong Coupling Regime

In this chapter, we study the problem of quasi-one dimensional analog of the standard optical polaron relevant to a cylindrical quantum well wire (QWW), we are using the strong-coupling theory, with infinite boundary potential [19]. 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 radius (R), and the units ($2m = \omega_{LO} = \hbar = 1$), where m is the effective mass of the electron.

The Hamiltonian of the polaron is given by

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

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

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

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

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

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

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

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

$$V_Q = \frac{\sqrt{4\pi\alpha}}{Q} \ . \qquad (2.5)$$

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

$$|\Psi_g\rangle = |\varphi_e\rangle|\varphi_{ph}\rangle \ , \qquad (2.6)$$

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

$$|\varphi_{ph}\rangle = U_Q|0\rangle \qquad (2.7)$$

Describes the phonon wave function. The ket $|0\rangle$ is 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).

U_Q is the unitary displacement operator which is given by,

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

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

$$\varphi_e(\vec{\rho}, z) = \varphi_e(\vec{\rho})\varphi_e(z) , \tag{2.9}$$

with

$$\varphi_e(\vec{\rho}) = n_\rho J_0(k\rho)\exp(-\tfrac{1}{2}\mu^2\rho^2) , \tag{2.10}$$

and

$$\varphi_e(z) = n_z\exp(-\tfrac{1}{2}\lambda^2 z^2) \quad , \tag{2.11}$$

where μ and λ are two variational parameters accounting for anisotropic nature of the system, J_0 is zeroth order cylindrical Bessel function of the first kind in which $(\mathrm{k}=\frac{j_{0.1}}{R})$ its first zero , $j_{0.1} = 2.4048$, R is radius of the cylinder and n_ρ, n_z are normalization constants of $\varphi_e(\vec{\rho}, z)$ which is normalized function, Applying the normalization condition ($\int \varphi^* \varphi dv = 1$) we will get, $\varphi_e(z)$ as

$$\varphi_e(z) = (\frac{\lambda^2}{\pi})^{\frac{1}{4}}\exp(-\tfrac{1}{2}\lambda^2 z^2) \tag{2.12}$$

and

$$\varphi_e(\vec{\rho}) = \frac{1}{\sqrt{2\pi\,\sigma_{00}^{(1)}(0)}} J_0(k\rho)\exp(-\tfrac{1}{2}\mu^2\rho^2) \tag{2.13}$$

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), taking the wave function of polaron as,

$$\Psi_g = \varphi_e U_Q |0\rangle \tag{2.14}$$

the energy can be obtained as

$$E_g = \langle 0|\langle \varphi_e | U_Q^{-1} H U_Q | \varphi_e \rangle |0\rangle \tag{2.15}$$

$$= \langle 0|\langle \varphi_e | H` | \varphi_e \rangle |0\rangle$$

where

$$H` \rightarrow U_Q^{-1} H U_Q$$

Now using the identity

$$e^{A} \mathrm{B} e^{-\mathrm{A}} = \mathrm{B} + \frac{1}{1!}[\mathrm{A}, \mathrm{B}] + \frac{1}{2!}\big[\mathrm{A}, [\mathrm{A}, \mathrm{B}]\big] + \frac{1}{3!}\Big[\mathrm{A}, \big[\mathrm{A}, [\mathrm{A}, \mathrm{B}]\big]\Big] + \cdots, \tag{2.16}$$

and equation (2.8) which explains the expression of U_Q [6], we obtained the following results

$$U^{-1} H_e U = H_e, \tag{2.17}$$

$$U^{-1} \sum_Q a_Q^\dagger a_Q U = \sum_Q a_Q^\dagger a_Q + \sum_Q u_Q^2 - \sum_Q u_Q (a_Q + a_Q^\dagger), \tag{2.18}$$

and

$$U^{-1}[\sum_Q V_Q (a_Q e^{i\vec{Q}.\vec{r}} + a_Q^\dagger e^{-i\vec{Q}.\vec{r}})]U = -\sum_Q V_Q u_Q \left(e^{i\vec{Q}.\vec{r}} + e^{-i\vec{Q}.\vec{r}}\right) + \sum_Q V_Q (a_Q e^{i\vec{Q}.\vec{r}} + a_Q^\dagger e^{-i\vec{Q}.\vec{r}}). \tag{2.19}$$

The last three equations will form the modified Hamiltonian as

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

which can be simplified to

$$H` = H_e + \sum_Q a_Q^\dagger a_Q + \sum_Q u_Q^2 - \sum_Q V_Q u_Q(e^{i\vec{Q}.\vec{r}} + e^{-i\vec{Q}.\vec{r}}) + \sum_Q\{\left[V_Q e^{(i\vec{Q}.\vec{r})} - u_Q\right] a_Q + \left[V_Q e^{(-i\vec{Q}.\vec{r})} - u_Q\right] a_Q^\dagger\} . \quad (2.21)$$

The energy will be then

$$E_g = \langle\varphi_e|H_e|\varphi_e\rangle + \sum_Q u_Q^2 - \sum_Q V_Q u_Q \left\langle\varphi_e\middle|e^{(i\vec{Q}.\vec{r})}\middle|\varphi_e\right\rangle - \sum_Q V_Q u_Q \left\langle\varphi_e\middle|e^{-(i\vec{Q}.\vec{r})}\middle|\varphi_e\right\rangle . \quad (2.22)$$

Defining

$$\epsilon_k = \langle\varphi_e|-\nabla^2|\varphi_e\rangle ,$$

and

$$S_Q = \left\langle\varphi_e\middle|e^{\mp(i\vec{Q}.\vec{r})}\middle|\varphi_e\right\rangle .$$

Then E_g, becomes

$$E_g = \epsilon_k + \sum_Q u_Q^2 - 2\sum_Q V_Q u_Q S_Q \quad (2.23)$$

By minimizing equation (2.23) with respect to u_Q, we can obtain u_Q as

$$u_Q = S_Q V_Q \ . \tag{2.24}$$

Substituting back in equation (2.23), for u_Q we obtain

$$E_g = \epsilon_k - \sum_Q V_Q^2 S_Q^2 \tag{2.25}$$

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

$$\begin{aligned}
\epsilon_k &= \langle \varphi_e(\vec{\rho}, z) | -\nabla^2 | \varphi_e(\vec{\rho}, z) \rangle \\
&= \left\langle \varphi_e(\vec{\rho}) \right| -\frac{1}{\rho}\frac{\partial}{\partial \rho}\left(\rho \frac{\partial}{\partial \rho}\right) \left| \varphi_e(\vec{\rho}) \right\rangle + \left\langle \varphi_e(z) \right| -\frac{\partial^2}{\partial z^2} \left| \varphi_e(z) \right\rangle \\
&= \left\langle \varphi_e(\vec{\rho}) \right| -\frac{1}{\rho}\frac{\partial}{\partial \rho}\left(\rho \frac{\partial}{\partial \rho}\right) \left| \varphi_e(\vec{\rho}) \right\rangle + \frac{\lambda^2}{2} \ .
\end{aligned}$$

Defining for notational convenience,

$$\sigma_{mm`}^{(n)}(x) = \int_0^{j_{0.1}} dt t^n J_m(t) J_{m`}(t) J_0(xt) \exp\left(-\frac{\mu^2}{k^2} t^2\right) . \tag{2.26}$$

Finally ϵ_k can be written as

$$\epsilon_k = k^2 + \mu^2 \left(2 - \frac{2\sigma_{10}^{(2)}(0) - \left(\mu/k\right)^2 \sigma_{00}^{(3)}(0)}{\sigma_{00}^{(1)}(0)} \right) + \frac{\lambda^2}{2} \tag{2.27}$$

For S_Q,we have

$$S_Q = \langle\varphi_e(\vec{\rho})|\langle\varphi_e(z)|e^{\pm i\vec{q}.\vec{\rho}}e^{\pm iq_z.z}|\varphi_e(z)\rangle|\varphi_e(\vec{\rho})\rangle$$

$$= \langle\varphi_e(\vec{\rho})|e^{\pm i\vec{q}.\vec{\rho}}|\varphi_e(\vec{\rho})\rangle\langle\varphi_e(z)|e^{\pm iq_z.z}|\varphi_e(z)\rangle$$

$$= r_q \langle\varphi_e(z)|e^{\pm iq_z.z}|\varphi_e(z)\rangle .$$

where

$$r_q = \langle\varphi_e(\vec{\rho})|e^{\pm i\vec{q}.\vec{\rho}}|\varphi_e(\vec{\rho})\rangle . \tag{2.28}$$

Equ. (2.28) can be written as

$$r_q = \frac{\sigma_{00}^{(1)}(\frac{q}{k})}{\sigma_{00}^{(1)}} \tag{2.29}$$

The final form of S_Q is now

$$S_Q = r_q e^{(-\frac{q_z^2}{4\lambda^2})} \tag{2.30}$$

Projecting out the $\vec{Q}$-summations in equation (2.25) using the transformation

$$\sum_Q \rightarrow \frac{1}{(2\pi)^3}\int_0^\infty \int_{-\infty}^\infty \int_0^{2\pi} q dq\, dq_z\, d\emptyset \tag{2.31}$$

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

$$E_g = \epsilon_k - \alpha \int_0^\infty dq\, r_q^2\, f_q \ , \tag{2.32}$$

where

$$f_q = \exp\left(\frac{q^2}{2\lambda^2}\right) erfc\left(\frac{q}{\sqrt{2}\,\lambda}\right), \tag{2.33}$$

with (erfc) denoting the complementary error function.

Chapter 3

The Effect of The Magnetic Field on Problem

The application of an external magnetic field on the problem puts a further confinement on the problem, this means that the effect of the magnetic field is expected to enhance the importance of the polaronic effect [21, 22].

We consider a constant and uniform magnetic field directed along the z-axis $\vec{B} = B\hat{z}$. Using the symmetric gauge [23],

$$\vec{A} = \frac{1}{2}\vec{B} \times \vec{r} = \frac{B}{2}(-y\,\hat{\imath} + x\,\hat{\jmath}) \tag{3.1}$$

For the vector potential, the electronic part of the Hamiltonian is given by

$$H_e = -\nabla^2 + \frac{\omega^2}{8}\rho^2 + \frac{\omega}{2}\,L_Z \tag{3.2}$$

Where $\vec{\rho}$ = (x,y) denotes the electron position in the transverse plane, $L_Z = (\,xP_y - yP_x)$ is the z-component of angular momentum, and ω is the dimensionless cyclotron frequency.

The expectation value of the electronic part of the Hamiltonian using the same wave-function defined in Eq. (2.9) is now given as

$$\langle\varphi_e|H_e|\varphi_e\rangle = \langle\varphi_e|-\nabla^2|\varphi_e\rangle + \left\langle\varphi_e\left|\frac{\omega^2}{8}\rho^2\right|\varphi_e\right\rangle + \frac{\omega}{2}\langle\varphi_e|L_Z|\varphi_e\rangle \tag{3.3}$$

But the first term of Eq.(3.3) is already calculated in Eq.(2.27) with

$$\epsilon_k = \langle\varphi_e|-\nabla^2|\varphi_e\rangle = k^2 + \mu^2\left(2 - \frac{2\sigma_{10}^{(2)}(0) - \left({}^{\mu}/_{k}\right)^2\sigma_{00}^{(3)}(0)}{\sigma_{00}^{(1)}(0)}\right) + \frac{\lambda^2}{2}, \qquad (3.4)$$

and knowing that

$$\langle\varphi_e|L_Z|\varphi_e\rangle = -\frac{i\hbar}{2}\left\langle\varphi_e\left|\frac{\partial}{\partial\varphi}\right|\varphi_e\right\rangle = 0\,, \qquad (3.5)$$

because φ_e does not depend on $\emptyset$.

To calculate the last term we have

$$\left\langle\varphi_e\left|\frac{\omega^2}{8}\rho^2\right|\varphi_e\right\rangle = \frac{\omega^2}{8}\int {\varphi_e}^*\rho^2\varphi_e d\tau$$

$$= \frac{\omega^2}{8}\int {\varphi_e}^*\rho^2\varphi_e\rho d\rho d\emptyset dz \qquad (3.6)$$

Integrating with respect to the azimuthal angel $\emptyset$ we obtain

$$\left\langle\varphi_e\left|\frac{\omega^2}{8}\rho^2\right|\varphi_e\right\rangle = \frac{\omega^2}{8}2\pi\int {\varphi_e}^*\rho^2\varphi_e\rho d\rho dz. \qquad (3.7)$$

Substituting about $\varphi_e(z)$ we get

$$\left\langle \varphi_e \left| \frac{\omega^2}{8}\rho^2 \right| \varphi_e \right\rangle =$$

$$\frac{\omega^2}{8} 2\pi \int \left(\frac{\lambda^2}{\pi}\right)^{\frac{1}{4}} \varphi(\rho)^* e^{\frac{-\lambda^2 z^2}{2}} e^{-i\omega z} \rho^3 \left(\frac{\lambda^2}{\pi}\right)^{\frac{1}{4}} \varphi(\rho) e^{\frac{-\lambda^2 z^2}{2}} e^{i\omega z} d\rho dz$$

$$= \frac{\omega^2}{8} 2\pi \left(\frac{\lambda^2}{\pi}\right)^{\frac{1}{2}} \int_{-\infty}^{\infty} e^{-\lambda^2 z^2} dz \int_0^R \varphi(\rho)^* \rho^3 \varphi(\rho) d\rho \qquad (3.8)$$

Now using Gaussian integral we get

$$\int_{-\infty}^{\infty} e^{-\lambda^2 z^2} dz = \frac{\sqrt{\pi}}{\lambda} \ . \qquad (3.9)$$

Substituting (3.9) in (3.8) we have

$$= \frac{\omega^2}{8} 2\pi \left(\frac{\lambda^2}{\pi}\right)^{\frac{1}{2}} \frac{\sqrt{\pi}}{\lambda} \int_0^R \varphi(\rho)^* \rho^3 \varphi(\rho) d\rho \ . \qquad (3.10)$$

After simplifying we obtain

$$\left\langle \varphi_e \left| \frac{\omega^2}{8}\rho^2 \right| \varphi_e \right\rangle = \frac{\omega^2}{4} \pi \int_0^R \varphi(\rho)^* \rho^3 \varphi(\rho) d\rho \qquad (3.11)$$

Now

$$n_\rho = \frac{1}{\sqrt{2\pi \sigma_{00}^{(1)}(0)}} \ . \qquad (3.12)$$

Substituting Form $\varphi(\rho)$ in (3.11) we get

$$\left\langle \varphi_e \left| \frac{\omega^2}{8}\rho^2 \right| \varphi_e \right\rangle = \frac{\omega^2}{8\sigma_{00}^{(1)}(0)} \int_0^R [J_0(k\,\rho)]^2\, e^{-\rho^2\mu^2} \rho^3 d\rho. \tag{3.13}$$

but

$$\int_0^R [J_0(k\,\rho)]^2\, e^{-\rho^2\mu^2} \rho^3 d\rho = \sigma_{00}^{(3)}(0)\,. \tag{3.14}$$

Substituting Equ. (3.14) in (3.13) we have

$$\left\langle \varphi_e \left| \frac{\omega^2}{8}\rho^2 \right| \varphi_e \right\rangle = \frac{\omega^2}{8\sigma_{00}^{(1)}(0)}\ \sigma_{00}^{(3)}(0)\,. \tag{3.15}$$

The ground state energy of problem now becomes

$$E_g = \epsilon_k + \frac{\omega^2}{8\sigma_{00}^{(1)}(0)}\ \sigma_{00}^{(3)}(0)\,, \tag{3.16}$$

Or which can be written as

$$E_g = k^2 + \mu^2 \left(2 - \frac{2\sigma_{10}^{(2)}(0) - \left(\mu/k\right)^2 \sigma_{00}^{(3)}(0)}{\sigma_{00}^{(1)}(0)} \right) + \frac{\omega^2}{8\sigma_{00}^{(1)}(0)}\ \sigma_{00}^{(3)}(0) + \frac{\lambda^2}{2}\,. \tag{3.17}$$

It should be noticed that even though the lattice part of the Hamiltonian seems not to be effected by the application of the magnetic field directly, the effect inter the problem indirectly through the variational parameters. The effect of the electron-phonon coupling constant α and the strength of the magnetic field ω enter the problem in an interrelated feature. The minimization of equation (3.17) will be done numerically.

Chapter 4

Results & Discussion

In order to obtain the binding energy, we numerically minimize equation (3.17) with respect to the variational parameters μ and λ. Then substituting the minimized value of E_g to obtain the binding energy which is defined as [11]

$$\varepsilon_p = \left(j_{0.1}/R\right)^2 - E_g \qquad (4.1)$$

By using Maple Programme, we obtain $\varepsilon_p = 3.34$ for a wire with $\alpha = 3$ and wire radius $R = 1$. This value is exactly the same as obtained by Ercelebi A. and Senger R.T [11]. 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 $\varepsilon_p = 5.51$ when $R = 0.5$ and $\varepsilon_p = 9.98$ when $R = 0.2$

A comparison of these values with the corresponding three-and two-dimensional values by using equations (1.9), (1.10), gives that $\varepsilon_p^{(3D)} = 0.955$, and $\varepsilon_p^{(2D)} = 3.534$.

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.

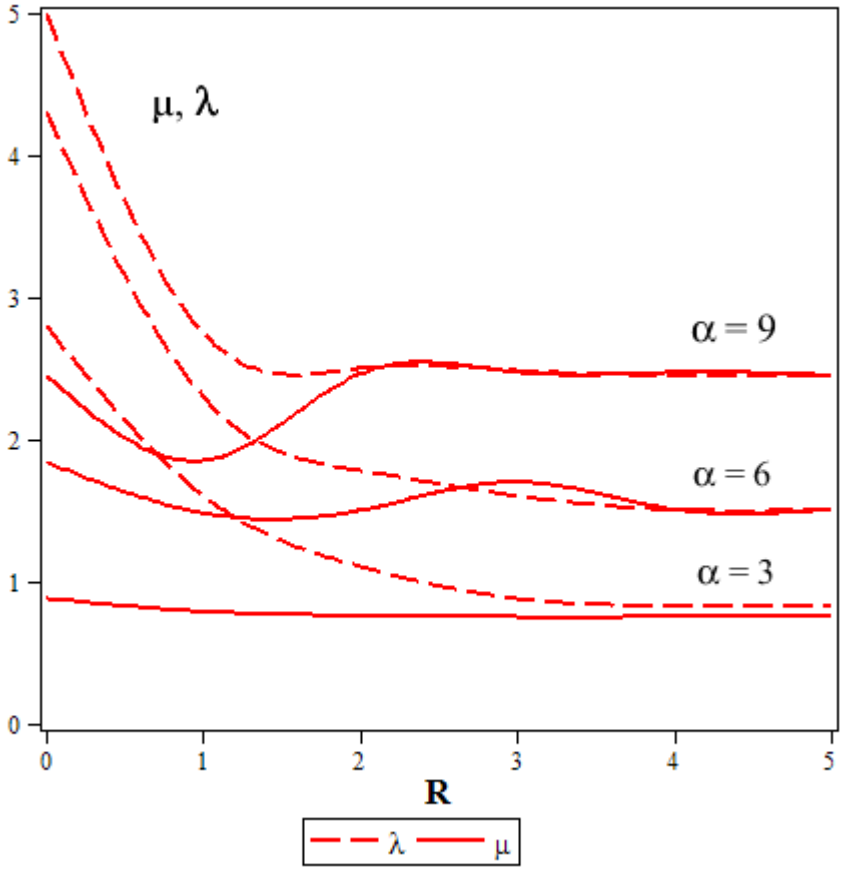

Figure 4.1: The variational parameters μ (solid curve) and λ (dashed Curve) as a function of the wire radius (R).

The relation between the variational parameters (μ, λ) and the radius of the wire R is displayed in figure (4.1). 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 getting smaller the curves begin to split, depicting the anisotropy due to the confinement imposed by the wire boundary.

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

So from the figure (4.1) we note at large values of R (the case approaches the bulk limit), ($\mu = \lambda$), 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 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 [figure (4.2)] the measures of localization of the electron coordinates expressed in terms of the corresponding root-mean-square (r.m.s) value which is given by

$$\xi_\rho = [\,\langle\varphi_e|\rho^2|\varphi_e\rangle\,]^{(\frac{1}{2})} = k^{-1}\sqrt{\sigma_{00}^{(3)}\Big/\sigma_{00}^{(1)}} \qquad (4.2)$$

and

$$\xi_z = [\,\langle\varphi_e|z^2|\varphi_e\rangle\,]^{(\frac{1}{2})} = (2\lambda^2)^{-\frac{1}{2}} \qquad (4.3)$$

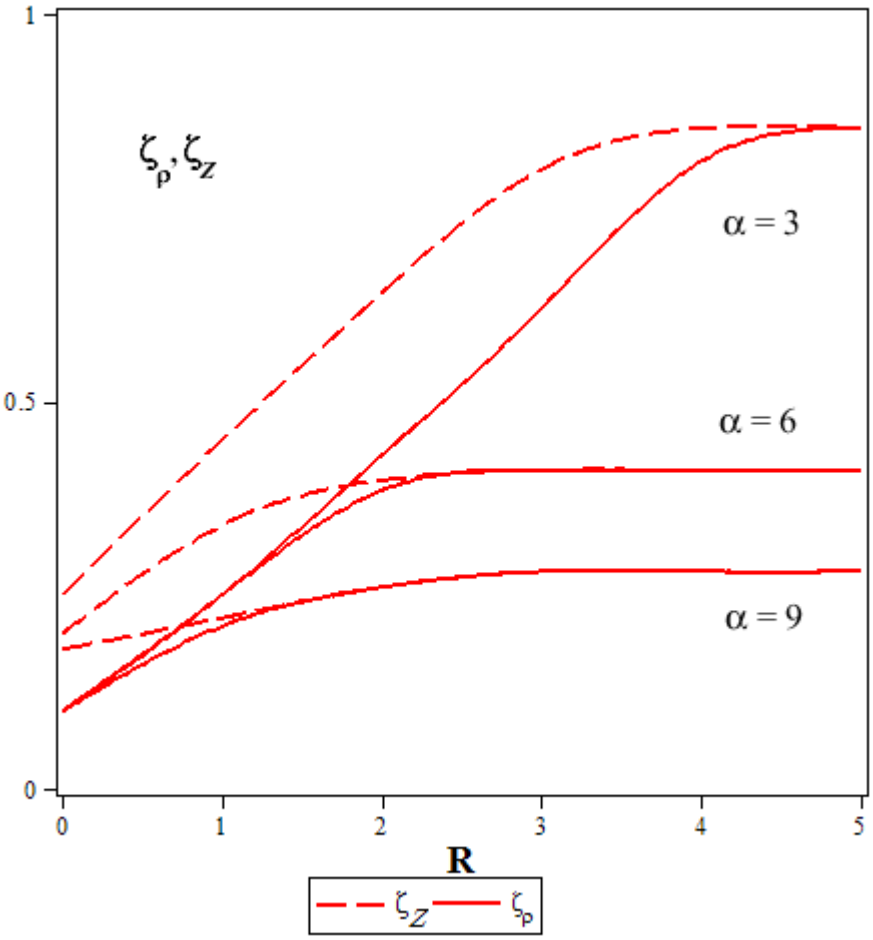

Figure 4.2: The spatial extends ξ_ρ (solid curve) and ξ_z (dashed curve) of the Polaron as a function of the wire radius

We plot the relation between the parameters (ξ_ρ, ξ_z and R). Thus the figures 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 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 on to origin (the polaron center) or will expand to relax itself in the longitudinal directions along the wire axis.

Starting from $R \gg 1$ and then restricting the transverse spread of the electron, the contribution coming from the tendency of the polaron to expand longitudinally is compensated for by the pseudo-enhancement in the effective phonon coupling due to lateral localization towards the wire axis, thus leading to an overall shrinking spatial extent in the $\pm Z$ direction. Meanwhile, with contracting wire size there are results an alteration in the lateral structure of the electron wave function as depicted by the μ-profile, displaying first a monotonic decrease and then an increase, implying that the radial part $\varphi(\rho)$, of the electron wave function conforms to a form structured more by its Bessel-function counterpart $J_0(k\rho)$, rather than a narrow Gaussian$\exp(-{\mu^2\rho^2}/{2})$, decaying far before the boundary is reached. This can alternatively be recognized from the fact that, regardless of α, the curves for ξ_ρ figure (4.2) all tend to the same asymptote, meaning that at small wire radii the lateral extent of polaron is governed mainly by geometric confinement rather than phonon coupling-induced localization.

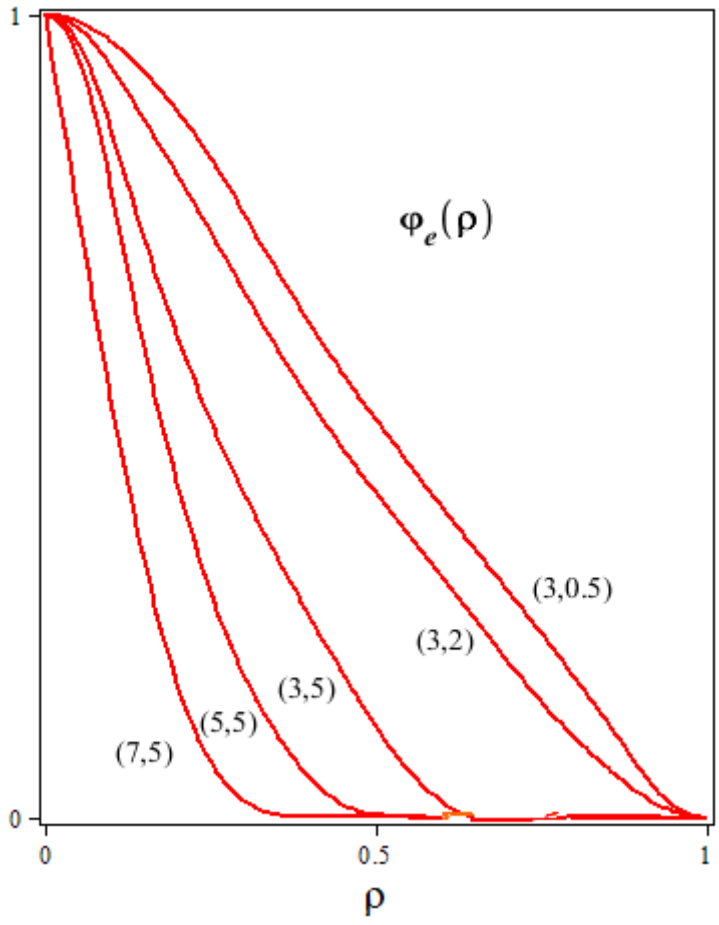

Figure (4.3): $\varphi(\rho)$ versus ρ for various pairs (α, R) of α (= 3, 5,7) and R(= 0.5, 2, 5). In the plots the peak value of φ is normalized to unity, and ρ is expressed in units of R.

For completeness, we also present a pictorial view of the phonon-coupling- induced potential well profiles along the radial and transverse direction.

$$V(\rho,z)=\frac{1}{e}\sum_{Q}\Gamma_{Q}\langle -0|U^{-1}(e^{iQ.r}a_{Q}+e^{-iQ.r}a_{Q}^{\dagger})U|0\rangle \qquad (4.4)$$

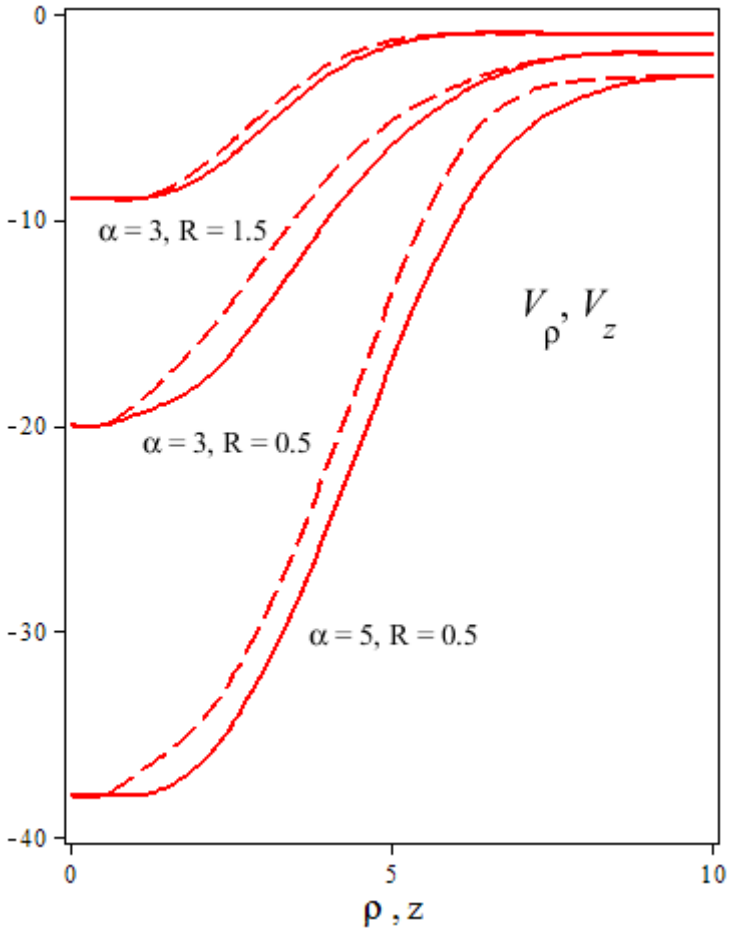

Figure (4.4): the phonon coupling-induced potential well profiles in the radial and longitudinal directions represented, respectively, by the upper and lower curves.

The potentials V_ρ and V_Z are given in arbitrary units on a linear scale, whereas ρ and z are expressed in terms of R. The spatial anisotropy mentioned in the preceding paragraph is also portrayed in the set of curves for the potential profiles in that V_Z lies deviated below V_ρ, the digression being most significant for small R values and at sites more on the boundary side rather than the axial region $(\rho/R, z\,|R \leq 0.1)$ where V_ρ and V_Z join and form spherically symmetric (isotropic) equipotential.

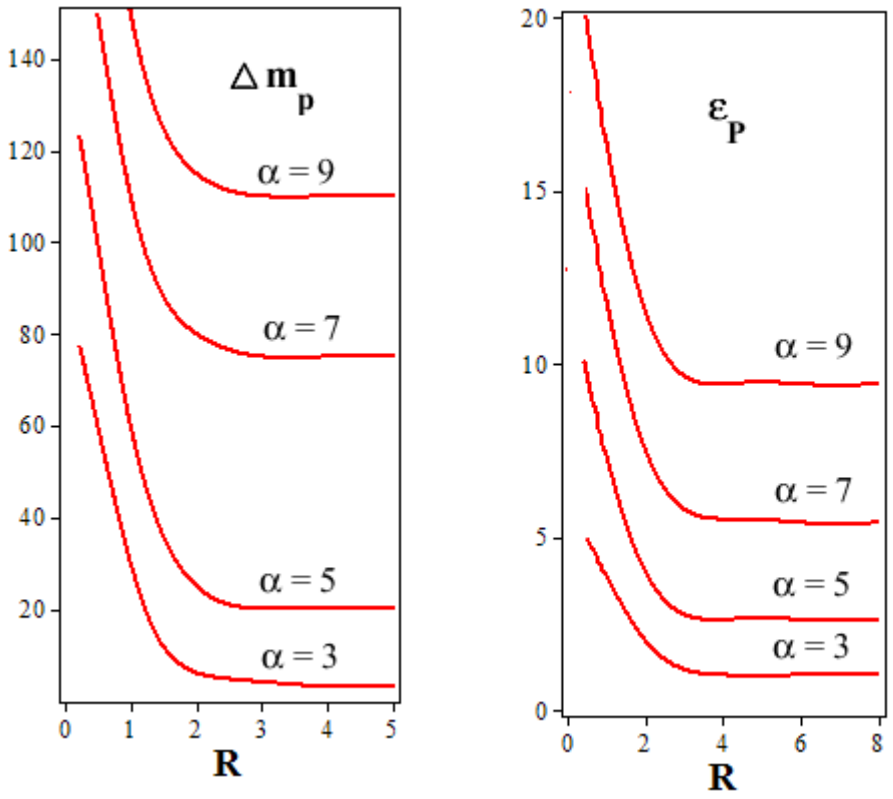

Figure (4.5): ε_ρ and Δm_ρ as function of R.

A more brief content of arguments given above is provided in fig.(4.5) where we plot the binding energy, $\varepsilon_p = (j_{0.1}/R)^2 - E_g$ (relative to the subband), and the polaronic contribution to the band mass, $\Delta m_\rho = m_\rho - 1$, against the wire radius for a set of distinctive α-values. We once again note the same qualitative behavior where the growth rates of ε_p and m_ρ are somewhat moderate for large R, but however on the opposite

extreme where R is tuned to smaller values both $\varepsilon_p$and $m_\rho$are observed to increase with very pronounced slopes the growth rates, which are significantly greater for strong α.

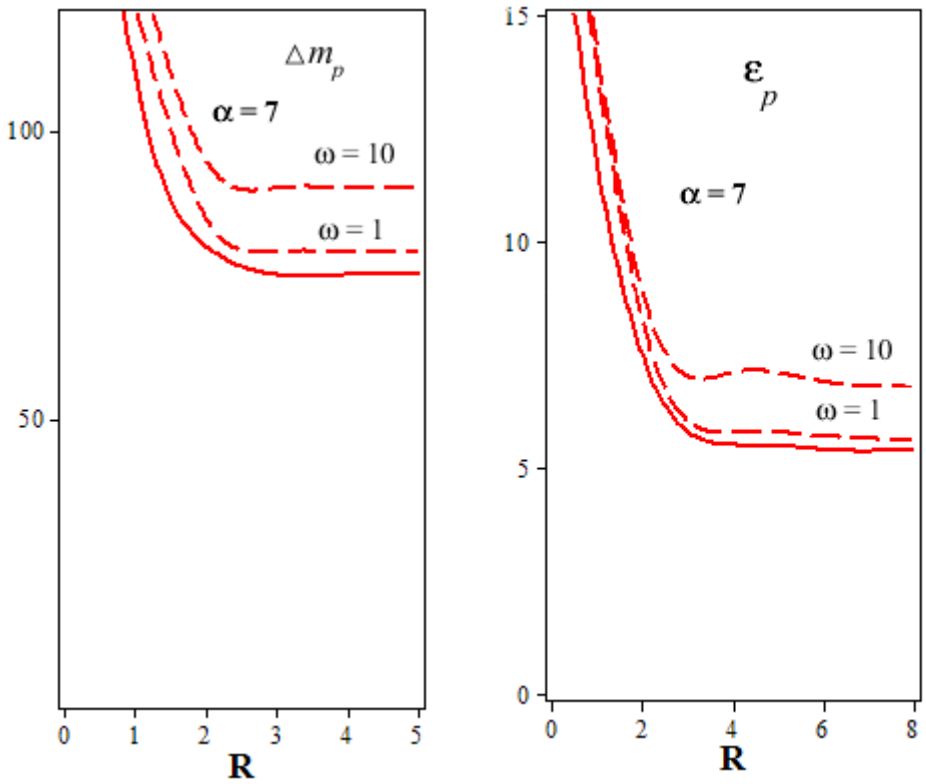

Figure (4.6): ε_ρ and Δm_ρ as function of R under external magnetic field.

It is expected that the application of an external magnetic field puts a further confinement on the problem making the polaronic effect more important. Even though, the problem is somewhat complicated due to the combined effect of the magnetic field and the electron-phonon interaction we will not go in detail for the extreme limits of the magnetic field.

In figure (4.6) the binding energy and the effective mass is plotted versus the radius of the wire for different values of the strength of the magnetic field, for $\alpha = 7$. As it is clear from the figure, the polaronic effect becomes more important for strong values of the magnetic field and large values of the wire radius. As R getting smaller the effect of the magnetic field becomes negligible. This because as the problem squeezes along the transverse of the confinement coming from the geometry of the problem becomes more dominant.

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