Islamic University-Gaza
Deanery of Graduate Science
Faculty of Science
Department of Physics

The Ground State Energy Of The Two Dimensional Polaron

Represented By

Amal Youssef Al-Batniji

Supervisor

Dr. Bassam H. Saqqa

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0.1 Dedication

To my parents, dear husband, and to my children Sara and Abdullah

Amal Y. Al-Batniji
0.2 Acknowledgement

First of all I thank God for all blessings he bestowed on me. I wish to extend my gratitude and appreciation to my supervisor Dr. Bassam Saqqa for his generous help, valuable guidance and his continued encouragement during the preparation of this thesis. I am also most grateful to all my teachers and all members of physics department in the Islamic University for their encouragement. Also I wish to thank my parents and my hole family for their continuous support, special thanks to my husband for his cooperation and patience that kept me productive during this work.
0.3 Abstract

The two-dimensional polaron ground state energy was retrieved using a variational technique proposed by Devreese et al. The calculations was based on a suitable modification of the strong coupling approximation, which enables the adiabatic theory to extrapolate towards the weak coupling approximation through a perturbative scheme. The results of the present work is compared with both the strong and the weak coupling approximations and with the results obtained by the Feynman path-integral.

Within the framework of strong coupling polaron theory the problem of a two-dimensional polaron is studied under the effect of an external magnetic field using two types of variational wavefunction. It is found that the polaronic effect is enhanced with the magnetic field.
0.4 Arabic Abstract
Chapter 1

Introduction

1.1 The Polaron Concept

Atoms or molecules in most solids are assembled in some characteristic regular patterns called crystals. The atoms in a crystal are located on certain positions called lattice points. At room temperature the atoms are not fixed, but rather vibrate about their equilibrium positions. The vibrations of the atoms will form a vector field called the displacement field, which can be quantized. Just as photons, the quanta of the electromagnetic radiation, phonons are the quanta of the displacement field.

An electron in a crystal interacts with these phonons in such a way that phonons clothe the electron to form what is called a polaron. This concept was first introduced by Landau in
1933[1]. According to Landau, the electron polarizes the lattice producing a potential well around itself in which it becomes trapped. This lattice deformation reacts back on the electron and affects the motion so that the electron wave function and the lattice deformation depend upon each other self-consistently.

### 1.2 The Size of the Polaron

The polaron can be classified according to its size (large or small). The small polaron is formed when an electron is trapped by its self-induced atomic displacement field in a region of dimensions in the order of the lattice constant, or we can say that the deformation of the lattice is small. On the other hand when the displacement of the ions are larger than the lattice constant, a large polaron is formed and the deformation of the lattice is large. The large polaron differs from the small polaron in many aspects. In large polaron regime the lattice can be replaced by a continuum which is not appropriate for the small polaron regime. The effective mass of the small polaron is large enough to drastically altering the transport properties of the crystal, while the large polaron has a much smaller ef-
fective mass which is slightly larger than that of the bare bond electron. There are many other types of polarons intermediate between the two extremes. Polarons can bind in pairs, the interaction of two electrons (or holes) with the phonon field may result in a composite quasiparticle called bipolaron. Studies of bipolarons are of interest due to their possible role in high-$T_c$ superconductivity, where $T_c$ is the critical temperature for the superconductivity phenomena [27]. In this work we shall be concerned only with the large polaron.

### 1.3 The Importance of the Study

The polaron theory is of important interest due to what it represents as a theoretical model of a particle interacting with a fluctuating medium. In fact, it was the first problem in condensed matter physics formulated within the framework of quantum field theory [2].

The applications of the problem in condensed matter physics are so significant that, since introduced in 1933, the polaron problem attracted much attention by researchers [2 – 12]. The
bipolaron problem is assumed to be responsible for the formation of the pairing system in the high-$T_c$ superconductivity [3].

The physical properties of the polaron differ from those of the band-electron. In particular, the polaron is characterized by its binding energy, effective mass, and by its response to external electric and magnetic fields.

Today electron systems in reduced dimensions e.g. in two dimensions, like in GaAs-AlGaAs or MOSFETS are of great interest, and the polaron effects should not be completely ignored. Das Sarma and Mason [4] has studied extensively the case of a dynamically two dimensional electron interacting via the Fröhlich Hamiltonian with the bulk longitudinal optical (LO) phonons. Their calculations were based on a strict two dimensional approximation for the electronic wavefunction, the relevant results in the weak, intermediate and strong coupling regimes provide the basic features of the polaron effect in confined structures. A comparison of their results with the corresponding three dimensional values reveals that electron-phonon coupling is considerably enhanced in two dimensions.

The problem of a polaron under the influence of a magnetic
field lays out distinctive qualitative features in the different limits of the magnetic field intensity and the polaron coupling strength. The magnetic field and the phonon coupling play an interrelated rule in the polaron binding.

1.4 The Polaron Theory

Within the framework of quantum field theory, Fröhlich et al [5], have derived the Hamiltonian of the large polaron. In deriving their Hamiltonian the crystal is treated as a continuous medium (continuum approximation). Within this approximation the electron is treated as an entity with an effective mass \( m^* \) reflecting the overall average effect of the lattice potential on the dynamical behavior of the electron (the effective mass approximation).

Using appropriate units \( (2m = \hbar = \omega_{LO} = 1) \), the Fröhlich Hamiltonian is given by

\[
H = H_{\text{electron}} + H_{\text{phonon}} + H_{\text{interaction}} \quad (1.1)
\]

where \( H_{\text{electron}} \) is the Hamiltonian of the electron in the absence
of the phonons, and

\[ H_{phonon} = \sum_Q (a_Q^\dagger a_Q) \]  

(1.2)

is that of the lattice vibrations alone, and

\[ H_{interaction} = \sum_Q V_Q (a_Q e^{i\mathbf{q}.\mathbf{r}} + a_Q^\dagger e^{-i\mathbf{q}.\mathbf{r}}) \]  

(1.3)

describes the electron-phonon interaction. Where \( a_Q^\dagger \) and \( a_Q \) are, respectively the creation and annihilation operators of a phonon, of wave-vector \( \mathbf{Q} \) and frequency \( \omega_{LO} \), and \( V_Q \) is the fourier component of the electron-phonon interaction given by

\[ V_Q = \left( \frac{4 \pi \alpha}{V} \right)^{\frac{1}{2}} / Q \]  

(1.4)

where \( V \) is the volume and

\[ \alpha = \frac{e^2}{2\hbar \varepsilon_0} \sqrt{\frac{2m}{\hbar \omega_{LO}}} \left( \frac{\varepsilon_0}{\varepsilon_\infty} - 1 \right) \]  

(1.5)

being the coupling constant, \( \varepsilon_0 \) and \( \varepsilon_\infty \) are the static and the high frequency dielectric constants, respectively.
Since the Fröhlich Hamiltonian given by eq.(1.1) has no exact solution, different approaches were developed to solve it, among these approaches are:

1. The strong coupling theory developed by Pekar [6]. This theory is valid when the electron’s kinetic energy in the potential well is much greater than the energy of the phonons contributing to the deformation.

2. The perturbation theory is appropriate if the coupling constant is weak. In this case the last term \( H_{interaction} \) of the Hamiltonian given in eq.(1.1), can be treated as a small perturbation. In this picture the lattice polarization tends to follow the electron as it moves, through the crystal.

3. In(1953) Lee, Low, and Pines [7] have derived a variational technique depends on a series of successive canonical transformations which gives good results for the intermediate coupling ie. \( \alpha \gtrsim 3 \). 

4. Feynman path integral method [8]: After studying the Fröhlich Hamiltonian, Feynman got the idea to formulate the polaron problem into the Lagrangian
form of quantum mechanics and then eliminated oscillators. The resulting path integral has a great intuitive appeal, it shows that the polaron as an equivalent one-particle problem, in which the interaction (non-local in time or retarded), is between the electron and itself. Subsequently Feynman showed how the variational principle of quantum mechanics could be adapted to the path integral. Over the years Feynman model for the polaron has remained in many respects the most successful approach to this problem, for the overall range of the coupling constant.

1.5 The Aim of the Work

In this work we attack three problems:

1. A review of the ground state properties of the two-dimensional polaron through a variational method for strong electron phonon coupling is presented in chapter (2). The calculations we use is of a variational nature starting with a localized polaron wavefunction which is good for strong coupling regime.
2. In chapter (3) the ground state properties will be extended for all values of the coupling constant, by an improvement including a first-order perturbative correction to the strong coupling trial state through which the results of the adiabatic theory conform to those obtained from second-order perturbation theory.

We formulate the algebra in a manner proposed by Devreese et al [10]. Our primary aim is to give a comparison of the formulation applied to free two-dimensional polaron with the relevant results obtained by weak and strong coupling theories.

3. Chapter (4) is devoted to the effect of a magnetic field on a two-dimensional polaron. The rules which the magnetic field and the phonon coupling play in the polaron binding is not completely independent, but rather they are interrelated to each other. Each one may dominates over the other. At weak phonon coupling, and moreover if the magnetic field is also weak, the problem can be characterized as consisting of an electron orbiting together with its concomitant lattice deformation with an effective polaron mass rather than the band mass. A contrasting aspect to such a description is the case where the electron goes into a bound
state with a highly localized wavefunction in the deep potential well induced by the lattice polarization.

Due to the distinguishing features of the theory in the extreme limits of the fields we think it is more appropriate to study the problem using two types for the electronic wavefunction.

(a) A gaussian trial wavefunction:

\[ \psi = Ne^{-\beta r^2} \] (1.6)

(b) A 1-s like trial wavefunction:

\[ \psi = Ne^{-\beta r} \] (1.7)

and the ground state energy will be calculated for different values of both the magnetic field strength (\(\omega_c\)), and the coupling constant (\(\alpha\)).

4. In chapter (5) we display the results of the work with a discussion of the physical interpretation of the problems. A concluding remarks are also presented in this last chapter.
Chapter 2

The Strong Coupling Regime

As an electron moves through a polar crystal it generates a distortion which acts back on the electron. For large enough coupling constants this lattice distortion forms such a deep potential well that the electron becomes self-trapped in this well. Since the ions are heavy, the lattice distortion which is associated with the polarization is assumed to remain at rest, so the electron moves in a static potential well centered around a fixed point in the crystal, taken as the origin of the axis. Inside the potential well the electron undergoes quantum fluctuations about the center. These fluctuations are due to emission and absorption of virtual phonons[13-16].

In the frame work of the adiabatic approximation, we start with the Hamiltonian of an optical polaron confined to a two-
dimensions well. The Hamiltonian of eq.(1.1) is rewritten as:

\[ H = H_e + \sum_Q a_Q^\dagger a_Q + \sum_Q V_Q (a_Q e^{iq.r} + a_Q^\dagger e^{-iq.r}) \] (2.1)

with

\[ H_e = -\frac{1}{r} \frac{\partial}{\partial r} (r \frac{\partial}{\partial r}) - \frac{1}{r^2} \frac{\partial^2}{\partial \phi^2} \] (2.2)

is the electronic part of the Hamiltonian, in cylindrical coordinates.

\(^{12}\)

\(a_Q^\dagger\) and \(a_Q\) are respectively, the creation and annihilation operators for a three-dimensional phonon of wavevector \(Q = (q, q_z)\) and frequency \(\omega_0\). The interaction amplitude is related to the electron-phonon coupling constant \(\alpha\) and the phonon wavevector \(Q\) through

\[ V_Q = \left( \frac{4\pi \alpha}{Q^2} \right)^{1/2} \] (2.3)

In the above relation, the normalization volume is set to unity for notational convenience.

To obtain the binding energy in the adiabatic approximation we take the Pekar-type [6] trial state which is separable into the
particle part $\phi_0$ and the phonon part $\phi_{ph}$, that is

$$\psi = \phi_0 \cdot \phi_{ph}$$

(2.4)

with

$$\phi_{ph} = U |0 >$$

(2.5)

The ket $|0 >$ describes the phonon vacuum state, simply because at low temperature ($KT << \hbar \omega_0$) there will be no effective phonons. The unitary operator $U$ is given by

$$U = \exp \left[ \sum_Q V_Q \sigma_q (a_Q - a_Q^\dagger) \right]$$

(2.6)

It is a displaced oscillator transformation which produces a lattice deformation centered at the origin[9].

Under the displaced oscillator transformation

$$H \Rightarrow \dot{H} = U^{-1} H U$$

and using the rule

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

(2.7)
we obtain

\[ U^{-1}H_eU = H_e \quad , \]  
(2.8)

\[ U^{-1}(\sum_Q a_Q^{\dagger}a_Q)U = \sum_Q a_Q^{\dagger}a_Q - \sum_Q V_Q\sigma_q a_Q^{\dagger} - \sum_Q V_Q\sigma_q a_Q + \sum_Q V_Q^2\sigma_q^2 \]  
(2.9)

and

\[ U^{-1}(\sum_Q V_Q(a_Qe^{iq.r} + a_Q^{\dagger}e^{-iq.r}))U = \sum_Q V_Qa_Qe^{iq.r} - \sum_Q V_Q^2\sigma_q e^{iq.r} \]  
\[ + \sum_Q V_Qa_Q^{\dagger}e^{-iq.r} - \sum_Q V_Q^2\sigma_q e^{-iq.r} \]  
(2.10)

Equations (2.7), (2.8), and (2.9) will form the modified Hamiltonian as

\[ \dot{H} = H_e + \sum_Q a_Q^{\dagger}a_Q - \sum_Q V_Q\sigma_q a_Q^{\dagger} - \sum_Q V_Q\sigma_q a_Q + \sum_Q V_Q^2\sigma_q^2 \]  
\[ - \sum_Q V_Q^2\sigma_q e^{iq.r} + \sum_Q V_Qa_Q e^{iq.r} + \sum_Q V_Qa_Q^{\dagger} e^{-iq.r} - \sum_Q V_Q^2\sigma_q e^{-iq.r} \]  
(2.11)
Defining

\[ \eta_q = (e^{i\mathbf{q} \cdot \mathbf{r}} - \sigma_q) \quad , \quad (2.12) \]

the Hamiltonian simplifies to

\[
\hat{H} = H e + \sum_Q a_Q^\dagger a_Q + \sum_Q V_Q^2 \sigma_q^2 - \sum_Q V_Q^2 \sigma_q (e^{i\mathbf{q} \cdot \mathbf{r}} + e^{-i\mathbf{q} \cdot \mathbf{r}}) \\
+ \sum_Q V_Q (\eta_q a_Q + \eta_q^* a_Q^\dagger) \\
(2.13)
\]

In the self trapping picture, the electron distribution and the lattice polarization influence each other in such away that a stable relaxed state is eventually attained.

Choosing a Gaussian trial wavefunction

\[
\phi_0 = \sqrt{\frac{2}{\pi \beta^2}} e^{-r^2/\beta^2} \quad (2.14)
\]

with \(\beta\) is a variational parameter, the expectation value of \(\hat{H}\) in the trial state is now given by
\[ <\psi|\hat{H}|\psi> = e_0 - \lambda_0 \quad (2.15) \]

where

\[ e_0 = \frac{2}{\beta^2} \quad (2.16) \]

and

\[ \lambda_0 = \sum_Q V_Q^2 \sigma_q^2 = \frac{\sqrt{\pi} \alpha}{\beta} \quad (2.17) \]

minimizing with respect to \( \beta \), we can establish an approximate result of the ground state energy of a strongly coupling 2D polaron as

\[ E = -\left(\frac{\pi}{8}\right) \alpha^2 \quad (2.18) \]
Chapter 3

The Extended Regime

In extending our work to be appropriate for all the values of the coupling constants, the procedure is to start with the standard canonical transformation of the strong coupling formulation and then modify the adiabatic polaron state via a variationally determined perturbative extension serving for the theory to interpolate in the overall range of the coupling constant.

As we go toward the case of weak coupling the degree of localization of the electron becomes reduced in a significant manner, eventually \( \sigma_q \to 0 \), then \( U \to 1 \), and thus \( \hat{H} \) converts back to the initial form of the Hamiltonian in eq.(2.1).

In view of this procedure, we are going to include a first or-
der correction to the trial state \((\phi_0|0>)\) with the last term in eq.(2.13) being a perturbation. We then have

\[
\delta \psi = \sum_Q V_Q \sum_i |i> \frac{<i|\eta_q^* a_Q|\phi_0>|0>}{\epsilon_0 - \epsilon_n - 1} \quad (3.1)
\]

The summation over the intermediate states \((|i>=\phi_n|1_Q>)\), can be projected out simply by replacing the energy denominator by an average quantity which in the calculation will be determined variationally. In complete form we write

\[
\delta \psi = \sum_Q V_Q g_q \eta_q^* a_Q^\dagger |\phi_0> |0> \quad (3.2)
\]

The trial wavefunction for the Hamiltonian is then extended to

\[
\psi_{ext} = c|\phi_0> |0> + \delta \psi = c|\phi_0> |0> + \sum_Q V_Q g_q \eta_q^* a_Q^\dagger |\phi_0> |0> \quad (3.3)
\]

where \(c\) is a normalization constant.

Applying the normalization condition \(\int \psi_{ext}^* \psi_{ext} dv = 1\) we will get
\[ c^2 + \sum_Q V_Q^2 g_q^2 h_q = 1 \]

where \((h_q = 1 - \sigma_q^2)\). Or we write

\[ F(c, g_q) = c^2 + \sum V_Q^2 g_q^2 h_q - 1 = 0 \quad , \quad (3.4) \]

and \(g_q\) is a variational parameter determining the fractional admixture of the strong and weak coupling counterparts of the problem\([9]\).

The optimal fit to \(g_q\) is achieved by minimizing the expectation value of \(\hat{H}\) subject to the constraint (3.4). Now, we find

\[ < \psi_{ext} | \hat{H} | \psi_{ext} > = c^2 e_0 + \lambda_0 (1 - 2 c^2) + 2c \sum V_Q^2 g_q h_q \]

\[ + \sum V_Q^2 g_q^2 (e_q + f_q + h_q) \quad (3.5) \]

where

\[ e_q = < \phi_0 | \eta_q \ H_e \ \eta_q^* | \phi_0 > = \frac{1}{2} q^2 + (\frac{1}{2} q^2 + e_0) h_q \quad , \quad (3.6) \]
\[ f_q = - \sum V_Q^2 \sigma_q < \phi_0 | \eta_q (e^{i\mathbf{q} \cdot \mathbf{r}} + e^{-i\mathbf{q} \cdot \mathbf{r}}) \eta_q^* | \phi_0 > \]

\[ = 2 \lambda_0 [2 e^\gamma I_0(\gamma) - 1] \sigma_q^2 - 2 \lambda_0 \]  

(3.7)

with \( \gamma = (\beta^2/32) q^2 \), and \( I_0 \) is zeroth order of modified Bessel function.

According to the variational procedure

\[ \frac{\partial}{\partial g_q} (E - \lambda F) = 0 \]  

(3.8)

with \( \lambda \) being a Lagrange multiplier, we get

\[ g_q/c = -h_q [(1 - e_0 + 2 \lambda_0 - \lambda) h_q + e_q + f_q]^{-1} \]  

(3.9)

with

\[ \lambda = \sum Q V_Q^2 (g_q/c) h_q \]  

(3.10)

The expression for the energy is then
\[ E = e_0 - \lambda_0 + \lambda, \quad (3.11) \]

which is to be further minimized, numerically, with respect to \( \beta \) and \( \lambda \).
Chapter 4

Two Dimensional Polaron in a Magnetic Field

For the case of a two-dimensional polaron under a magnetic field the binding energy is expected to get even deeper due to the additional degree of localization brought about by the magnetic field. A way to investigate this totally distinctive aspect is either to imagine a rather strong coupling to the lattice or to go over to the high magnetic field limit where the lattice can only respond to the mean charge density of the rapidly orbiting electron and hence acquire a static deformation over the entire Landau orbit.

An important contribution to the theoretical study of polarons in magnetic fields was made by Larsen [26]. In particu-
lar he was the first to point out the level of repulsion close to the crossing of the levels at \((\omega_c = \omega_{LO})\).

Using the symmetric gauge \(\vec{A} = \frac{B}{2}(-y, x, o)\) for the vector potential[9], the Hamiltonian of a two-dimensional polaron immersed in a magnetic field \(\vec{B} = B \hat{Z}\) is:

\[
H = H_e + \sum_Q a_Q^\dagger a_Q + \sum_Q V_Q\left(a_Q e^{iq\cdot\vec{r}} + a_Q^\dagger e^{-iq\cdot\vec{r}}\right) \quad (4.1)
\]

with

\[
H_e = P^2 + \frac{1}{4} \left(\frac{\omega_c}{2}\right)^2 r^2 + \left(\frac{\omega_c}{2}\right) l_Z \quad (4.2)
\]

where \(\vec{r} = (x, y)\) denotes the electron position in the transverse plane, \((L_Z = x P_y - y P_x)\) is the angular momentum, and \(\omega_c = eB/mc\omega_{LO}\) is the dimensionless cyclotron frequency.

Using cylindrical coordinates, the electronic Hamiltonian is written as

\[
H_e = \left(-\frac{1}{r} \frac{\partial}{\partial r} (r \frac{\partial}{\partial r}) - \frac{1}{r^2} \frac{\partial^2}{\partial \phi^2}\right) + \frac{1}{4} \left(\frac{\omega_c}{2}\right)^2 r^2 - i\hbar \left(\frac{\omega_c}{2}\right) \frac{\partial}{\partial \phi} \quad (4.3)
\]
Applying the same procedure of chapter (2), we will modify our Hamiltonian under the same displaced oscillator transformation ($U$), but since ($U$) does not affect the electronic Hamiltonian, our modified Hamiltonian ($\hat{H}$) will be the same as in eq.(2.4).

The expectation value under the same Gaussian wave function defined in eq.(2.14) is

$$< \psi | H | \psi > = e_0 - \lambda_0 = \frac{2}{\beta^2} + \frac{1}{4} \left( \frac{\omega_c}{2} \right)^2 \frac{\beta^2}{2} - \frac{\sqrt{\pi \alpha}}{\beta}$$  \hspace{1cm} (4.4)

Here we notice that $e_0$ has been modified under the effect of the magnetic field to be

$$e_0 = \frac{2}{\beta^2} + \frac{1}{4} \left( \frac{\omega_c}{2} \right)^2 \frac{\beta^2}{2}$$  \hspace{1cm} (4.5)

Notice that in the absence of the magnetic field ($\omega_c = 0$), $e_0$ conforms back to eq.(2.16) as expected.

To find the ground-state energy we will minimize with respect to $\beta$. The energy for different values of $\omega_c$ and $\alpha$ was calculated numerically.
To give a comprehensive picture of the influence of the magnetic field on the polaron problem, we recalculated the energy of our problem using a 1-s like trial wavefunction, which is expected to be appropriate for the case of weak magnetic field densities. The wavefunction is

\[ \phi_0 = N e^{-r/\beta^2}, \quad (4.6) \]

with

\[ N = (2/\pi \beta^4)^{1/2}, \quad (4.7) \]

is the normalization constant of the above wavefunction.

Using this new wavefunction we find

\[ \sigma_q = \langle \phi_0 | e^{\pm i\mathbf{q} \cdot \mathbf{r}} | \phi_0 \rangle = 1/\left(1 + \frac{\beta^4 q^2}{4}\right)^{3/2}, \quad (4.8) \]

and the ground state-energy is

\[ E = e_0 - \lambda_0 = \frac{1}{\beta^4} + \frac{3}{8} \left(\frac{\omega_c}{2}\right)^2 \beta^4 - \frac{3}{8} \left(\frac{\alpha \pi}{\beta^2}\right) \quad (4.9) \]
where $e_0 = \frac{1}{\beta^4} + \frac{3}{8} \left( \frac{\omega_c}{2} \right)^2 \beta^4$, and $\lambda_0 = \frac{3}{8} \left( \frac{\alpha \pi}{\beta^2} \right)$

Again the minimization process will be done numerically.
Chapter 5

Results and Discussion

5.1 Strong and Weak Coupling Results

The strong coupling binding energy that obtained eq.(2.18) is exactly the same as obtained by Das Sarma and Mason [4]. The same problem has been studied by Xiaoguang et al [23] utilizing what they refer to as the modified Pekar-type ansatz:

\[ \phi_0 = [1 + br + a(br)^2 + c(br)^3 + d(br)^4]e^{-br} \]  \hspace{1cm} (5.1)

The presumably exact result they obtained is \( E_g = -0.4047\alpha^2 \).

Even though the usage of such a four-parameter form for the electronic wavefunction would have been more appropriate here, we have chosen to use the approximate Gaussian form to facilitate our calculation so that we can obtain the results analytically which would be very tedious otherwise. Yet, in spite of
this simplification, we see that for large $\alpha$ ($\alpha = 10$ for instance) the discrepant is not more than 3%. The corresponding result for the 3D case is $E_g = -0.106 \alpha^2$. Thus the strong-coupling polaron binding energy is about four times larger in 2D compared with that of 3D case. This leads to the conclusion that the polaronic effect is more pronounced in low dimensional systems due to the further confinement brought about by the low dimensionality.

Examining the extended regime result eq.(3.11) we see that it differs from the strong-coupling result eq.(2.15) only by the last term $\lambda$, which depends, implicitly on $\alpha$ via eq.(3.10). For large coupling-constant $\alpha$, $\lambda \rightarrow 0$ and the strong coupling limit is readily obtained. For loosely bound electron however, (for small $\alpha$), the rule $\lambda$ plays becomes very prominent and the polaron binding energy is determined dominantly by this term. For instance, for $\alpha = 10$, $\lambda = -0.98$, which represents (2.4%) of the energy. However, for $\alpha = 0.01$, $\lambda = -1.5 \times 10^{-2}$, that represents (99.7%) of the energy. Due to the analytic complexity, the minimization of eq.(3.11) with respect to the parameters $\beta$ and $\alpha$ is performed numerically.
In Figure (5.1) we display the present theory compared with the strong and the weak coupling results of Xiaoguang [23]. As it is clear from the figure, the present theory tends to the strong coupling limit for $\alpha \gg 1$ and coincide with the weak coupling results for $\alpha \ll 1$.

In order to test the validity of the present formalism for intermediate values of the coupling constant we tabulate in Table (5.1) our results with the corresponding results of the Feynman path integral and also with the results of the Gaussian approximation, which is a special case of the Feynman polaron model. The results of both the Feynman and Gaussian approximations written in the table is obtained by translating the $3D$-values already obtained by the two approximations to the $2D$-case through the scaling relation derived by Xiaoguang et al [23], given by $E_{2D}(\alpha) = \frac{2}{3} E_{3D}(\frac{3\pi}{4} \alpha)$, which relates the $3D$ and the $2D$ polaron ground state energies. A comparison of the corresponding values in the table reveals that the agreement is fairly good for the extreme limits of the coupling constant. For not too weak coupling the present theory may not be as successful as in the $\alpha \to 0$ limit, since the trial wavefunction given by eq.(3.3) involves a perturbative correction to the adiabatic
Figure 5.1: The 2D polaron binding energy in $\hbar \omega$ versus $\alpha$. The solid curve represents the present calculations, whereas the dashed and the dotted curves respectively provide the weak and the strong coupling approximations.
state $\phi_0|0\rangle$ up to first order only. An improvement would be achieved if one extend the trial state further to cover higher order perturbation corrections.

Table 5.1: The 2D polaron binding energy of the present calculation compared with that of the Feynman and Gaussian approximations [9]. Energies are given in units of $\hbar\omega$.

<table>
<thead>
<tr>
<th>$\alpha$</th>
<th>present work</th>
<th>Feynman</th>
<th>Gaussian</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.424</td>
<td>0.539</td>
<td>0.675</td>
<td>0.667</td>
</tr>
<tr>
<td>1.273</td>
<td>1.543</td>
<td>2.089</td>
<td>2.000</td>
</tr>
<tr>
<td>2.122</td>
<td>2.807</td>
<td>3.627</td>
<td>3.333</td>
</tr>
<tr>
<td>2.971</td>
<td>4.536</td>
<td>5.409</td>
<td>4.905</td>
</tr>
<tr>
<td>3.820</td>
<td>6.801</td>
<td>7.657</td>
<td>7.144</td>
</tr>
<tr>
<td>4.669</td>
<td>9.624</td>
<td>10.470</td>
<td>10.000</td>
</tr>
</tbody>
</table>

### 5.2 The Effect of an External Magnetic Field

The application of an external magnetic field on the polaron problem brings about very interesting physical features due to the interrelation between the strength of the magnetic field and the coupling strength of the polaron. Let us first test the present approach for the extreme limits of the strong and weak fields. For weak electron-phonon coupling and large magnetic field strength,
the first and second terms in eq.(4.4) play the main rule to find the expectation value of the energy, so we can neglect the too small third term. The optimal value of $\beta$ which minimizes the dominant part is $\beta^2 = 8/\omega_c$. Substituting in eq.(4.4) we obtain

$$E = \frac{\omega_c}{2} - \frac{1}{2} \alpha \sqrt{\frac{\pi \omega_c}{2}}$$

(5.2)

which differs from the results of the second-order perturbation of Larsen [26] just by the factor 2 in the dominator in the square root. The reason in our opinion for this difference is that in this limit the lattice deformation should not be treated as surrounding the mean density of the electron. This means that the unitary operator defined in eq.(2.6) should be modified such that the lattice deformation taken to be centered on the Landau orbit center rather than at the origin (A.Erçelebi and B.Saqqa)[11].

On the other extreme of the magnetic field, $\alpha \gg 1$ and $\omega_c$ is too small, the dominant terms in eq.(4.4) are the first and the third, and the second one is only a small correction, then the optimal $\beta$ value is $4/(\alpha \sqrt{\pi})$, yielding

$$E = -\frac{\pi \alpha^2}{8} + \frac{\omega_c^2}{2\pi \alpha^2}$$

(5.3)
which is the $2D$-analogue of the corresponding $3D$ value.

In order to explore the ground state energy for the overall range of the fields we minimize eq.(4.4) numerically.

**Table 5.2:** Comparison between the present calculations with the Feynman approximation. The first, second and third rows, represent respectively, our results, using Gaussian, using 1s and the Feynman results of[22]. Energies are given in units of $\hbar \omega$.

<table>
<thead>
<tr>
<th>$\alpha \backslash \omega_c$</th>
<th>0.1</th>
<th>0.2</th>
<th>1</th>
<th>2</th>
<th>10</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.1</td>
<td>0.0291</td>
<td>0.0709</td>
<td>0.4360</td>
<td>0.9100</td>
<td>4.8008</td>
</tr>
<tr>
<td></td>
<td>0.0396</td>
<td>0.0924</td>
<td>0.5462</td>
<td>1.1316</td>
<td>5.9167</td>
</tr>
<tr>
<td></td>
<td>-0.109</td>
<td>-0.061</td>
<td>0.3224</td>
<td>0.8030</td>
<td>4.6826</td>
</tr>
<tr>
<td>1</td>
<td>-0.391</td>
<td>-0.386</td>
<td>-0.266</td>
<td>-0.0116</td>
<td>2.9094</td>
</tr>
<tr>
<td></td>
<td>-0.3443</td>
<td>-0.3364</td>
<td>-0.1564</td>
<td>0.1963</td>
<td>3.9675</td>
</tr>
<tr>
<td></td>
<td>-1.592</td>
<td>-1.560</td>
<td>-1.307</td>
<td>-0.983</td>
<td>1.8262</td>
</tr>
<tr>
<td>4</td>
<td>-6.283</td>
<td>-6.282</td>
<td>-6.273</td>
<td>-6.243</td>
<td>-5.399</td>
</tr>
<tr>
<td></td>
<td>-5.551</td>
<td>-5.550</td>
<td>-5.534</td>
<td>-5.484</td>
<td>-4.159</td>
</tr>
</tbody>
</table>

In Table (5.2) we tabulate our results for the two choices of the wavefunction together with that obtained by the generalized
Feynman approximation [22]. First we notice that the discrepancy between the two choices is very large for large $\alpha$ and large $\omega_c$ which we expected since in these two limits the problem is approximately harmonic oscillator. A comparison with the results of [22] shows that the present model is capable of reproducing similar qualitative features as obtained by Xiaoguang. et al [22], but however yields higher values for the energy. The reason for the difference is mostly due to the superiority of the Feynman path integral theory which proven to be valid for all values of the polaron coupling constant.

In order to make the comparison more constructive we tabulate our results together with that obtained using eq.(15) of [22]

\[
E_{wpd} = -\frac{\pi}{8} \alpha^2 - 2 \ln 2 - \frac{1}{2} + \frac{\omega_c}{2 v^2}
\]  
(5.4)

with \(v = \pi \alpha^2/4 - 1.773\)

which is expected to be valid for \(\alpha \gg 1\) and \(\omega_c \ll \omega_c = 0.1\) and large values of \(\alpha\) which is the scope of this work, [Table(5.3)]

As it is clear from the table the present work gives approximately similar results for large values of \(\alpha\). For instance the difference between the two results decreases from about 23% for \(\alpha = 4\) to just 4.6% for \(\alpha = 10\).
Table 5.3: Comparison between the present calculations for $\omega_c = 0.1$ using the two choices of the wavefunction and that obtained by Wu et al. (22).

<table>
<thead>
<tr>
<th>$\alpha$</th>
<th>$E_{Gaussian}$</th>
<th>$E_{1s}$</th>
<th>$E_{wpd}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>4</td>
<td>-6.283</td>
<td>-5.551</td>
<td>-8.169</td>
</tr>
<tr>
<td>5</td>
<td>-9.817</td>
<td>-8.674</td>
<td>-11.703</td>
</tr>
<tr>
<td>6</td>
<td>-14.137</td>
<td>-12.491</td>
<td>-16.023</td>
</tr>
<tr>
<td>7</td>
<td>-19.242</td>
<td>-17.002</td>
<td>-21.128</td>
</tr>
<tr>
<td>8</td>
<td>-25.132</td>
<td>-22.206</td>
<td>-27.018</td>
</tr>
<tr>
<td>9</td>
<td>-31.808</td>
<td>-28.105</td>
<td>-33.694</td>
</tr>
<tr>
<td>10</td>
<td>-39.269</td>
<td>-34.697</td>
<td>-41.155</td>
</tr>
</tbody>
</table>

In Figure (5.2) we display the binding energy versus the coupling constant $\alpha$ for two different values of the magnetic field ($\omega_c = 0.1, 10$). We see that the two curves matches for large $\alpha$ and this leads to the conclusion that for large coupling constant the polaronic effect becomes dominant and plays the main rule in determining the ground state energy over the effect of the magnetic field. Therefore, the effect of the magnetic field on the polaron problem is pronounced for weak coupling limits only.
Figure 5.2: The binding energy calculated for the Gaussian wavefunction in units of $\hbar \omega$ versus $\alpha$. The dotted curve represents $\omega_c = 0.1$, whereas the solid curve represents $\omega_c = 10$. 
5.3 Conclusions

We have studied the problem of the 2D polaron using the variational approach of Devreese et al [10]. In view of the results that obtained, we conclude that the theory sets 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 the perturbation theory. The shortcoming encountered here is essentially due to the extended trial wavefunction given by eq.(3.3) which involves a perturbative correction to the adiabatic state up to first order only. In our opinion an improvement would be achieved by extending the trial state of Devreese et al [10] so as to cover higher order corrections.

The problem of a 2D-polaron in a magnetic field is revised using the strong-coupling regime with two types of the variational wavefunction, a Gaussian wavefunction and a H-like wavefunction. It has been observed that the magnetic field put additional confinement to the problem making the polaronic effect more important. We believe that further improvement and considerably better results should be achieved if one adopts a suit-
ably modified coherent phonon state which takes into account whether the lattice deformation tends to cover the entire Landau orbit or the average electron position. The problem can be reconsidered using the modified trial state of Devreese et al [10] to cover the overall range of the coupling constant. Even though the procedure is straight-forward, the corresponding algebra is somewhat tedious.
Bibliography


