PHONON-COUPLING AND MAGNETIC FIELD EFFECTS ON THE BINDING ENERGY OF A HYDROGENIC IMPURITY IN TWO DIMENSIONS

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By

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ABSTRACT

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M.S. in Physics
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September, 2006

Electron-phonon interaction and magnetic field effects on a two-dimensional electron bound to a Coulomb center is studied within the framework of a variational approximation consisting of an adiabatic polaronic wave function corrected by a first order perturbative extension by which it is possible to interrelate the strong and weak coupling counterparts of the coupled electron-phonon system. Various aspects of the problem is considered depending on the Coulomb interaction, magnetic field, and electron-phonon coupling strength.

Keywords: Electron-phonon interaction strength, Coulomb interaction, magnetic field strength, perturbative extension, strong and weak coupling, Fröhlich Hamiltonian.

ÖZET

İKİ BOYUTLU HİDROJENİK SAFSIZLIĞIN BAĞLANMA ENERJİSİNE POLARON VE MANYETİK ALAN ETKİSİ

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Çiftleşimli elektron-fonon sisteminin, kuvvetli ve zayıf etkileşim durumlarını birbiriyle bağdaştırmayı mümkün kılan, birinci dereceden tedirgeme genişletmesi sayesinde düzeltilen adiyabatik polaronik dalga fonksiyonunu kapsayan, Coulomb merkezine bağlı iki boyutlu elektron üzerine olan elektron-fonon etkileşimi ve manyetik alan etkisi, çeşitli kuramsal yaklaşımlar altında çalışıldı. Coulomb etkileşimi, manyetik alan ve elektron-fonon etkileşim kuvvetlerine bağlı olarak problemin çeşitli safhaları gözönüne alındı.

Anahtar sözcükler: Elektron-fonon etkileşim kuvveti, Coulomb etkileşmesi, manyetik alan kuvveti, tedirgeme genişletmesi, kuvvetli ve zayıf etkileşim, Fröhlich Hamiltonu.

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Contents

List of Figures

List of Tables

Chapter 1

INTRODUCTION

1.1 Historical Introduction

The problem of the motion of an electron in an ionic crystal has been of interest ever since solid state physics began to develop in the early 1930's. The interest in this problem has continued to the present day for two main reasons. Firstly, and more obviously, it is relevant to the applied physics of semiconductors. Secondly, it provides a simple model of a particle interacting with a quantum field, and serves as a testing ground for new methods.

In this historical sketch we hope to illustrate how the attitudes and procedures involved in the development of a physical theory may fail to be reflected in the final solution; conversely, much time and effort may have been taken on what, in retrospect, seems an obvious step. As an example let us look briefly at the concept of free electrons in the theory of metals. By neglecting Coulomb interactions, the free-electron model appeared for many years to be based on inconsistent approximations; Wigner's calculation of the correlation energy (in 1933) showed that Coulomb effects were far from negligible. It was only in the early 1950's that the application of the plasma concept and the understanding of the screening effect in the electron gas effectively validated the independent-electron concept. Both the physical concept and the mathematical techniques had been familiar for

many years, yet the essential step was slow in coming.

An optical polaron is an electron interacting with the longitudinal optical lattice vibrations of an ionic crystals. Historically, the polaron problem has been approached from two points of view. One idea is the self-trapped electron. The other is based on the idea of electron-phonon scattering.The idea of self-trapped electron was first introduced by Landau in 1933 [1] in order to explain F centers. Pekar [2] worked this theory in detail. His work is the extreme strong coupling theory of the polaron. Bogolubov and Plechko [3] extended Pekar's theory towards lower coupling constants by developing a method for writing the polaron energy as an infinite series in inverse power at the coupling constant α in 1949.

The idea of electron phonon interaction was first introduced by Bloch in 1930. The interaction of such electrons with the thermal vibrations of the lattice was calculated and used to find the electron scattering, and hence the mobility.

In 1937, Fröhlich [5] gave a quantitative treatment of electron scattering in ionic crystals. In considering the interaction of the electrons with the vibrating lattice, the concept of the field of lattice displacements (polarization field) was introduced. It was eleven years later that the application of field-theoretic concepts was introduced to the subject as a preliminary investigation in an attempt to approach the problem of superconductivity. In this work, not only was scattering treated, but the electron self energy in the lattice was calculated. A variational approach based on the wave functions of perturbation theory was used: it was found that the perturbation theory energy was lower than that obtained variationally. It was subsequently found that new methods were required to treat the intermediate-coupling problem. The critical step in the theoretical problem had been the formulation of the problem of electrons interacting with the field of lattice vibrations (phonons) in Hamiltonian form:

$$H = H_{electron} + H_{phonon} + H_{e-p\ interaction}. \tag{1.1}$$

This Hamiltonian is used as a basis for all present day work on the polaron.

This non-relativistic problem is of general field-theoretical interest, in so far as the self energy does not diverge as it apparently does in all relativistic field theories. A striking example of the use of polarons as a testing ground for new methods is provided by Feynman's application of the path-integral method.

The above methods treat the polarization field as a continuum, which becomes unrealistic in the case of strong coupling. A new and more realistic approach in this limit was first introduced by Fröhlich in connection with an interpretation of Debye-type dielectric loss due to electrons which is observed in a number of ionic crystals.

The polaron problem raises several intriguing general questions. It is not always obvious how self-energy and scattering effects are to be separated in a field theory. For the polaron, one must determine how the energy level densities are affected by the lattice vibrations, and determine whether the resulting complex has particle-like behavior. There is the problem of determining the effective interaction which operates in scattering and mobility theory. The customary use of the Boltzmann equation raises profound difficulties. The Boltzmann equation is concerned with the distribution function in phase space and with the scattering probability for electrons in a phonon gas. Initially one considers the distribution in the absence of interaction. According to the usual procedure, one then switches the interaction on for a short time, and looks at the resulting distribution, forgetting about the phases set up during the interaction. While such a procedure may be justified in treating a single particle scattering process, it is not obvious how it can be justified straightforwardly for the continuing process. Density-matrix methods make a correct treatment of weakly interacting systems possible; however at present they are essentially perturbative and fail in the strong-coupling limit. One would hope that it might be possible to eliminate most of the interaction in some reasonable approximation in terms of self energy, leaving for scattering a residual weak interaction to be treated by existing methods.

In 1957, the BCS superconductivity theory appeared and was successful, as function alternating to apply polaron theory to superconductivity were dropped.

In 1953, Lee, Low, and Pines (LLP) [7] developed a variational intermediate

coupling theory, which assumes that an electron interacts with states containing any number of phonons.

Perturbation theory gives the polaron energy as an infinite series in powers of α. Both the perturbation theory and LLP theory extend from weak coupling toward intermediate coupling.

The most successful theory that interpolates between weak and strong coupling theories is the Feynmann path integral formalism.

To be more clear, the idea of the self-trapping can be expressed physically by considering the total energy of the electron plus lattice.

1. Kinetic energy due to localization of the electron.

$$\Delta p \Delta x = \hbar, \qquad \Delta p = \frac{\hbar}{\Delta x}, \qquad E_k = \frac{(\Delta p)^2}{\tau m} = \frac{\hbar^2}{2ml^2}. \tag{1.2}$$

2. Potential energy of electron distribution.

$$\int \frac{\widetilde{E}.\widetilde{D}}{8\pi} = \int \frac{D^2}{8\pi\epsilon}. \tag{1.3}$$

3. Interaction energy of electron with lattice.

$$E_{int} = -\int \frac{D^2}{8\pi\epsilon} \tag{1.4}$$

then

$$E_{tot} = \frac{\hbar^2}{2mR^2} - \frac{1}{8\pi}\left(1 - \frac{1}{\epsilon}\right)\int D^2 d^3\Omega \tag{1.5}$$

where Ω is the radius of electron distribution.

The rest of this thesis is organized as follows: In the next sections of this chapter, the Fröhlich Hamiltonian will be derived starting from the basic principles, and then coupling of electron to ionic lattice and coupling constant of optical mode electron interaction will be presented. Moreover, small and large polaron concepts will be explained and finally a brief summary about the perturbation and strong coupling theory methods will be presented in this chapter. The

Chapters 2, 3 and 4 are devoted to different theoretical approaches, each chapter starting with a short presentation of the essential points of the methodology, is accompanied with an application in two and three dimensions. In the fourth chapter we will consider the problem of a polaron in a magnetic field. And we will give a brief conclusion.

1.2 Fröhlich Hamiltonian

In this section we derive the Hamiltonian operator for the interaction between electrons and lattice vibrations. We represent the motion of the electrons and of the lattice vibration in the simplest possible form. For this reason, we will consider the electrons lying at the lower edge of the band which means the Bloch functions have a small k-vector resulting large wavelength compared with the lattice constant, and we treat all electrons as individual dipoles.

By considering polarization oscillations, the model we use for the polarization $P(x)$ of a medium are individual dipoles. The basis of such a dipole can be written as the vector q with its vibrating mass m and frequency w.

Then the total energy is

$$E_{tot} = \frac{1}{2}m(\dot{q}^2 + \omega^2 q^2). \tag{1.6}$$

But recall that in this scheme we assume that the dipoles are not coupled. Since we try to derive an equation for the dipole moment, we should replace dipole moments by dipole densities. If the charge appears in the dipole moment is e^*;

$$e^* q_n \to P(x). \tag{1.7}$$

And similarly, by taking into account the mass density

$$m = \rho d^3 x. \tag{1.8}$$

If, in addition, we write

$$\frac{m}{e^{*2}} = \gamma d^3 x, \tag{1.9}$$

Then the total energy becomes

$$H_{ph} = \frac{1}{2}\gamma \int (\dot{P}(x)^2 + w^2 P^2(x)) d^3x. \tag{1.10}$$

Here the constant γ is to be found from phenomenological theory.

The interaction energy of an electronic charge e at the point x and a dipole moment P at the point x' is

$$E_{e-ph} = e\frac{(x-x')}{|x-x'|^3}P. \tag{1.11}$$

For the continuously distributed charge density

$$E_{e-ph} = \int\int \rho(x)\frac{(x-x')}{|x-x'|^3}P(x')d^3x d^3x'. \tag{1.12}$$

The Lagrangian is written as

$$L = T - U - E_i \tag{1.13}$$

and the equations of motions are

$$\frac{d}{dt}\frac{\partial L}{\partial \dot{P}_j} - \frac{\partial L}{\partial P_j}. \tag{1.14}$$

By using this equation with (1.10) and (1.12) the equation of motion becomes

$$\gamma(\ddot{P}(x') + w^2 P(x')) = -\int \frac{(x-x')}{|x-x'|^3}\rho(x)d^3x. \tag{1.15}$$

Recall that the right hand-side of the equation is the dielectric displacement. And also notice that in the static case, where $\dot{P}(x') = 0$, we can obtain the value of constant γ, i.e;

$$\gamma\omega^2 P(x') = D(x'). \tag{1.16}$$

Using the relation between field strength and the dielectric displacement

$$D = E + 4\pi P_{tot} = \varepsilon E, \tag{1.17}$$

we get

$$4\pi P_{tot} = \left(1 - \frac{1}{\varepsilon}\right) D. \tag{1.18}$$

P_{tot}, in the above equation is the total polarization coming from the polarization of the electrons in the ionic shells and from the ionic displacements. With an

applied static field both polarization contributions develop fully, so ε is the static dielectric constant.

Notice that in this approach we are interested in only with the contribution coming from the lattice. To single this out; think of the field as having been applied slowly and then rapidly removed. Only the electrons are able to keep up with this sudden switch-off of the field. And as a result we obtain

$$4\pi\delta P = -\left(1 - \frac{1}{\epsilon_\infty}\right) D. \tag{1.19}$$

Now P_{tot} is replaced by δP which refers only to the polarization of the electrons. And also one another difference with Eq. (1.18) is that, now, ε is replaced by the dielectric constant for very high frequencies.

Adding 1.18 to 1.19 we obtain the polarization due to lattice vibrations

$$4\pi P = 4\pi(P_{tot} + \delta P) = \left(\frac{1}{\epsilon_\infty} - \frac{1}{\epsilon_0}\right) D. \tag{1.20}$$

This equation is in the same form with Eq. (1.16). So if we compare 1.16 with 1.20 we get the value of the constant γ

$$\gamma = \frac{4\pi}{\omega^2}\left(\frac{1}{\epsilon_\infty} - \frac{1}{\epsilon_0}\right) = \frac{4\pi\epsilon}{\omega^2}. \tag{1.21}$$

We still have one step left to obtain the total Hamiltonian operator for polarization oscillations plus electrons. So we should add the contribution of the energy of the electrons. At the beginning we have taken the electrons at the lower edge of the band and long wavelengths are concerned in the interaction with the lattice vibrations. For this reason we may use effective mass method and neglect the potential field and describe the electrons by their effective masses m^*

$$H_{el} = \int \Psi^\dagger(x)\left(\frac{-\hbar^2}{2m^*}\nabla^2\right)\Psi(x)d^3x, \tag{1.22}$$

$$\rho(x) = e\Psi^\dagger(x)\Psi(x). \tag{1.23}$$

Substituting equation (1.22) to (1.23) and integrating by parts with respect to x', H_I becomes

$$H_{el-ph} = \int\int\{\Psi^\dagger(x)\Psi(x)\frac{e}{|x-x'|}(-\nabla'_x P(x'))d^3x d^3x'. \tag{1.24}$$

This equation can be written by using the relation

$$\begin{aligned}\nabla_x \left(\frac{1}{|x-x'|}\right) P(x') &= -\nabla'_x \left(\frac{1}{|x-x'|}\right) P(x') \\ &= -\nabla'_x \left(\frac{P(x')}{|x-x'|}\right) + \frac{1}{|x-x'|}\nabla'_x P(x') \end{aligned} \tag{1.25}$$

the contribution coming from the first term becomes zero due to boundary conditions. This result shows that the plane wave expansion of the term $\nabla'_x P(x')$ contains only longitudinal waves. We therefore restrict our total Hamiltonian operator from the start to the case of longitudinal lattice vibrations.

After having found γ and the interaction Hamiltonian H_{e-ph}, we can now form the total Hamiltonian operator. But before this, let us replace $\dot{P}$ in the expression 1.10 by the canonically conjugate momentum $\prod$ to P

$$\prod = \dot{\mathbf{P}}/\gamma, \tag{1.26}$$

the polarization Hamiltonian 1.10 becomes

$$H_{ph} = \int \left(\frac{1}{2\gamma}\prod^2 + \frac{\gamma\omega^2}{2}P^2\right) d^3x. \tag{1.27}$$

So, the total Hamiltonian is

$$\begin{aligned} H &= \int \Psi^\dagger(x) \left(\frac{-\hbar^2}{2m^*}\nabla^2\right) \Psi(x) d^3x. + \int \left(\frac{1}{2\gamma}\prod^2 + \frac{\gamma\omega^2}{2}P^2\right) d^3x \\ &+ \int\int \{\Psi^\dagger(x)\Psi(x)\frac{e}{|x-x'|}(-\nabla'_x P(x'))d^3x d^3x'. \end{aligned} \tag{1.28}$$

From now on we need one more step to reach the exact form of the Fröhlich Hamiltonian. We now use the commutator relations. For the quantization of the field we may assume that the commutators involving only the fields and also those involving only the canonically conjugate momenta vanish:

$$[\prod_i, P_j] = -i\hbar\delta_{ij}, \qquad i,j = x,y,z \tag{1.29}$$

The phonon annihilation and creation operators are defined as

$$\begin{aligned} A(x) &= \sqrt{\frac{\gamma\omega_{LO}}{2\hbar}}\mathbf{P(x)} + \frac{i}{\sqrt{2\gamma\omega_{LO}}}\pi(x), \\ A^\dagger(x) &= \sqrt{\frac{\gamma\omega_{LO}}{2\hbar}}\mathbf{P(x)} - \frac{i}{\sqrt{2\gamma\omega_{LO}}}\pi(x) \end{aligned} \tag{1.30}$$

with $[A_i(x), A_j^\dagger(x)] = \delta_{ij}(x - x')$.

By using the plane waves, the operators become

$$A(x) = \frac{1}{\sqrt{V}} \sum_Q \frac{\mathbf{Q}}{Q} a_Q e^{iQr},$$
$$A^\dagger(x) = \frac{1}{\sqrt{V}} \sum_Q \frac{\mathbf{Q}}{Q} a_Q^\dagger e^{-iQr} \tag{1.31}$$

where V is the normalization volume and $\overrightarrow{Q}$ is the phonon wave vector. The commutation relation becomes

$$[a_i, a_j] = \delta_{ij} \qquad and \qquad [a_i, a_j] = [a_i^\dagger, a_j^\dagger] = 0. \tag{1.32}$$

Inverting the set of equations 1.30 and substituting $A(x)$ and $A^\dagger(x)$ as given in (1.31) we have

$$P(\mathbf{x}) = \sqrt{\frac{\hbar}{2\gamma\omega V}} \sum_Q \frac{\mathbf{Q}}{Q} (a_Q e^{i\mathbf{Q}.\mathbf{r}} + a_Q^\dagger e^{-i\mathbf{Q}.\mathbf{r}}),$$
$$\prod(x) = i\sqrt{\frac{\gamma\hbar\omega}{2V}} \sum_Q \frac{\mathbf{Q}}{Q} (a_Q^\dagger e^{-i\mathbf{Q}.\mathbf{r}} - a_Q e^{i\mathbf{Q}.\mathbf{r}}). \tag{1.33}$$

Inserting these equations in (1.27), we get

$$H_{ph} = \hbar\omega_{LO} \sum_Q a_Q^\dagger a_Q,$$
$$H_{e-ph} = \sum_Q V_Q a_Q e^{i\mathbf{Q}.\mathbf{r}} + V_Q^* a_Q^\dagger e^{-i\mathbf{Q}.\mathbf{r}}. \tag{1.34}$$

Here, $V_Q = -i4\pi\sqrt{e^2\hbar/2\gamma\omega_{LO}}(1/Q)$ is the interaction amplitude. By choosing $\hbar\omega_{LO}$ as a unit of energy ; $l = \sqrt{\frac{\hbar}{2m^*\omega_{LO}}}$ as a unit of length and with the value of constant γ in Eq. (1.21) we an complete the derivation of the dimensionless Fröhlich Hamiltonian by following scaling transformations

$$H \to \hbar\omega_{LO} H, \qquad x \to lx, \qquad \mathbf{Q} \to \mathbf{Q}/l, \qquad V \to l^3 V \tag{1.35}$$

The Fröhlich Hamilonian at the end takes the form

$$H = p^2 + V_{conf}(x; \Omega_i) + \sum_Q a_Q^\dagger a_Q + \sum_Q V_Q (a_Q e^{i\mathbf{Q}.\mathbf{r}} + a_Q^\dagger e^{-i\mathbf{Q}.\mathbf{r}}) \tag{1.36}$$

and now the dimensionless interaction amplitude becomes $V_Q = \sqrt{\frac{4\pi\alpha}{V}}\frac{1}{Q}$ and

$$\alpha = \frac{e^2}{2}\left(\frac{1}{\epsilon_\infty} - \frac{1}{\epsilon_0}\sqrt{\frac{2m^*\omega_{LO}}{\hbar}}\right)\frac{1}{\hbar\omega_{LO}} \tag{1.37}$$

is the dimensionless electron-phonon coupling constant.

1.3 Coupling of Electron to Ionic Lattice

The way an electron moves through an ionic crystal has been of considerable interest over a period of more than 35 years. This is due both the fundamental interest in the many-body problem which it turns out to constitute, and also to its importance in our understanding of the physics of semiconductors and general low-mobility solids.

As in many aspects of the theory of solids and fluids, early work of outstanding significance was that of Landau [1] (1933) who introduced the notion of the self-trapped electron. The idea is simple enough; namely that an electron,by its Coulomb interaction with the ions in a crystal having appreciable ionicity, produces a polarization. In the potential field resulting from this polarization, the electron cloud, it was suggested, become bound. Then, as the electron moves in the potential, the ions, being much more massive than the electron, do not take up their equilibrium positions again in a time of the order of the period of the electronic motion.

The next important step came when Fröhlich [5] (1937) gave a quantitative treatment of the way electrons are scattered in ionic crystals. In this work, the interaction between the electrons with the vibrating lattice was treated via the use of the polarization field.

While it is useful, in many cases, to treat the polarization field as a continuum, this becomes a rather poor approximation in the case of strong coupling and this requires a basically different method of treatment.

1.4 Coupling Constant of Optical Mode-Electron Interaction

The measure of the interaction between electrons and optical mode vibrations is given by the coupling constant

$$\alpha = \frac{e}{h}\left(\frac{m}{2h}\right)^{\frac{1}{2}}\left(\frac{1}{\varepsilon_\infty}-\frac{1}{\varepsilon_s}\right)\left(\frac{m^*}{m\omega_1}\right)^{\frac{1}{2}} = 1.4\times 10^8\left(\frac{\varepsilon_s-\varepsilon_\infty}{\varepsilon_\infty\varepsilon_s}\right)\left(\frac{m^*/m}{\omega_1}\right)^{\frac{1}{2}}, \quad (1.38)$$

where ε_∞ and ε_s represent respectively the optical and static dielectric constants, ω_1 is the longitudinal mode frequency $\left(\frac{\varepsilon_s}{\varepsilon_\infty}\right)^{\frac{1}{2}}\omega_0$ and $m*$ is the band mass of the electron mass.

It is useful to make a very rough separation into highly polar substances such as alkali halides, $\alpha > 3$, intermediate coupling cases where $\alpha \sim 1.5$, such as the silver halides, and weakly polar crystals such as compound semiconductors. In a material like PbS, α is small because the optical dielectric constant is almost as large as the static constant. there are certain materials such as NiO in which one expects to find highly localized polarons.

1.5 Small Polaron

There are two limiting approximations. In the first, the effective mass, m^* of the electron is assumed to be so high that the kinetic energy due to its localization in the well is negligible.Then r_p must be the order of the interionic distance, generally a little less.

We thus arrive at the concept of the small polaron, the energy of which can be written as a sum of

(i) The energy required to polarize the medium is

$$(\frac{1}{2}e^2/r_p)\left(\frac{1}{\varepsilon_\infty}-\frac{1}{\varepsilon_s}\right). \quad (1.39)$$

(ii) The lowering of the potential energy of the electron,

$$-\frac{e^2}{r_p}\left(\frac{1}{\varepsilon_\infty}-\frac{1}{\varepsilon_s}\right). \tag{1.40}$$

This gives us a rough continuum theory of the polaron energy -W as

$$-W=-\frac{1}{2}\frac{e^2}{r_p}\left(\frac{1}{\varepsilon_\infty}\right)-\left(\frac{1}{\varepsilon_s}\right) \tag{1.41}$$

We can develop a more exact method of treating the interaction of the electron with the whole spectrum of optical phonons. If we then make an approximation for the phonon spectrum, then we obtain equation (1.41), with r_p given by

$$r_p=\frac{1}{2}\left(\frac{\pi}{6}\right)^{\frac{1}{3}}l, \tag{1.42}$$

where l^{-3} is the number of centers per unit volume.

1.6 Large Polaron

This is the other limit when the effective mass m^* is not large. The kinetic energy $\hbar^2\pi/2m^*r_p^2$ of an electron confined in a sphere of radius r_p is now an essential feature, and we can write

$$-W=-\frac{1}{2}\frac{e^2}{r_p}\left(\frac{1}{\varepsilon_\infty}-\frac{1}{\varepsilon_s}\right)+\frac{\hbar^2\pi^2}{2m^*r_p^2}. \tag{1.43}$$

This is minimized when

$$r_p=2\pi^2\hbar^2\left(\frac{1}{\varepsilon_\infty}-\frac{1}{\varepsilon_s}\right)^{-1}/m^*e^2. \tag{1.44}$$

Hence the magnitude of the polaron energy is given by

$$w=\left(\frac{1}{4}e^2/r_p\right)\left(\frac{1}{\varepsilon_\infty}-\frac{1}{\varepsilon_s}\right). \tag{1.45}$$

1.7 Approximation Methods

In the Fröhlich Hamiltonian, when expressed in units of $\hbar\omega_{LO}$, all the material dependent parameters are summed up into the dimensionless constant α. The numerical value of this electron-phonon interaction constant can be quite different for different types of materials, ranging from ~ 0.01 up to ~ 10. It is large for highly polar materials such as alkali halides, whereas it is small for compound semiconductors. In Table 1.1 we list the values of α and the energy unit $\hbar\omega LO$ for several common materials, as calculated with the given data in a review article by Karthauser [43], in Table 1.1.

Table 1.1: Coupling constants and LO-phonon frequencies of some common materials

Material	α	$\hbar\omega_{LO}$
KCl	5.6	26.7
NaCl	5.5	33.6
AgBr	1.56	17.1
CdTe	0.40	20.8
InP	0. 11	43.3
GaAs	0.07	36.8
InAs	0.05	30.2

The interpretation of the polaron problem and its mathematical structure are relatively simple and well understood in the asymptotic limits of the interaction strength. One of the basic points of the view is the case where the kinetic energy of the electron is much smaller than the energy of the phonon modes, and $\alpha \ll 1$. In this case the lattice deformation tends to follow the electron, as it moves through the crystal. A reasonable treatment to such a case is to take the electron-phonon interaction, H_{e-ph}, as a perturbation and to calculate the corrections to the energy eigenvalues brought about by the polaron effect.

A contrasting point of view originates from the idea that for a strong enough electron-phonon interaction ($\alpha \gg 1$) the electron goes into a bound state with a highly localized wavefunction in the self-induced potential, which is built up by the field of correlated virtual phonons. If the electron is really deeply bound, one

expects the lattice deformation to react back and produce some structure in the electronic wavefunction, and the presence of the electron in turn determines and maintains the size and shape of the deformation. The point of view presented by these arguments is referred to as strong coupling (adiabatic) theory. The method, basically consists of proposing a trial wavefunction for the electron with some parameters, and making use of the variational principle, to calculate the ground state polaron properties.

The results of the perturbation and strong coupling theories, up to leading order in α, for the ground state energy and the effective mass of the polaron, are summarized in Table 1.2. We have provided the results of 2-dimensional (2D) polaron as well as those of the bulk (3D) polaron.

Table 1.2: Results of perturbation and strong coupling theories for the polaron properties

		E_g	$m_p - 1$
$\alpha \ll 1$	2D	$-(\pi/2)\alpha$	$(\pi/8)\alpha$
	3D	$-\alpha$	$(1/6)\alpha$
$\alpha \gg 1$	2D	$-(\pi/8)\alpha^2$	$(\pi^2/16)\alpha^4$
	3D	$-(1/3\pi)\alpha^2$	$(16/81\pi^2)\alpha^4$

It is seen that the functional dependence of the ground state energy and phonon contribution to the effective mass $(m_p - 1)$, on α, are quite different at the two limiting regimes.

Recently, Peeters *et al.* [26] have derived an interesting scaling relation for (2D) polaron properties, taking (3D) case as a reference;

$$\begin{aligned} E_g^{(2D)}(\alpha) &= \frac{2}{3} E_g^{(3D)}\left(\frac{3\pi}{4}\alpha\right), \\ m_p^{(2D)}(\alpha) &= m_p^{(3D)}\left(\frac{3\pi}{4}\alpha\right). \end{aligned} \tag{1.46}$$

Chapter 2

PERTURBATION THEORY

In section 1.1 we derived the Hamiltonian operator for the interaction between electrons and lattice vibrations. Although this Hamiltonian operator still looked fairly simple, it transpired that the corresponding Schrödinger equation could not be solved exactly. We are, therefore, left with the problem of developing suitable methods of approximation to treat the interaction between lattice vibrations and electrons. For a first attempt, it seems appropriate to use perturbation theory, where the interaction energy may be regarded as being very small. However, to apply this theory the electron-phonon coupling constant α must be small. Then the electron-phonon interaction term in the Fröhlich Hamiltonian is treated as a perturbation. The other remaining terms which are H_e and H_{ph} are unperturbed Hamiltonian. Let us, therefore, resolve the Hamiltonian operator as usual into

$$H = H_0 + H_1, \tag{2.1}$$

where H_0 describes the unperturbed problem, while H_1 is regarded as referring to a small perturbation. In our case,i.e; for the polaron problem

$$H_0 = H_e + H_{ph}, \qquad H_1 = H_{e-ph}. \tag{2.2}$$

We begin with an unperturbed Hamiltonian H_0, which is also assumed to have no time dependence. It has known energy levels and eigenstates, arising from the

time-independent Schrödinger equation;

$$H_0|n^{(0)}\rangle = E_n^{(0)}|n^{(0)}\rangle, \qquad n = 1, 2, 3, ... \tag{2.3}$$

$$H = H_0 + H_1 \tag{2.4}$$

where H_1 is perturbed Hamiltonian. The energy levels and eigenstates of the perturbed Hamiltonian are given by

$$(H_0 + H_1)|n\rangle = E_n|n\rangle. \tag{2.5}$$

If the perturbation is sufficiently weak, we can write them as power series

$$E_n = E_n^{(0)} + E_n^{(1)} + E_n^{(2)} + ..., \tag{2.6}$$

$$|n\rangle = |n^{(0)}\rangle + |n^{(1)}\rangle + |n^{(2)}\rangle + ... \tag{2.7}$$

Plugging the power series into the Schrödinger equation, we obtain

$$\begin{aligned}(H_0 + H_1)(|n^{(0)}\rangle + |n^{(1)}\rangle + |n^{(2)}\rangle + ...) &= (E_n^{(0)} + E_n^{(1)} + E_n^{(2)} + ...) \\ &\times (|n^{(0)}\rangle + |n^{(1)}\rangle + |n^{(2)}\rangle + ...).\end{aligned} \tag{2.8}$$

The zeroth-order equation is simply the Schrödinger equation for the unperturbed system

$$H_0|n^{(0)}\rangle = E_n^{(0)}|n^{(0)}\rangle. \tag{2.9}$$

The first-order equation is

$$H_0|n^{(1)}\rangle + H_1|n^{(0)}\rangle = E_n^{(0)}|n^{(1)}\rangle + E_n^{(1)}|n^{(0)}\rangle. \tag{2.10}$$

This leads to the first-order energy shift

$$E_n^{(1)} = \langle n^{(0)}|H_1|n^{(0)}\rangle. \tag{2.11}$$

But as it will be seen later, for the polaron problem the first-order correction equals to zero, so we need second-order correction.

$$E_n^{(0)} = \sum_{k\neq n} \frac{|\langle k^{(0)}|H_1|n^{(0)}\rangle|^2}{E_n^{(0)} - E_k^{(0)}} \tag{2.12}$$

And for the eigenstates, according to the perturbation theory the correction term becomes

$$|n^{(1)}\rangle = \sum_{k\neq n} \frac{\langle k^{(0)}|H_1|n^{(0)}\rangle}{E_n^{(0)} - E_k^{(0)}}|k^{(0)}\rangle. \tag{2.13}$$

The first-order change in the n-th energy eigenket has a contribution from each of the energy eigenstates $k \neq n$. Each term is proportional to the matrix element $\langle k^{(0)}|H_1|n^{(0)}\rangle$, which is a measure of how much the perturbation mixes eigenstate n with eigenstate k, it is also inversely proportional to the energy difference between eigenstates k and n, which means that perturbation deforms the eigenstate to a greater extent if there are more eigenstates at nearby energies.

Chapter 3

STRONG COUPLING THEORY

The total polaron Hamiltonian as it is derived in section 1.1 can be written as

$$H = H_e + H_{ph} + H_{e-ph},$$
$$H_e = \frac{p^2}{2m^*} + V_{conf}(\vec{r}; \Omega_i). \tag{3.1}$$

The Fröhlich Hamiltonian

$$H = H_e + \sum_Q a_Q^\dagger a_Q + \sum_Q V_Q (a_Q e^{i\mathbf{Q}.\mathbf{r}} + a_Q^\dagger e^{-i\mathbf{Q}.\mathbf{r}}), \tag{3.2}$$

$$V_Q = \sqrt{4\alpha\pi/V}(1/Q) \qquad ; \qquad \alpha = \frac{e^2}{2}\left(\frac{1}{\epsilon_\infty} - \frac{1}{\epsilon_0}\right)\sqrt{\frac{2m^*\omega_{LO}}{\hbar}}\frac{1}{\hbar\omega_{LO}} \tag{3.3}$$

where α is the dimensionless electron-phonon coupling constant.

In the Fröhlich Hamiltonian when expressed in units of $\hbar\omega_{LO}$ all the material dependent parameters are summed up into the dimensionless constant α.

One of the basic points of view is the case where the kinetic energy of the electron is much smaller than the energy of the phonon modes, and $\alpha << 1$. In this case the lattice deformation tends to follow the electron, as it moves through the crystal. A reasonable treatment to such a case is to take the electron-phonon interaction, H_{e-ph}, as a perturbation and to calculate the corrections to the energy eigenvalues brought about by the polaron effect as it is mentioned in the previous chapter.

For strong enough electron-phonon interaction ($\alpha >> 1$) the electron goes into a bound state with a highly localized wave function in the self induced potential. The point of view presented by these arguments is referred to as strong-coupling (adiabatic) theory. The method, basically consists of proposing a trial wave function for the electron with some parameters, and making use of the variational principle, to calculate the ground state polaron properties.

Before discussing he details of these arguments, let us first consider the standard canonical transformation of strong coupling theory.

3.1 Displaced Oscillator Transformation

The Hamiltonian used for the polaron can also be interpreted by the use of harmonic oscillators interacting with the electron. Then the Fröhlich Hamiltonian can be expressed by

$$H_Q\Psi_Q = \left(-\nabla^2_{\xi_Q} + (1/4)\xi^2_Q - u_Q\xi_Q\right)\Psi_Q = \epsilon_Q\Psi_Q, \tag{3.4}$$

where ξ_Q and u_Q are the dimensionless coordinate and the energy of the oscillators, and u_Q is also the interaction force term.

Completing Eq.(3.4) to a square, the equation becomes

$$\left(-\nabla^2_{\xi_Q} + (1/4)(\xi_Q - 2u_Q)^2 - u^2_Q\right)\Psi_Q = \epsilon_Q\Psi_Q. \tag{3.5}$$

From this equation it can be seen easily that $2u_Q$ is equilibrium coordinate. By taking all the phonon modes behave independently in the same way, in terms of the phonon creation and annihilation operators, the total Hamiltonian can be written as

$$H = \sum_Q a^\dagger_Q a_Q - u_Q(a^\dagger_Q + a_Q). \tag{3.6}$$

The terms linear in $a^\dagger_Q$ and a_Q can easily made to disappear by defining the

set of new operators,

$$\tilde{a}_Q = a_Q - u_Q, \qquad \tilde{a}_Q^\dagger = a_Q^\dagger - u_Q \tag{3.7}$$

which can be obtained through a canonical transformation of the previous ones,

$$\tilde{a}_Q = \mathbf{U}^{-1} a_Q \mathbf{U}, \qquad \tilde{a}_Q^\dagger = \mathbf{U}^{-1} a_Q^\dagger \mathbf{U} \tag{3.8}$$

where

$$\mathbf{U} = exp \sum_Q u_Q (a_Q - a_Q^\dagger). \tag{3.9}$$

Instead of transforming the phonon operators, one can equivalently consider the phonon ground state to be chosen as $\mathbf{U}|0\rangle$ rather than the bare phonon vacuum $|0\rangle$, where the origin is shifted over to the equilibrium coordinates. This kind of representation is known as displaced oscillator transformation.

The amount by which the origin is to be displaced depends on the interaction strength and further on the electronic charge density in a somewhat implicit manner. As a result, the procedure of strong coupling theory will consist of proposing a variational wave function for the electron and through the minimization of the ground state energy, determining the variational parameters and the terms u_Q.

3.2 Adiabatic Formulation

The adiabatic polaron ground state is given through a product ansatz consisting of the electron and phonon parts, i.e.,

$$\Psi_g = \Phi_e(\mathbf{r})|0\rangle, \tag{3.10}$$

together with the Hamiltonian subjected to the displaced oscillator transformation,

$$H \longrightarrow \widetilde{H} = e^{-S} H e^{S} \tag{3.11}$$

where

$$S = \exp \sum_Q u_Q(\Phi_e)[a_Q - a_Q^\dagger]. \tag{3.12}$$

Here, $u_Q(\Phi_e)$ is the lattice variational parameter, which will depend on $\mathbf{r}$, since it is via this parameter an interrelation establishes between the potential well set up by the lattice polarization and the electron which, in turn, becomes trapped in this well. It then follows that, for each choice of Φ_e, there is an optimal fit to u_Q and, therefore, the transformed Hamiltonian depends on Φ_e, implicitly.

Now if $u_Q(\Phi_e)$ is defined as below;

$$u_Q(\Phi_e) = S_Q e^{i\mathbf{Q}.\mathbf{r}} + hc, \tag{3.13}$$

then S takes the new form given as

$$S = \exp \sum_Q S_Q(a_Q e^{i\mathbf{Q}.\mathbf{r}} - a_Q^\dagger e^{-i\mathbf{Q}.\mathbf{r}}). \tag{3.14}$$

Hence, the transformed Hamiltonian becomes

$$\begin{aligned} H \longrightarrow \widetilde{H} &= e^{-S} H e^{S}, \\ \widetilde{H} &= p^2 + V_{conf} + \sum_Q V_Q(a_Q e^{i\mathbf{Q}.\mathbf{r}} + a_Q^\dagger e^{-i\mathbf{Q}.\mathbf{r}}). \end{aligned} \tag{3.15}$$

The Fröhlich Hamiltonian is given by

$$\begin{aligned} \widetilde{H} &= H_e + H_{ph} + H_{e-ph} \\ &= p^2 + V_{conf} + \sum_Q V_Q(a_Q e^{i\mathbf{Q}.\mathbf{r}} + a_Q^\dagger e^{-i\mathbf{Q}.\mathbf{r}}) \\ &= -\nabla^2 + \sum_Q V_Q(a_Q e^{i\mathbf{Q}.\mathbf{r}} + a_Q^\dagger e^{-i\mathbf{Q}.\mathbf{r}}) \end{aligned} \tag{3.16}$$

where we have taken $V_{conf} = 0$.

3.3 Application: Strong Coupling Polaron Theory of Two Dimensional Polaron

We consider a 2D electron gas in the $x - y$ plane in the presence of a hydrogenic potential representing the interaction between a conduction electron and a donor.

The eigenstates of a 2D hydrogen atom are described by the Schrödinger equation, in polar coordinates,

$$\left[-\frac{\hbar^2}{2m}\left(\frac{\partial}{\partial r^2}+\frac{1}{r}\frac{\partial}{\partial r}+\frac{1}{r^2}\frac{\partial}{\partial \varphi^2}\right)-\frac{Ze^2}{r}\right]\psi(r,\varphi)=E\psi(r,\varphi). \tag{3.17}$$

Using separation of variables

$$\psi(r,\varphi)=R(r)\Phi(\varphi), \tag{3.18}$$

we obtain

$$\Phi(\varphi)=\frac{1}{(2\pi)^{1/2}}e^{il\varphi}, l=0,\pm1,\pm2,... \tag{3.19}$$

and

$$\frac{d^2}{dr^2}R(r)+\frac{1}{r}\frac{d}{dr}R(r)+\left[\frac{2m}{\hbar^2}\left(E+\frac{Ze^2}{r}\right)-\frac{l^2}{r^2}\right]R(r)=0. \tag{3.20}$$

Equation (3.20) is the 2D radial Schrödinger equation; its solution $R(r)$, depends only on $|l|$. Solution (3.19) is also the eigenfunction of the angular momentum along the z-direction

$$\hat{L_z}=-i\hbar\frac{\partial}{\partial\varphi}, \tag{3.21}$$

which commutes with the Hamiltonian. Hence l is a good quantum number.

Now, let us define

$$R(x)=x^{|l|}e^{-x/2}G(x). \tag{3.22}$$

Equation (3.20) then becomes

$$x\frac{d^2G}{dx^2}+[(2\,|l|+1)-x]\frac{dG}{dx}-(-N+|l|+\frac{1}{2})G=0. \tag{3.23}$$

The solution of Eq.(3.23), which is regular at $x=0$, is the confluent hypergeometric function [12]

$$G(x)=F_1(-N-|l|+\frac{1}{2},2|l|+1,x). \tag{3.24}$$

The normalized radial eigenfunction is given by [13]

$$\begin{aligned} R_{nl}(r) &= \frac{\beta_{nl}}{(2|l|)!}\left[\frac{(n-|l|-1)!}{(2n-1)(n-|l|-1)!}\right]^{1/2} \\ &\times (\beta_n r)^{|l|}exp(-\beta_n r/2) \\ &\times F_1(-n+|l|+1,2|l|+1,\beta|nr), \end{aligned} \tag{3.25}$$

where

$$\beta_n = \frac{2Z}{n-\frac{1}{2}}\frac{me^2}{\hbar^2}. \tag{3.26}$$

3.3.1 Trial Wavefunction for Two Dimension

In the previous section we have derived the wavefunction for two-dimensional as

$$\begin{aligned}\psi(r,\varphi) &= R(r)\Phi(\varphi) \\ &= Ne^{il\varphi}\times\frac{\beta_{nl}}{(2|l|)!}\left[\frac{(n-|l|-1)!}{(2n-1)(n-|l|-1)!}\right]^{1/2} \\ &\times (\beta_n r)^{|l|}\exp(-\beta_n r/2) \\ &\times F_1(-n+|l|+1, 2|l|+1, \beta|nr),\end{aligned} \tag{3.27}$$

for the ground-state Hydrogen atom this becomes

$$\psi = \left(\frac{2}{\pi\sigma^2}\right)^{1/2} e^{-r/\sigma} \tag{3.28}$$

where $l = 0$ for the ground-state.

The Hamiltonian without polaronic contribution is

$$H = -\frac{\hbar^2}{2m}\nabla^2 - \frac{e^2}{\varepsilon_0 r} \tag{3.29}$$

and

$$-\nabla^2 = -\frac{1}{r}\frac{\partial}{\partial r}r\frac{\partial}{\partial r}, \tag{3.30}$$

since there is no φ dependence in the wavefunction we used. The expectation value of $-\nabla^2$ is

$$\begin{aligned}\langle -\nabla^2\rangle &= N^2\int_0^\infty re^{-2r/\sigma}dr\int_0^{2\pi}d\varphi \\ &= \frac{1}{\sigma^2}\end{aligned} \tag{3.31}$$

where N^2 is the normalization constant and is given by $N^2 = \frac{2}{\pi\sigma^2}$. For the Coulomb potential term we calculate

$$-\frac{e^2}{\varepsilon_0}\langle\frac{1}{r}\rangle = -\frac{2e^2}{\varepsilon_0\sigma}. \tag{3.32}$$

Then

$$E = \langle H \rangle = \frac{\hbar^2}{2m^*\sigma^2} - \frac{2e^2}{\varepsilon_0 \sigma}. \tag{3.33}$$

Minimizing this equation with respect to σ,

$$\frac{\partial \langle H \rangle}{\partial \sigma} = 0 \tag{3.34}$$

gives us two dimensional Bohr radius as

$$a_{2D} = \frac{\varepsilon_0 \hbar^2}{2m^* e^2}. \tag{3.35}$$

Inserting this equation into the energy expression, the two dimensional Rydberg constant which we will use as a unit of energy becomes

$$R_{2D} = -\frac{2m^* e^4}{\varepsilon_0^2 \hbar^2}. \tag{3.36}$$

For polaron units we use $E = \hbar\omega$, and $l = \left(\frac{\hbar}{2m^*\omega}\right)^{1/2}$ as a unit of energy and length respectively, and $\hbar = 2m^* = 1$. So the Hamiltonian is

$$H = -\nabla^2 - \frac{\beta}{r} \tag{3.37}$$

where

$$\beta = \frac{e^2}{\varepsilon_0 \hbar} \left(\frac{2m^*}{\hbar\omega}\right)^{1/2} \tag{3.38}$$

The Fröhlich Hamiltonian can now be written for the strong coupling case as

$$H = -\nabla^2 - \frac{\beta}{r} + \sum_Q a^{\dagger Q} a_Q + \sum_Q V_Q (a_Q e^{i\mathbf{Q}.\mathbf{r}} + a^{\dagger Q} e^{-i\mathbf{Q}.\mathbf{r}}) \tag{3.39}$$

where

$$V_q = \left(\frac{2\pi\alpha}{AQ}\right)^{1/2}. \tag{3.40}$$

In the previous chapter we have defined e_0 as

$$e_0 = \langle \psi | H_0 | \psi \rangle, \tag{3.41}$$

where

$$H_0 = -\nabla^2 - \frac{\beta}{r}. \tag{3.42}$$

Then

$$e_0 = \frac{1}{\sigma^2} - \frac{2\beta}{\sigma}. \tag{3.43}$$

Minimizing this equation with respect to σ,

$$\frac{\partial e_0}{\partial \sigma} = 0 \tag{3.44}$$

we get

$$\sigma = \frac{1}{\beta}. \tag{3.45}$$

Plugging this into the e_0 expression we get

$$e_0 = \beta^2 - 2\beta^2 = -\beta^2. \tag{3.46}$$

And

$$\begin{aligned} \sigma_Q &= \langle\psi|e^{i\mathbf{Q}.\mathbf{r}}|\psi\rangle \\ &= \frac{1}{\left(1+\frac{1}{4}\sigma^2 Q^2\right)^{3/2}} \end{aligned} \tag{3.47}$$

Remember

$$\lambda_0 = \sum_Q V_Q^2 \sigma_Q^2, \tag{3.48}$$

and it is equal to

$$\lambda_0 = \frac{3\pi\alpha}{8\sigma}. \tag{3.49}$$

So we have now get the result of strong coupling energy which is given by

$$E_{sc} = e_0 - \lambda_0 = \frac{1}{\sigma^2} - \frac{2\beta}{\sigma} - \frac{3\pi\alpha}{8\sigma}. \tag{3.50}$$

Minimizing this equation with respect to σ, gives σ as

$$\sigma = \frac{16}{16\beta + 3\pi\alpha}. \tag{3.51}$$

Putting this value into Eq. (3.47) we have derived Eq. (4.58); that is,

$$E_{sc}^{(2D)} = -\beta^2 - (3/8)\pi\alpha\beta - (9/256)\pi^2\alpha^2. \tag{3.52}$$

3.3.2 Trial Wavefunction for Three Dimensional Polaron

If we use the same wavefunction for three dimensional case, that is, $\psi = Ne^{-r/\sigma}$ and follow the same procedure we get the normalization constant as

$$N = \left(\frac{1}{\pi\sigma^3}\right)^{1/2} \tag{3.53}$$

and the Bohr radius and the corresponding Rydberg constant calculated as

$$a_{3D} = \frac{\varepsilon_0\hbar^2}{m^*e^2}; R_{3D} = -\frac{m^*e^4}{2\varepsilon_0^2\hbar^2} \tag{3.54}$$

which is $\frac{1}{4}$ of the two dimensional Rydberg constant. I mean,

$$R_{2D} = 4R_{3D}. \tag{3.55}$$

The three dimensional $-\nabla^2$ is

$$-\nabla^2 = -\frac{1}{r^2}\frac{\partial}{\partial r}r^2\frac{\partial}{\partial r} \tag{3.56}$$

again because of no θ and φ dependence we did not take the corresponding parts of $-\nabla^2$. Then

$$\begin{aligned} e_0 &= \langle\psi|H_0|\psi\rangle \\ &= N^2\int_0^\infty r^2e^{-r/\sigma}(-\nabla^2)e^{-r/\sigma}dr\int_0^\pi sin\theta d\theta\int_0^{2\pi}d\varphi \\ &= \frac{1}{\sigma^2} - \frac{\beta}{\sigma}. \end{aligned} \tag{3.57}$$

Minimizing this result with respect to σ, we get

$$\sigma = \frac{2}{\beta}. \tag{3.58}$$

Inserting this value in Eq.(3.57) we get

$$e_0 = -\frac{\beta^2}{4} \tag{3.59}$$

which is again $\frac{1}{4}$ of the two dimensional energy.

The result of 3D σ_Q

$$\begin{aligned} \sigma_Q &= \langle\psi|e^{i\mathbf{Q}.\mathbf{r}}|\psi\rangle \\ &= \frac{16}{(4+\sigma^2Q^2)^2}. \end{aligned} \tag{3.60}$$

The three dimensional interaction potential is $V_Q = \sqrt{\frac{4\pi\alpha}{V}}\frac{1}{Q}$. So $\lambda_0 = \sum_Q V_Q^2 \sigma_Q^2$ becomes

$$\lambda_0 = \frac{5\alpha}{8\sigma}. \tag{3.61}$$

Then

$$E_{sc} = e_0 - \lambda_0 = \frac{1}{\sigma^2} - \frac{\beta}{\sigma} - \frac{5\alpha}{8\sigma}. \tag{3.62}$$

Minimizing this equation with respect to σ, we get

$$\sigma = \frac{16}{8\beta + 5\alpha} \tag{3.63}$$

and

$$E_{sc}^{(3D)} = -\frac{\beta^2}{4} - \frac{5}{16}\alpha\beta - \left(\frac{5}{16}\right)^2 \alpha^2 \tag{3.64}$$

which is given in Eq. (4.57).

Chapter 4

PERTURBATIVE VARIATIONAL APPROACH

We have seen that for not too weak electron-phonon interaction the strong coupling polaron theory, though not capable of reflecting a totally dependable quantitative description, may serve so as to provide some qualitative insight into the study of polarons. On the other hand, a pure perturbation treatment may also be not perfectly appropriate except for too weak phonon coupling. The formalism we follow in this chapter consists of the usage of a perturbative variational approach used previously dy Devreese *et al.* [6]. the procedure is structured on basing the starting ansatz on the standard displaced oscillator transformation of the Pekar strong coupling theory [44] and then modify the adiabatic polaron state by a variationally determined perturbative extension serving for the theory to interpolate in the overall range of the coupling constant.

4.1 Formulation

In the most commonly studied compound materials the electron-phonon coupling is rather weak, an appropriate approach is to treat the Fröhlich interaction as a

perturbation. Using units for which

$$2m^* = \hbar = \omega_{LO} = 1 \tag{4.1}$$

the Hamiltonian describing the confined electron coupled to LO-phonons is given by

$$H = H_e + \sum_Q a_Q^\dagger a_Q + H_{e-ph}, \tag{4.2}$$

$$H_e = -\frac{1}{\rho}\frac{\partial}{\partial\rho}\left(\rho\frac{\partial}{\partial\rho}\right) - \frac{1}{\rho^2}\frac{\partial^2}{\partial\varphi^2} - \frac{\partial^2}{\partial z^2} - \frac{\beta}{r}, \tag{4.3}$$

$$H_{e-ph} = \sum_Q V_Q[a_Q \exp(i\mathbf{Q}.\mathbf{r}) + HC] \tag{4.4}$$

is the Fröhlich interaction.

Here we use $\hbar\omega$ as a unit of energy and $(\hbar/2m^*\omega_0)^{1/2}$ as a unit of length. The operators $a_Q^\dagger$ and a_Q respectively create and annihilate a phonon wavevector $\mathbf{Q}$ and frequency ω_0.With the normalization volume set to unity for notational convenience, the electron- phonon interaction amplitude is $V_Q = \sum_Q (4\pi\alpha)^{1/2}/Q$. The dimensionless parameter $\beta = (e^2/\kappa)(2m^*/\hbar^3\omega_0)^{1/2}$ gives the strength of the Coulomb attraction screened by the static dielectric constant κ of the material.

To obtain the binding energy in the adiabatic approximation we take the Pekar-type trial ansatz [44] which is separable into the particle part φ_0 and the phonon part. We choose

$$\psi_{sc} = \varphi_0 e^S |0\rangle \tag{4.5}$$

wherein the exponential operator e^S, S is given by

$$S = \sum_Q V_Q \sigma_Q (a_Q - a_Q^\dagger), \tag{4.6}$$

where

$$\sigma_Q = \langle\varphi_0| \exp(\pm i\mathbf{Q}.\mathbf{r})|\varphi_0\rangle \tag{4.7}$$

determines the optimal lattice deformation surrounding the electric charge density. A further optimization with respect to the parameters contained in φ_0 leads

to the relaxed state of the system describing the composite behavior of the electron and the surrounding polarization field.

Under the displaced oscillator transformation

$$H' = U^{-1}HU \tag{4.8}$$

where $U = e^S$

$$H' \to e^{-S}He^S. \tag{4.9}$$

$$H' = H - [S,H] + \frac{1}{2}[S,[S,H]] - ..., \tag{4.10}$$

$$\begin{aligned} [S,H] &= [\sum_Q V_Q\sigma_Q a_Q - \sum_Q V_Q\sigma_Q a_Q^\dagger, H] \\ &= \sum_Q V_Q\sigma_Q(a_Q + a_Q^\dagger) + \sum_Q V_Q^2\sigma_Q(e^{i\mathbf{Q}.\mathbf{r}} + e^{-i\mathbf{Q}.\mathbf{r}}), \end{aligned} \tag{4.11}$$

$$\begin{aligned} [S,[S,H]] &= [\sum_Q V_Q\sigma_Q a_Q - \sum_Q V_Q\sigma_Q a_Q^\dagger, \sum_Q V_Q\sigma_Q a_Q \qquad (4.12) \\ &+ \sum_Q V_Q\sigma_Q a_Q^\dagger + \sum_Q V_Q^2\sigma_Q e^{i\mathbf{Q}.\mathbf{r}} + \sum_Q V_Q^2\sigma_Q e^{-i\mathbf{Q}.\mathbf{r}}] \\ &= 2\sum_Q V_Q^2\sigma_Q^2. \qquad (4.13) \end{aligned}$$

Since this term is a constant i.e, involving no such annihilation or creation operator all other terms are zero.

Then Hamiltonian H' becomes

$$\begin{aligned} H' &= H_e + \sum_Q a_Q^\dagger a_Q + \sum_Q V_Q^2\sigma_Q^2 - \sum_Q V_Q^2\sigma_Q(e^{i\mathbf{Q}.\mathbf{r}} + e^{-i\mathbf{Q}.\mathbf{r}}) \\ &+ \sum_Q V_Q a_Q(e^{i\mathbf{Q}.\mathbf{r}} - \sigma_Q) + \sum_Q V_Q a_Q^\dagger(e^{-i\mathbf{Q}.\mathbf{r}} - \sigma_Q). \end{aligned} \tag{4.14}$$

Define

$$e^{i\mathbf{Q}.\mathbf{r}} - \sigma_Q = \eta_Q, \tag{4.15}$$

$$e^{-i\mathbf{Q}.\mathbf{r}} - \sigma_Q = \eta_Q^*. \tag{4.16}$$

Then the final form of the Hamiltonian becomes

$$H' = H_e + \sum_Q a_Q^\dagger a_Q + \sum_Q V_Q^2 \sigma_Q^2 - \sum_Q V_Q^2 \sigma_Q (e^{i\mathbf{Q}.\mathbf{r}} + e^{-i\mathbf{Q}.\mathbf{r}}) + \sum_Q V_Q (\eta_Q a_Q + \eta_Q^* a_Q^\dagger). \tag{4.17}$$

Without perturbation;

$$E_0 = \langle \Psi | H | \Psi \rangle, \tag{4.18}$$

$$|\Psi\rangle = e^S \Phi_0 |0\rangle. \tag{4.19}$$

Then the expectation value of the above Hamiltonian becomes

$$\begin{aligned} E_0 &= \langle \Phi_0 | H_e | \Phi_0 \rangle + \langle 0 | e^{-S} \sum_Q a_Q^\dagger a_Q e^S | 0 \rangle + \sum_Q V_Q \sigma_Q \langle 0 | e^{-S} a_Q e^S | 0 \rangle \\ &+ \sum_Q V_Q \sigma_Q \langle 0 | e^{-S} a_Q^\dagger e^S | 0 \rangle. \end{aligned} \tag{4.20}$$

By using Baker-Haussdorf formula this can easily be written as

$$\begin{aligned} E_0 &= \langle \Psi | H | \Psi \rangle = \langle \Phi_0 | H_e | \Phi_0 \rangle + \sum_Q V_Q^2 \sigma_Q^2 - 2 \sum_Q V_Q^2 \sigma_Q^2 \\ &= \langle \Phi_0 | H_e | \Phi_0 \rangle - \sum_Q V_Q^2 \sigma_Q^2 \\ &= e_0 - \lambda_0 \end{aligned} \tag{4.21}$$

where σ_Q is

$$\sigma_Q = \langle \Phi_0 | e^{iQ.r} | \Phi_0 \rangle. \tag{4.22}$$

We now extend the formulation to the case of weak coupling wherein what is more appropriate is the perturbation theory with H_{e-ph} in the Hamiltonian taken as perturbation. It should be noted, however, that with decreasing degree of localization of the electron, σ_Q which is given in Eq. (4.22) tends to zero on average and consequently H' reduces to the starting Hamiltonian. One is therefore led to include the first-order correction to the trial state $\Phi_0|0\rangle$ with the last term in Eq. (4.17) being a perturbation. We then have

$$\delta\Psi = \sum_Q \sum_i |i\rangle \frac{\langle i | \eta_Q^* a_Q^\dagger | \Phi_0 \rangle | 0 \rangle}{\varepsilon_0 - \varepsilon_n - 1} \tag{4.23}$$

in which the energy eigenvalues $\varepsilon_n (n = 0, 1, 2, ...)$ of the unperturbed part of H' depend on α and the lattice coordinates in an involved manner. The summation

over the intermediate states can be projected out simply by replacing the energy denominator by an average quantity which in the calculation will be determined variationally. Using completeness we write

$$\delta\Psi = \sum_Q g_Q V_Q \eta_Q^* a_Q^\dagger \Phi_0|0\rangle. \tag{4.24}$$

The trial wavefunction for the Hamiltonian H' is the extended to

$$\Psi_{exc} = c\Phi_0|0\rangle + \delta\Psi = c\Phi_0|0\rangle + \sum_Q g_Q V_Q \eta_Q^* a_Q^\dagger \Phi_0|0\rangle \tag{4.25}$$

where c is normalization constant given by

$$f(c, g_Q) = c^2 + \sum_Q V_Q^2 g_Q^2 h_Q - 1 = 0 \tag{4.26}$$

with

$$h_Q = 1 - \sigma_Q^2. \tag{4.27}$$

The variational parameter g_Q sets up a fractional admixture of the strong and weak coupling counterparts of the coupled electron-phonon system and thus is expected to serve for the theory to interpolate between the extreme limits of the coupling constant.

In order to find the optimal fit to g_Q one has to minimize the expected value of H' in state 4.25 subject to the constraint 4.26

$$E(c, g_Q) = \langle\Psi_{exc}|H'|\Psi_{exc}\rangle. \tag{4.28}$$

After some simple algebra we reach

$$\begin{aligned} E(c, g_Q) &= c^2\langle\Phi_0|H_0|\Phi_0 - c^2\sum_Q V_Q^2\sigma_Q^2 + 2c\sum_Q V_Q^2 g_Q\langle\Phi_0|\eta_Q\eta_Q^*|\Phi_0\rangle \\ &+ \sum_Q V_Q^2 g_Q^2\langle\Phi_0|\eta_Q H_0\eta_Q^*|\Phi_0\rangle + \sum_Q V_Q^2 g_Q^2\langle\Phi_0|\eta_Q\eta_Q^*|\Phi_0\rangle \\ &+ \sum_Q V_Q^2 g_Q^2 V_Q^2\sigma_Q\langle\Phi_0|\eta_Q\eta_Q^*|\Phi_0\rangle \\ &- \sum_Q V_Q^2 g_Q^2 V_Q^2\sigma_Q\langle\Phi_0|\eta_Q(e^{i\mathbf{Q}.\mathbf{r}} + e^{-i\mathbf{Q}.\mathbf{r}})\eta_Q^*|\Phi_0\rangle. \end{aligned} \tag{4.29}$$

For the energy, after some definitions we obtain

$$E(c, g_Q) = \langle\Psi_{exc}|H'|\Psi_{exc}\rangle$$

$$
\begin{aligned}
&= c^2 e_0 + (1-2c^2)\lambda_0 + 2c\sum_Q V_Q^2 g_Q h_Q \\
&+ \sum_Q V_Q^2 g_Q^2 (e_Q + f_Q + h_Q)
\end{aligned} \tag{4.30}
$$

where

$$
\begin{aligned}
\lambda_0 &= \sum_Q V_Q^2 \sigma_Q^2, \\
e_0 &= \langle \Phi_0 | H_0 | \Phi_0 \rangle, \\
e_Q &= \langle \Phi_0 | \eta_Q H_0 \eta_Q^* | \Phi_0 \rangle, \\
f_Q &= -\sum_{Q'} V_{Q'}^2 \sigma_{Q'} \langle \Phi_0 | \eta_Q (e^{i\mathbf{Q}'.\mathbf{r}} + e^{-i\mathbf{Q}'.\mathbf{r}}) \eta_Q^* | \Phi_0 \rangle.
\end{aligned} \tag{4.31}
$$

The variational procedure then requires $\partial / \partial g_Q (E - \lambda F) = 0$, with λ being a Lagrange multiplier. We find

$$
g_Q / c = \frac{-h_Q}{h_Q (1 - e_0 + 2\lambda_0 - \lambda) + e_Q + f_Q} \tag{4.32}
$$

where

$$
\lambda = \sum_Q V_Q^2 (g_Q / c) h_Q \tag{4.33}
$$

and the expression

$$
E = e_0 - \lambda_0 - \lambda \tag{4.34}
$$

for the energy, which is to be minimized further with respect to Φ_0.

The additive term λ, by means of which the adiabatic theory goes over to the weak-coupling regime, depends implicitly on α and β through the transcendental Eq (4.33). For strong enough Coulomb attraction and/or large coupling constant, λ tends to zero and the strong coupling limit is readily obtained. However, as the coupling constant is shifted down to realistic values, the polaronic correction deviates considerably from λ_0. For a loosely bound electron the strong-coupling approximation loses its validity, since in this limit the charge density fluctuations of the electron are no longer faster than the phonon frequencies. In a perturbation theoretic calculation this feature shows up in that the corresponding perturbation series becomes poorly convergent and one needs to include the remaining terms, other than $n = 0$, as well. This is accomplished in the present formulation, however, by solving the transcendental Eq. (4.33) for the Lagrange multiplier λ.

4.2 Application: A Variational Treatment of a Two Dimensional Polaron

The case of a dynamically two dimensional electron interacting via the Fröhlich Hamiltonian with the bulk LO-phonons has already been studied extensively by Das Sarma and Mason [10]. Even though their calculations were based on a strict two-dimensional approximation for the electronic wavefunction, the relevant results in the weak and strong-coupling regimes provide the basic qualitative features of the polaron effect in confined structures. In this work we focus our attention on the same problem and present a review of the ground state properties of the 2D-polaron through an approach intended to work for arbitrary electron-phonon coupling. The calculation we use is of a variational nature, and the procedure is to start with the localized polaron wavefunction, which evidently is a poor approximation for not-too-strong coupling. In the intermediate and weak-coupling regimes an improvement can, however, be achieved by 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. In the following, we formulate the algebra in the manner proposed by Devreese et al. [9], where they resolve the problem of a bulk donor impurity for arbitrary Coulomb potentials and electron-phonon coupling strengths. Our primary aim is to give a comparison of the formulation applied to a free 2D-polaron with the relevant results obtained by weak- and strong-coupling theories.

For typical materials of interest such as GaAs ($\alpha = 0.07$), for instance, the electron-phonon coupling is too weak and consequently the most natural and straightforward way of handling the problem is to develop a systematic perturbation expansion in α. Regardless of the strength of the electron-phonon coupling we start with a strongly-coupled (adiabatic) polaron state where the electron is taken to be fluctuating within a self-induced potential well built up by the field of correlated virtual phonons. Such an ansatz for the composite behavior of the electron and the surrounding cloud of virtual phonon is expected to yield a reasonable description of the polaron effect only in the limit of large α. For small

coupling constants, one, therefore, expects an increasingly large deviation of the adiabatic theory from intermediate-LLP theory or from theoretical perturbation calculations. In what follows this short-coming is eliminated by an appropriate modification of the adiabatic polaron state which allows the theory itself to make an extrapolation towards the weak-coupling results.

For a choice of a Gaussian trial wavefunction

$$\psi_0 = \left(\frac{\sigma}{2\pi}\right)^{1/2} \exp(-r^2\sigma/4) \tag{4.35}$$

we obtain

$$\sigma_Q = \exp\left(-\frac{Q^2}{2\sigma}\right), \tag{4.36}$$

$$\langle\Psi|H|\Psi\rangle = e_0 - \lambda_0, \tag{4.37}$$

where

$$e_0 = \langle\psi_0|H_0|\psi_0\rangle = \frac{\sigma}{2} - \beta\sqrt{\frac{\pi\sigma}{2}} - \alpha\frac{\sqrt{\pi\sigma}}{2} \tag{4.38}$$

and

$$\lambda_0 = \sum_Q V_Q^2\sigma_Q^2 = \alpha\frac{\sqrt{\pi\sigma}}{2}. \tag{4.39}$$

Minimization with respect to σ yields the well established approximate result for strongly coupled 2D-polaron:

$$\frac{\partial E}{\partial\sigma} = 0 \tag{4.40}$$

gives

$$\sigma = \frac{\alpha^2\pi}{4}. \tag{4.41}$$

Then inserting this into Eq. (4.38) with β=0, we get

$$E_{sc} = -(\pi/8)\alpha^2. \tag{4.42}$$

We now extend the formulation to the case of a weak coupling. No matter how small α is, we still continue with our discussions from Eq. (4.31), since with decreasing α the degree of localization of the electron becomes reduced in a significant manner, eventually σ_Q tends to zero on average and thus H' converts back to the Eq. (4.2).

The perturbational term e_Q is

$$\begin{aligned} e_Q &= \langle\psi_0|\eta_Q H_0 \eta_Q^*|\psi_0\rangle \\ &= \frac{1}{2}Q^2 + \left(\frac{1}{2}Q^2 + e_0\right) h_Q - \beta\sqrt{2\pi\sigma}\sigma_Q^{3/2}\left[\sigma_Q^{1/2} - I_0\left(\frac{Q^2}{4\sigma}\right)\right]. \end{aligned} \quad (4.43)$$

Then

$$f_Q = -\sum_Q V_{Q'}^2 \sigma'_Q \langle\psi_0|\eta_Q(e^{i\mathbf{Q}'.\mathbf{r}} + e^{-i\mathbf{Q}'.\mathbf{r}})\eta_Q^*|\psi_0\rangle. \quad (4.44)$$

Taking

$$\eta_Q(e^{i\mathbf{Q}'.\mathbf{r}} + e^{-i\mathbf{Q}'.\mathbf{r}})\eta_Q^* \quad (4.45)$$

gives

$$\begin{aligned} &= e^{i\mathbf{Q}'.\mathbf{r}} - \sigma_Q e^{i(\mathbf{Q}+\mathbf{Q}').\mathbf{r}} + e^{-i\mathbf{Q}'.\mathbf{r}} - \sigma_Q e^{-i(\mathbf{Q}+\mathbf{Q}').\mathbf{r}} - \sigma_Q^2 e^{i\mathbf{Q}'.\mathbf{r}} \\ &- \sigma_Q e^{i(\mathbf{Q}-\mathbf{Q}').\mathbf{r}} - \sigma_q e^{-i(\mathbf{Q}-\mathbf{Q}').\mathbf{r}} - \sigma_Q^2 e^{-i\mathbf{Q}'.\mathbf{r}}. \end{aligned} \quad (4.46)$$

Sandwiching this with the wavefunction, we get

$$2(\sigma'_Q - \sigma_Q\sigma_{Q+Q'} - \sigma_Q\sigma_{Q-Q'} + \sigma_Q^2\sigma'_Q). \quad (4.47)$$

Then

$$f_Q = -2\sum_Q V_{Q'}^2(\sigma_{Q'}^2 - \sigma_{Q'}\sigma_Q\sigma_{Q+Q'} - \sigma_{Q'}\sigma_Q\sigma_{Q-Q'} + \sigma_Q^2\sigma_{Q'}^2). \quad (4.48)$$

Using Eq. (4.39), f_Q becomes

$$f_Q = -2\lambda_0 - 2\lambda_0\sigma_Q^2 + 2\sigma_Q + 2\sum_{Q'} V_{Q'}^2[\sigma_Q\sigma_{Q'}\sigma_{Q+Q'} + \sigma_Q\sigma_{Q'}\sigma_{Q-Q'}]. \quad (4.49)$$

The value of σ_Q is given in Eq. (4.36), so we now can find $\sigma_{Q'}$, $\sigma_{Q+Q'}$, and $\sigma_{Q-Q'}$

$$\sigma_{Q'} = \exp\left(-\frac{Q'^2}{2\sigma}\right), \quad (4.50)$$

$$\sigma_{Q+Q'} = \exp\left(-\frac{(\mathbf{Q}'+\mathbf{Q})^2}{2\sigma}\right) = \sigma_{Q'}\sigma_Q e^{-\frac{1}{\sigma}\mathbf{Q}.\mathbf{Q}'}, \quad (4.51)$$

$$\sigma_{Q-Q'} = \exp\left(-\frac{(\mathbf{Q}'-\mathbf{Q})^2}{2\sigma}\right) = \sigma_{Q'}\sigma_Q e^{\frac{1}{\sigma}\mathbf{Q}.\mathbf{Q}'}. \quad (4.52)$$

Converting summation into the integral we get

$$f_Q = 2\lambda_0\sigma_Q^2[2e^\gamma I_0(\gamma) - 1] - 2\lambda_0 \quad (4.53)$$

where I_0 denotes the zeroth order modified Bessel function and

$$\gamma = \left(\frac{Q^2}{8\sigma}\right). \quad (4.54)$$

4.3 Application: Polaron Effects on the Binding Energy of a Hydrogenic Impurity

In this work we consider the problem of a two-dimensional hydrogenic impurity. We formulate the theory again in the manner proposed by Devreese et al. [9]. The calculation is of variational nature, and even for small coupling constant ($\alpha \ll 1$) the procedure is to start with the strong coupling approximation. The small α limit is handled by a suitable modification of the adiabatic polaron state which allows the theory itself to make an extrapolation towards the weak-coupling regime.

As it is derived in the previous section; under displaced oscillator transformation $H \rightarrow e^{-S} H e^{S}$ the Hamiltonian becomes

$$\begin{aligned} H' &= H_e + \sum_Q a_Q^\dagger a_Q + \sum_Q V_Q^2 \sigma_Q^2 - \sum_Q V_Q^2 \sigma_Q (e^{i\mathbf{Q}.\mathbf{r}} + e^{-i\mathbf{Q}.\mathbf{r}}) \\ &+ \sum_Q V_Q a_Q (e^{i\mathbf{Q}.\mathbf{r}} - \sigma_Q) + V_Q a_Q^\dagger (e^{-iQ.r} - \sigma_Q) \end{aligned} \tag{4.55}$$

where

$$\eta_Q = e^{i\mathbf{Q}.\mathbf{r}} - \sigma_Q. \tag{4.56}$$

Minimization of $\langle 0|\langle\psi_0|H'|\psi_0\rangle|0\rangle$ with respect to ψ_0 leads to strong coupling result for the energy. Taking the hydrogen-like behavior, $\psi_0 = N \exp(-r/\sigma)$, we obtain

$$E_{sc}^{(3D)} = -(\beta^2/4) - (5/16)\alpha\beta - (5/16)^2\alpha^2 \tag{4.57}$$

for the bulk case and

$$E_{sc}^{(2D)} = -\beta^2 - (3/8)\pi\alpha\beta - (9/256)\pi^2\alpha^2 \tag{4.58}$$

when ψ_0 is taken to be strictly two-dimensional.

To obtain the weak coupling result we should follow the perturbational terms such as e_Q, f_Q, and λ. To begin with e_Q,

$$e_Q = \langle\psi_0|\eta_Q H_0 \eta_Q^*|\psi_0\rangle \tag{4.59}$$

where

$$H_0 = -\nabla^2 - \frac{\beta}{r}. \tag{4.60}$$

Multiplying this Hamiltonian from left by η_Q and then from right by η_Q^* and finally sandwiching the result into the wavefunction we get

$$\begin{aligned} &= \langle\psi_0| - e^{i\mathbf{Q}.\mathbf{r}}\nabla^2 e^{-i\mathbf{Q}.\mathbf{r}}|\psi_0\rangle + \sigma_Q\langle\psi_0|e^{i\mathbf{Q}.\mathbf{r}}\nabla^2|\psi_0\rangle \\ &- \langle\psi_0|\frac{\beta}{r}|\psi_0\rangle + 2\sigma_Q\langle\psi_0|\frac{\beta}{r}e^{i\mathbf{Q}.\mathbf{r}}|\psi_0\rangle + \sigma_Q\langle\psi_0|\nabla^2 e^{-i\mathbf{Q}.\mathbf{r}}|\psi_0\rangle \\ &+ \sigma_Q^2 e_0. \end{aligned} \tag{4.61}$$

Now if we do the calculation term by term e_Q becomes

$$e_Q = (Q^2 + e_0)h_Q + \sigma\beta Q^2\sigma_Q^2. \tag{4.62}$$

What is left is to calculate f_Q. Remember we define f_Q as;

$$f_Q = -\sum_{Q'} V_{Q'}^2\sigma_{Q'}\langle\psi_0|\eta_Q(e^{i\mathbf{Q}'.\mathbf{r}} + e^{-i\mathbf{Q}'.\mathbf{r}})\eta_Q^*|\psi_0\rangle. \tag{4.63}$$

Taking $\eta_Q(e^{i\mathbf{Q}'.\mathbf{r}} + e^{-i\mathbf{Q}'.\mathbf{r}})\eta_Q^*$, first;

$$\begin{aligned} &= (e^{i\mathbf{Q}.\mathbf{r}} - \sigma_Q)[e^{i\mathbf{Q}'.\mathbf{r}} + e^{-i\mathbf{Q}'.\mathbf{r}}](e^{-i\mathbf{Q}.\mathbf{r}} - \sigma_Q) \\ &= (e^{i\mathbf{Q}.\mathbf{r}} - \sigma_Q)[e^{i(\mathbf{Q}'-\mathbf{Q}).\mathbf{r}} - \sigma_Q e^{i\mathbf{Q}'.\mathbf{r}} + e^{-i(\mathbf{Q}'+\mathbf{Q}).\mathbf{r}} - \sigma_Q e^{-i\mathbf{Q}'.\mathbf{r}}] \\ &= e^{i\mathbf{Q}'.\mathbf{r}} - \sigma_Q e^{i(\mathbf{Q}+\mathbf{Q}').\mathbf{r}} + e^{-i\mathbf{Q}'.\mathbf{r}} - \sigma_Q e^{i(\mathbf{Q}-\mathbf{Q}').\mathbf{r}} - \sigma_Q e^{-i(\mathbf{Q}-\mathbf{Q}').\mathbf{r}} \\ &+ \sigma_Q^2 e^{i\mathbf{Q}'.\mathbf{r}} - \sigma_Q e^{-i(\mathbf{Q}+\mathbf{Q}').\mathbf{r}} + \sigma_Q^2 e^{-i\mathbf{Q}'.\mathbf{r}} \end{aligned} \tag{4.64}$$

Inserting this into the wave equation we reach

$$2\sigma'_Q - 2\sigma_Q\sigma_{Q+Q'} - 2\sigma_Q\sigma_{Q-Q'} + 2\sigma_Q^2\sigma'_Q, \tag{4.65}$$

where $\sigma_Q = \langle\psi_0|e^{i\mathbf{Q}.\mathbf{r}}|\psi_0\rangle$. Then, we can write f_Q as;

$$\begin{aligned} f_Q &= -2\sum_{Q'} V_{Q'}^2(\sigma_{Q'}^2 - \sigma_Q\sigma_{Q'}\sigma_{Q+Q'} - \sigma_Q\sigma_{Q'}\sigma_{Q-Q'} + \sigma_Q^2\sigma_{Q'}^2) \\ &= -2\lambda_0 - 2\lambda_0\sigma_Q^2 + 2\sum_{Q'} V_{Q'}^2[\sigma_Q\sigma_{Q'}\sigma_{Q+Q'} + \sigma_Q\sigma_{Q'}\sigma_{Q-Q'}]. \end{aligned} \tag{4.66}$$

To calculate f_Q we now have to take the summation. After converting the summation into an integral we come across ϕ integral since both Q and Q' are vectors.

The result of that integral gives us the complete integral of second kind $E(m)$ with parameter

$$m = \sin^2\left[\frac{\sigma}{\mu_+}(QQ')^{1/2}\right] \tag{4.67}$$

where

$$\mu_\pm = 1 + \frac{\sigma^2}{4}(Q \pm Q')^2 \tag{4.68}$$

so the final form of f_Q is

$$f_Q = 2\lambda_0(1+\sigma_Q^2) - \frac{8}{\pi}\alpha\sigma_Q \int_0^\infty dQ' \frac{\sigma_{Q'}}{\mu_+\mu_-^2} E(m) \tag{4.69}$$

where

$$\sigma_Q = \left(1 + \frac{\sigma^2}{4}Q^2\right)^{-3/2}. \tag{4.70}$$

Because of the analytic complexity, the optimal fits to λ and σ have been performed numerically. Without the polaron effect ($\alpha = 0$) we obtain trivially $\lambda_0 = 0$, $\lambda = 0$ and hence $E = -\beta^2$: the two dimensional Rydberg which is four times that for the bulk case.

4.4 Effective Mass of the Polaron

Fröhlich, Pelzer and Zienau [4] treat the interaction term of the Fröhlich Hamiltonian as a perturbation so that as it is mentioned,

$$H = H_0 + H_1, \tag{4.71}$$

where

$$\begin{aligned} H_0 &= -\nabla^2 + \sum_q a_q^\dagger a_q, \\ H_1 &= \sum_q V_q(\exp(i\mathbf{q}.\mathbf{r})a_q + H.c). \end{aligned} \tag{4.72}$$

The total momentum of the system

$$\hat{P} = \hat{p} + \sum_q q a_q^\dagger a_q = -i\nabla_r + \sum_q q a_q^\dagger a_q \tag{4.73}$$

commutes with the Hamiltonian H ($[\hat{P}, H] = 0 = [\hat{P}, H_0]$) and is therefore a constant of motion. Taking as basis the unperturbed eigenstates ψ of H_0 and $\hat{P}$ given by

$$\psi = \frac{1}{\sqrt{V}} exp\left[i \left(\mathbf{P} - \sum_q \mathbf{q} n_q \right) .\mathbf{r} \right] \prod_q |n_q\rangle, \tag{4.74}$$

where the phonon eigenstates $|n_q\rangle$ satisfy

$$a_q^\dagger a_q |n_q\rangle = n_q |n_q\rangle, \;\; n_q = 0, 1, 2, ..., \tag{4.75}$$

and

$$\begin{aligned} H_0\psi &= E_0\psi = \left[\left(\mathbf{P} - \sum_q \mathbf{q} n_q \right)^2 + \sum_q n_q \right] \psi, \\ \hat{P}\psi &= P\psi. \end{aligned} \tag{4.76}$$

FPZ [4] obtain the lowest order perturbed state ψ_{pert} and energy $E_{pert(\mathbf{p})}$ corresponding to an initial electron momentum $\mathbf{p}$ in the zero phonon state ($\psi = (1/\sqrt{V}) exp(i\mathbf{p}.\mathbf{r}) \prod_q |0_q\rangle$)

$$\psi_{pert} = \frac{exp(i\mathbf{p}.\mathbf{r})}{\sqrt{V}} \left\{ 1 - \left(\frac{4\pi\alpha}{V} \right)^{1/2} \sum_q \frac{exp(-i\mathbf{q}.\mathbf{r}) a_q^\dagger}{q[(p-q)^2 + 1 - p^2]} \right\} \prod_q |0_q\rangle, \tag{4.77}$$

$$E_{pert}(\mathbf{p}) = p^2 - \frac{4\pi\alpha}{V} \sum_q \frac{1}{q^2[(\mathbf{p}-\mathbf{q})^2 + 1 - p^2]} \tag{4.78}$$

$$= \begin{cases} p^2 - \alpha \frac{sin^{-1} p}{p} = -\alpha - p^2 \left(1 - \frac{\alpha}{6} \right) + O(p^4), & \text{p}<1, \qquad \alpha \to 0; \\ p^2 - \frac{\alpha}{p} \frac{\pi}{2}, & \text{p}\geq 1, \qquad \alpha \to 0. \end{cases} \tag{4.79}$$

Validity of Rayleigh Schrödinger Perturbation Theory requires that $\alpha \to 0$ and furthermore p must be kept less than unity in order to exclude the degeneracy with the real phonon states. Therefore, the solution compatible with the above constraints is given by the first line of the above equation whose expansion to order p^2 is sufficient for a low-lying electron ($p \ll 1$). In this way an effective mass is defined

$$m^* = 1/(1 - \alpha/6). \tag{4.80}$$

4.5 Variational State for Arbitrary Coupling

Regardless of the value of α, no matter how small it is, the procedure is still to continue with our considerations from Eq. 4.17, since with decreasing α the degree of localization of the electron becomes reduced in a significant manner; eventually σ_Q tends to zero on the average and thus H' converts back to its original form H stripped from the displaced oscillator transformation. In view of this reasoning one is led to include a first order correction to trial state

$$\Psi_g = \psi_e|0\rangle \tag{4.81}$$

with the last term in Eq. (4.17) treated as a perturbation as formulated in Section 1.

Then, for not too strong α the pure strong coupling treatment of the problem is totally inadequate to reflect any weak coupling aspect and this shortcoming is eliminated in the perturbative variational approach by solving the transcendental Eq. (4.33) for the term λ in the energy expression, since it is only through this term that a detailed interbalance is set up between the strong and weak coupling counterparts of the coupled electro-phonon system. As α is shifted down to small values the role of λ plays becomes very prominent and in case the electron is loosely bound the polaron binding is mostly determined by this term.

In particular, at weak coupling ($\alpha \ll 1$), it is easy to see that the terms e_0, λ_0 and λ become far too small to yield any significant contribution to the summand in the transcendental Eq. (4.32). Therefore in Eq. (4.27) retaining only $h_Q \approx 1$ and $e_Q \approx q^2$ in Eq. (4.43).

Chapter 5

MAGNETIC FIELD

The problem of a magnetic field on impurity states has been of considerable interest. The basic difficulty in calculating the energy levels of a donor atom subjected to a simultaneous Coulomb and magnetic field is that Schrödinger's equation is not completely separable. In the low magnetic field limit, where the states are mostly hydrogenic, the problem is treated by a perturbational method.

On the other extreme of strong enough fields, the electronic charge distribution condenses on to impurities in the directions perpendicular to the field leading to a stronger binding of the electrons. In this limit, oscillations in the field direction are much slower than the cyclotron frequency and consequently the electronic states can be described by the Landau levels.

The Hamiltonian consisting of a bound electron in a constant magnetic field $B\hat{z}$ is given by

$$H_0 = \frac{1}{2m^*}\left(\overrightarrow{p} - \frac{eB}{2c}\hat{z} \times \overrightarrow{r}\right)^2 - \frac{\beta}{r}. \tag{5.1}$$

After taking the square and grouping the terms together we get;

$$H_0 = \frac{p^2}{2m^*} + \frac{1}{2}m^*\left(\frac{w_c^0}{2}\right)^2 (x^2 + y^2) + \frac{1}{2}w_c^0 L_z - \frac{\beta}{r}. \tag{5.2}$$

where $w_c^0 = \frac{eB}{m^* c}$ is the cyclotron frequency, m^* is the band mass and L_z is the z-component of the angular momentum. The Coulomb interaction is screened

by the static dielectric constant of the material $\beta = \frac{e^2}{\varepsilon_0}$. The variational method has been used by several authors to calculate the magnetic field dependence of the ground-state energy of a donor atom. Yafet et al, have pointed out that in the strong magnetic field limit the eigenfunctions of H_0 take the product form: $f(x,y)g(z)$. They used the simple form

$$\Psi \propto exp[-a(x^2+y^2)-bz^2] \tag{5.3}$$

for the ground state and showed that the ionization potential increases considerably at high fields. There has been many later investigations on hydrogenic energy levels in high magnetic fields with an increasing degree of sophistication for the wavefunctions used.

In a deformable lattice, the interaction of the electron with the phonon field posses an additional yet interesting problem which affects the localized electronic spectrum. Much of the work done along this line concerns optical phonons. We would like to handle this problem for the case where the electron couples the acoustic phonons via deformation potential. Introducing the Fröhlich phonon energy and the electron-phonon interaction terms the Hamiltonian is extended to

$$H = H_0 = \sum_Q \hbar w(Q) a_Q^\dagger a_Q + H_{e-ph}. \tag{5.4}$$

Since the energy of the most important acoustic phonons contributing to a deformation around the electron impurity system is small in comparison with the ionization energy, the charge density fluctuations of the electron are too fast for the lattice to follow. Consequently, the lattice responds to the average position of the electron, and the electron in turn goes into a bound state in the deep attractive potential well set up by itself. A reasonable treatment to such a case can, therefore, be given by the strong coupling theory of Pekar [2].

5.1 Application: Polaron Effects on the Binding Energy of a Hydrogenic Impurity in Two Dimensions under Weak Magnetic Fields

We will now again consider the same problem which is treated in Chapter 4 but now with an additional potential due to an external magnetic field. The Hamiltonian under external magnetic field is given as

$$H_e = \frac{p^2}{2m^*} + \frac{1}{2}m^* \left(\frac{w_c^0}{2}\right)^2 (x^2 + y^2) + \frac{1}{2}w_c^0 L_z - \frac{\beta}{r}. \tag{5.5}$$

In polaron units ($2m^* = \hbar = 1$) and $E = \hbar\omega_0$ and $L \sim (\hbar/2m^*\omega_0)^{1/2}$, this equation becomes

$$H_e = \nabla^2 + \frac{1}{4}\left(\frac{\omega_c^0}{2}\right)^2 \rho^2 + \frac{1}{2}\omega_c^0 L_z - \frac{\beta}{\rho} \tag{5.6}$$

where

$$\beta = \frac{e^2}{\varepsilon_0 \hbar}\left(\frac{2m^*}{\hbar\omega_0}\right)^{1/2}. \tag{5.7}$$

For this problem we again use the perturbational theory to calculate the ground state energy, i.e; e_0, λ_0, e_Q, f_Q will be calculated in the same way. The difference is the additional terms in the kinetic part of the Hamiltonian as can be seen in Eq. (5.6). The remaining part of the Hamiltonian is the same with Fröhlich Hamiltonian because these terms are coming because of the polaronic contribution.

The wavefunction is

$$\psi = (\frac{2}{\pi\sigma^2})^{1/2} e^{-\rho/\sigma}. \tag{5.8}$$

We know that

$$\begin{aligned} e_0 &= \langle\psi|H_e|\psi\rangle \\ &= \langle\psi| - \nabla^2 + \frac{1}{4}\left(\frac{\omega_c^0}{2}\right)^2 \rho^2 + \frac{1}{2}\omega_c^0 L_z - \frac{\beta}{\rho}|\psi\rangle \\ &= \frac{1}{\sigma^2} - \frac{2\beta}{\sigma} + \frac{3}{8}\left(\frac{\omega_c}{2}\right)^2 \sigma^2. \end{aligned} \tag{5.9}$$

If now we take the Coulombic interaction zero, e_0 becomes

$$e_0 = \frac{1}{\sigma^2} + \frac{3}{8}\left(\frac{\omega_c}{2}\right)^2 \sigma^2. \tag{5.10}$$

The next step is the calculation of e_Q by the same procedure. So from now on I will give only the result of the relevant terms.

$$e_Q = (Q^2+e_0)h_Q+\sigma\beta Q^2\sigma_Q^2+\frac{3}{8}\left(\frac{\omega_c}{2}\right)^2 \sigma^2(1+\sigma_Q^2)-\frac{3}{8}\left(\frac{\omega_c}{2}\right)^2 \sigma^2\sigma_Q^{1/3}P_3(\sigma^{1/3}) \tag{5.11}$$

where P_3 is the third order Legendre polynomial.

Since magnetic field effect cause no contribution to the term f_Q,

$$f_Q = 2\lambda_0(1+\sigma_Q^2) - \frac{8}{\pi}\alpha\sigma_Q\int_0^\infty dQ' \frac{\sigma_{Q'}}{\mu_+\mu_-^2}E(m). \tag{5.12}$$

5.2 Application: Polaron Effects on the Binding Energy of a Gaussian Wavefunction in Two Dimensions under Strong Magnetic Fields

When we take ω_c strong enough we should change the form of the wavefunction we use, so from now on for strong magnetic field we will consider gaussian wavefunction which is given by

$$\psi_0 = \left(\frac{\sigma}{2\pi}\right)^{1/2} exp(-r^2\sigma/4). \tag{5.13}$$

Following the same procedure as the previous section we will first calculate e_0.

$$\begin{aligned} e_0 &= \langle\Psi|H_0|\Psi\rangle \\ &= \langle\Psi|-\nabla^2 - \frac{\beta}{r} + \frac{1}{4}\left(\frac{w_c^0}{2}\right)^2(x^2+y^2) + \frac{1}{2}\left(\frac{w_c^0}{2}\right)L_z|\Psi\rangle \end{aligned} \tag{5.14}$$

Because our wavefunction is symmetric due to x and y we get no contribution from L_z term. From the calculation of the rest three terms we get

$$e_0 = \frac{\sigma}{2} - \beta\sqrt{\frac{\pi\sigma}{2}} + \frac{\omega_c^2}{2}. \tag{5.15}$$

Then, from the definition of σ_Q, we get

$$\begin{aligned}\sigma_Q &= \langle\Psi|e^{i\mathbf{Q}.\mathbf{r}}|\Psi\rangle \\ &= \frac{\sigma}{2\pi}\int_0^\infty re^{-r^2\sigma/2}dr\int_0^{2\pi}e^{iQrcos\theta}d\theta \\ &= \frac{\sigma}{2\pi}2\pi\int_0^\infty re^{-r^2\sigma/2}J_0(Qr)dr \\ &= e^{-Q^2/2\sigma}. \end{aligned} \tag{5.16}$$

And,

$$\lambda_0 = \sum_Q V_Q^2\sigma_Q^2 = \frac{\alpha\sqrt{\pi\sigma}}{2} \tag{5.17}$$

where

$$V_Q = \left(\frac{2\pi\alpha}{Q}\right)^{(1/2)}. \tag{5.18}$$

So the strong coupling energy result is found as

$$\begin{aligned}E_{sc} &= e_0 - \lambda_0 \\ &= \frac{\sigma}{2} - \beta\sqrt{\frac{\pi\sigma}{2}} + \frac{1}{2}\left(\frac{\omega_c}{2}\right)^2\sigma^{-1} - \frac{\alpha\sqrt{\pi\sigma}}{2}. \end{aligned} \tag{5.19}$$

Taking $\alpha = \beta = 0$ and then minimizing energy with respect to σ we get

$$\sigma = 2\omega_c, \tag{5.20}$$

and

$$\begin{aligned}e_Q &= \frac{1}{2}Q^2 + (\frac{1}{2}Q^2 + e_0)h_Q - \beta\sqrt{2\pi\sigma}\sigma_Q^{3/2}\left[\sigma_Q^{1/2} - I_0\left(\frac{Q^2}{4\sigma}\right)\right] \\ &+ \frac{1}{2}\left(\frac{\omega_c}{2}\right)^2\frac{Q^2}{4\omega_c^2}\sigma_Q^2. \end{aligned} \tag{5.21}$$

And finally the last term f_Q is

$$f_Q = 2\lambda_0\sigma_Q^2[2e^\gamma I_0(\gamma) - 1] - 2\lambda_0. \tag{5.22}$$

Before we present our results considering the coupled effect of both the electron-phonon interaction and a magnetic field on the binding energy, we would like to test the validity of the present formulation by referring to some special cases where the situation is more clear and simple.

5.2.1 Bare Donor ($\alpha = 0$)

Even with no phonon coupling yet introduced into the problem, one has several distinguishing features.

i- $(\beta = 0)$ **case of a free electron in a magnetic field.**

Minimizing Eq. (5.10), the optimal σ-value is $\omega_c/2$, yielding the lowest Landau orbit energy.

$$e_0 = \frac{\omega_c}{2}. \tag{5.23}$$

ii- $(\beta \neq 0)$ **case of a bound electron in a magnetic field.**

Introducing

$$\gamma = \frac{\omega_c/2}{\beta^2} \tag{5.24}$$

as measure of the strength of the magnetic field relative to the two-dimensional effective Rydberg, we refer to the limits of strong and weak fields.

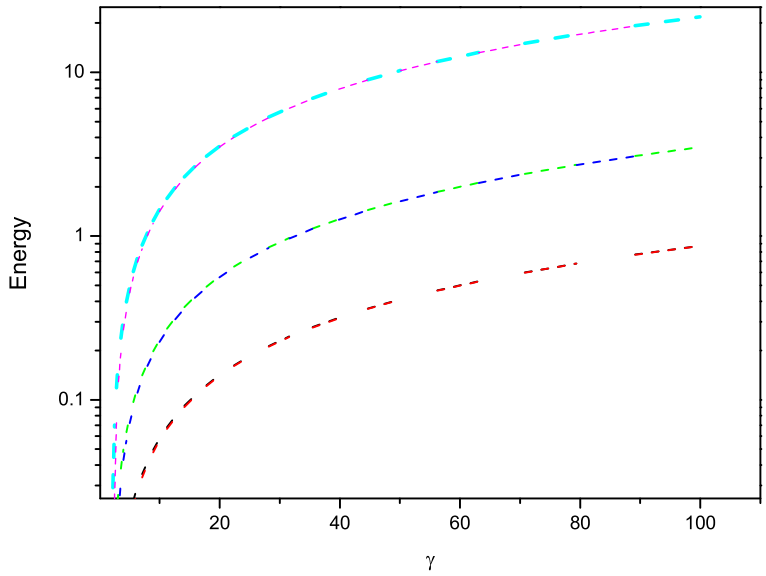

Figure 5.1: Energy versus γ for β =0.1, 0.2, 0.3 for $\alpha = 0$ from bottom to top. The results obtained from MacDonald an Ritchie [16] and our present theory match with each other and placed on the same line for different β values.

Figure 5.1 shows the energy characteristics against γ. Since we get a great agreement with MacDonald and Ritchie [16], their and our results are completely on the same line. We draw this for three different β values which are β=0.1, 0.2, and 0.3. The bottom line is for β=0.1 case and the top line is for β=0.3. Here because of the results are so close together we cannot see the small difference between the two energies. This small difference can be seen more clearly in Table 5.1.

Table 5.1: The change of the theoretical values of energy obtained by MacDonald and Ritchie [16] and our computed energy for β=0.1, 0.2, 0.3 and for different γ values, γ =10, 20, 50.

β	γ=10	γ=20	γ=50	
0.1	(-1)0.581880	(0)0.141409	(0)0.410417	present
	(-1)0.565250	(0)0.139796	(0)0.408848	M-R
0.2	(0)0.232752	(0)0.565635	(1)0.164167	present
	(0)0.226100	(0)0.559182	(0)0.163539	M-R
0.3	(1)0.145470	(1)0.353522	(2)0.102604	present
	(1)0.141312	(1)0.349489	(2)0.102212	M-R

a- weak field limit ($\gamma \ll 1$)

In this limit the donor state is mostly hydrogenic and the dominant terms in Eq. (5.10) are the first two and the last is only a small correction. We find that the optimal σ-value which minimizes the dominant part is β^{-1}: the effective two-dimensional Bohr radius.

Replacing σ by β^{-1} in Eq.(5.10) gives

$$E = -\beta^2 \left(1 - \frac{3}{8}\gamma^2\right). \tag{5.25}$$

This expression is identical to that given by MacDonald and Ritchie [16].

Figure 5.2 is for α=0.05, Figure 5.3 is for α=0.10 and Figure 5.4 is for α=0.20. As it is seen increasing α values causes to increase the gap between the two results. This again can be seen more clearly from the Table 5.2 for different ω_c and β values.

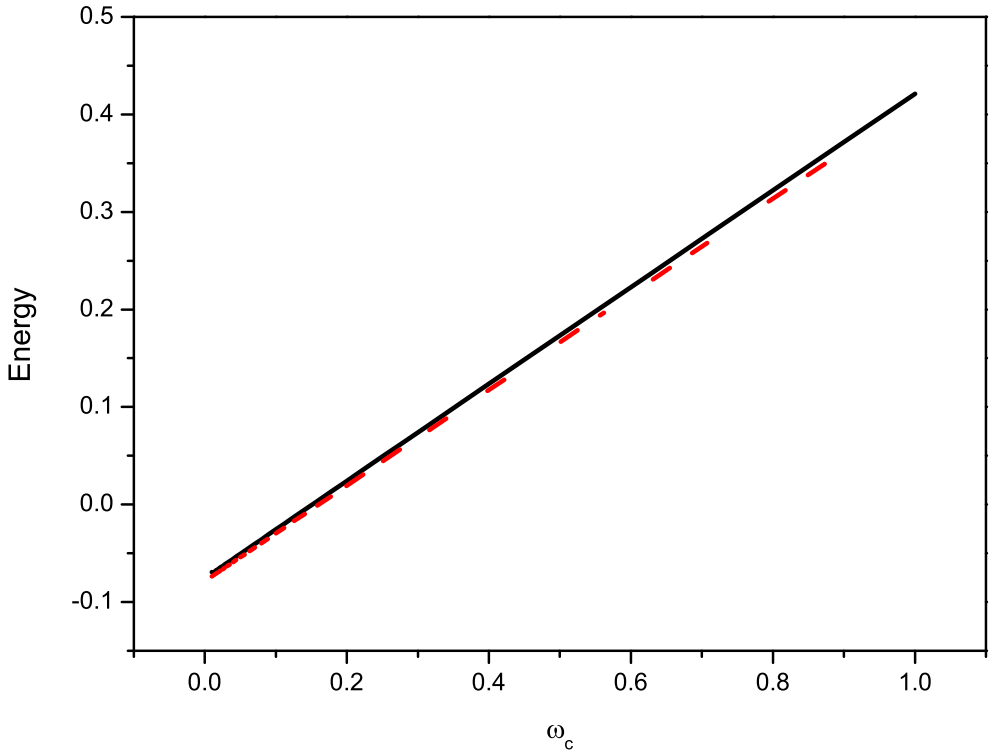

Figure 5.2: Energy versus ω_c for α=0.05 under weak magnetic field. The solid line represents M-R [16] results and the dashed line is for our results.

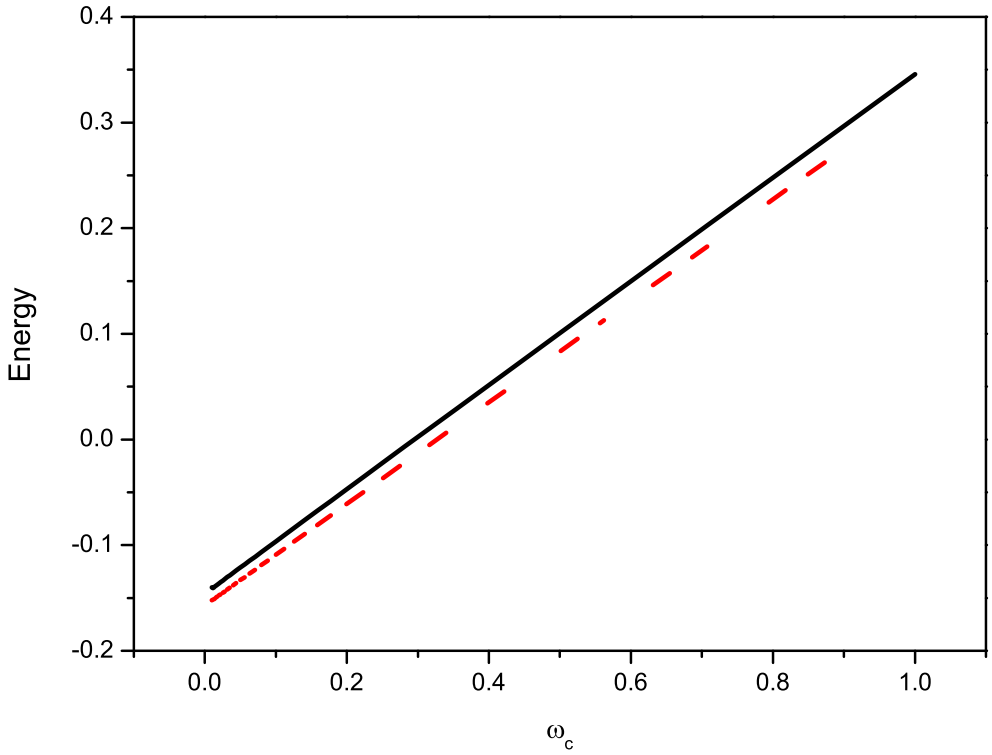

Figure 5.3: Energy versus $\omega_c$for α=0.10 under weak magnetic field. The solid line is for M-R [16] and the dashed line is for ours. The gap between the two is larger than for α=0.05.

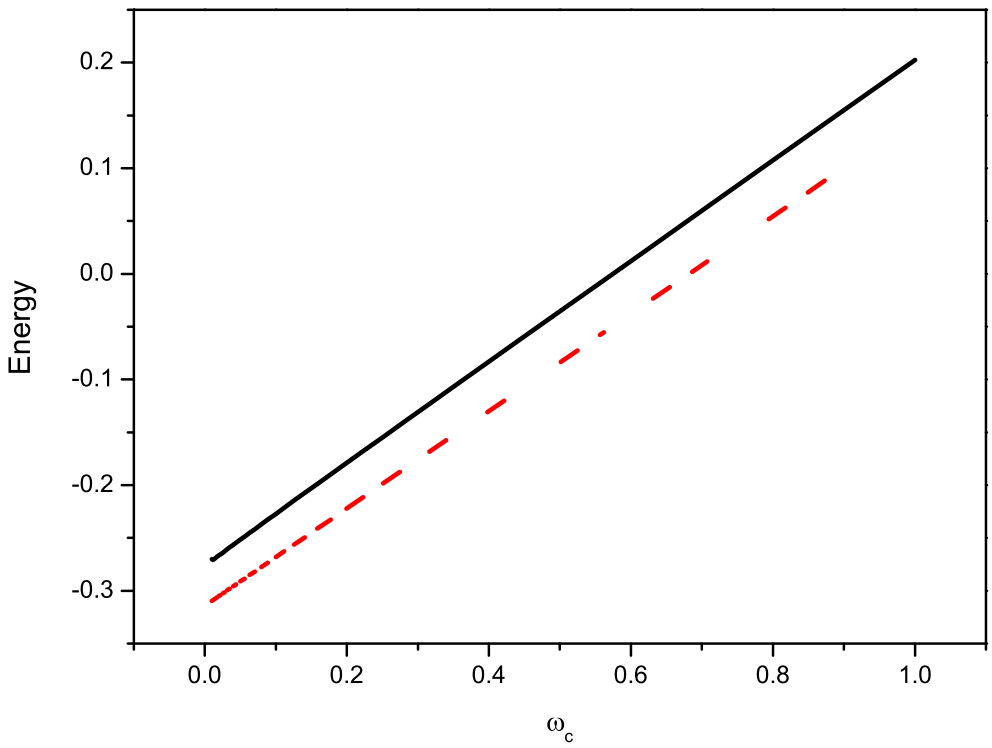

Figure 5.4: Energy versus ω_c for α=0.20 under weak magnetic field. The solid line is for M-R [16] and the dashed line is for ours. The gap between the two is larger than for α=0.05 and α=0.10.

Table 5.2: Comparison of the result of MacDonald and Ritchie [16] and our calculated energy values for γ=0.01

γ	β	ω_c	E_{M-R}	$E_{present}$
0.01	0.1	0.0002	0.009999625	0.0099630
0.01	0.2	0.0008	0.0399985	0.0399985
0.01	0.5	0.0050	0.24990625	0.249991
0.01	1.0	0.0020	0.9999624	0.999963

Table 5.3: Comparison of the result of MacDonald and Ritchie [16] and our calculated energy values for γ=0.02

γ	β	ω_c	E_{M-R}	$E_{present}$
0.02	0.1	0.0004	0.0099985	0.0099985
0.02	0.2	0.0016	0.039940	0.039940
0.02	0.5	0.0100	0.2499625	0.249963
0.02	1.0	0.0800	0.99985	0.99940

By using Eq. (5.25), we can compare the results by MacDonald and Ritchie [16] with our work in Table 5.2.

Table 5.4: Comparison of the result of MacDonald and Ritchie [16] and our calculated energy values for γ=0.05

γ	β	ω_c	E_{M-R}	$E_{present}$
0.05	0.1	0.0010	0.009990625	0.00999063
0.05	0.2	0.004	0.0399625	0.0399625
0.05	0.5	0.025	0.249765625	0.249766
0.05	1.0	0.100	0.9990625	0.999063

Table 5.5: Comparison of the result of MacDonald and Ritchie [16] and our calculated energy values for γ=0.1

γ	β	ω_c	E_{M-R}	$E_{present}$
0.1	0.1	0.002	0.0099625	0.00996264
0.1	0.2	0.008	0.03985	0.0398506
0.1	0.5	0.050	0.2490625	0.249066
0.1	1.0	0.200	0.99625	0.996264

Table 5.6: Comparison of the result of MacDonald and Ritchie [16] and our calculated energy values for γ=0.2

γ	β	ω_c	E_{M-R}	$E_{present}$
0.2	0.1	0.004	0.009850	0.00985215
0.2	0.2	0.016	0.039400	0.0394086
0.2	0.5	0.100	0.24625	0.246304
0.2	1.0	0.400	0.985000	0.985215

b- strong field limit ($\gamma \gg 1$)

To provide an insight into the validity of our results we once again refer to the paper by MacDonald and Ritchie [16]. In the high field extreme they obtain

$$E = 2\gamma\beta^2 \left(\frac{1}{2} - x - 0.4401x^2 - 0.2331x^3 - 0.0727x^4 - ...\right) \tag{5.26}$$

where

$$x = \left(\frac{\pi}{8\gamma}\right)^{1/2}. \tag{5.27}$$

Table 5.7: The change of the theoretical values of energy obtained by MacDonald and Ritchie [16] by using Eq. (5.26) , and our results obtained by extended theory

	γ=5	γ=10	γ=20	
β=0.1	0.0181	0.0565	0.1398	M-R
	0.0198	0.0582	0.1414	present
β=0.2	0.0722	0.2261	0.5592	M-R
	0.0791	0.2328	0.5656	present
β=0.5	0.4512	1.4131	3.4949	M-R
	0.4945	1.4547	3.5352	present

5.2.2 Polaronic Donor ($\alpha \neq 0$)

When the Fröhlich interaction is turned on the problem displays further distinguishing features pertinent to electron-phonon coupling. As preliminary simple cases we refer to the individual ones where either $\beta = 0$ or $\omega_c = 0$.

i- ($\beta = 0$) **case of a polaron in a magnetic field.**

At weak coupling the state of the system can be thought of as consisting of a polaron orbiting in the lowest Landau level with frequency ω_c corrected by replacing the effective electron mass by the polaron mass.

Thus, with the polaron of self energy

$$E_p \simeq -\frac{\pi}{2}\alpha \tag{5.28}$$

and mass

$$m_p = 1 + \frac{\pi}{8}\alpha, \tag{5.29}$$

orbiting as a rigid entity with frequency $\omega_c m_p^{-1}$, one writes

$$\begin{aligned} E &= \frac{1}{2}\left(\frac{\omega_c}{m_p}\right) + E_p \\ &= \frac{\omega_c}{2}\left(1+\frac{\pi}{8}\alpha\right)^{-1} - \frac{\pi}{2}\alpha \\ &\simeq \frac{\omega_c}{2} - \frac{\pi}{2}\alpha\left(1+\frac{\omega_c}{8}\right). \end{aligned} \tag{5.30}$$

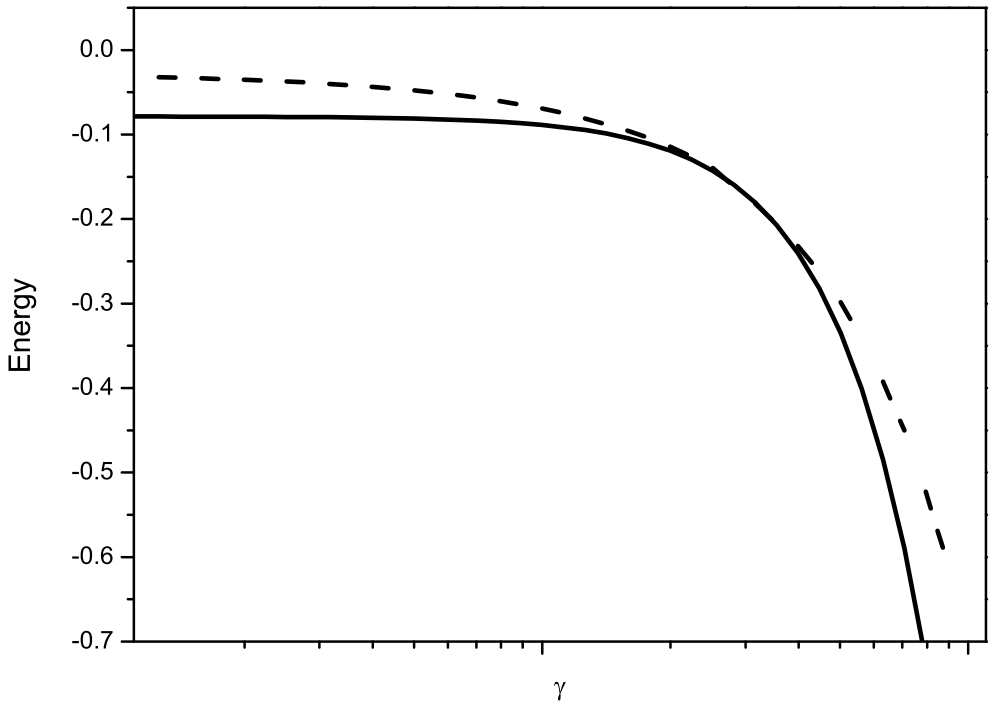

Figure 5.5: Comparison between the energy and the polaronic energy against γ by using Eq. (5.30). the solid line is the energy without polaron mass correction and the dashed line if for the energy with effective mass approximation.

Table 5.8: The change of the theoretical values of energy obtained by MacDonald and Ritchie [16] and our computed energy

ω_c	α=0.01	α=0.10	α=0.50	
0.01	(-2)-0.931212	(0)-0.139910.	(0)-0.606251	present
	(-1)-0.107276	(0)-0.152276	(0)-0.781380	mass app.
0.02	(-2)-0.556060	(0)-0.136149	(0)-0.602477	present
	(-2)0.574723	(0)-0.147472	(0)-0.777362	mass app.
0.05	(-2)0.943078	(0)-0.121222	(0)-0.588103	present
	(-2)0.919386	(0)-0.133061	(0)-0.765307	mass app.
0.10	(-1)0.344219	(-1)-0.964241	(0)-0.565912	present
	(-1)0.340957	(0)-0.1090431	(0)-0.745216	mass app.
0.20	(-1)0.843989	(-1)-0.470042	(0)-0.523509	present
	(-1)0.838999	(-1)-0.610066	(0)-0.705033	mass app.
0.50	(0)0.234273	(0)0.100620	(0)-0.399107	present
	(0)0.233310	(-1)0.831029	(0)-0.584486	mass app.
1.00	(0)0.483934	(0)0.345760	(0)-0.190920	present
	(0)0.482329	(0)0.3232851	(0)-0.383573	mass app.

Figure 5.5 displays the energy against γ for $\beta = 0.1, 0.2, 0.5$. We readily note that the present results are very close to those obtained from Eq. (5.15), and for even stronger fields the agreement is perfect.

For a further verification we refer to the paper by Larsen [20] where the problem of a polaron in a magnetic field is treated within the second-order perturbation approximation. He finds

$$E = \frac{\omega_c}{2} - \frac{1}{2}\pi\alpha \frac{\Gamma(\omega_c^{-1})}{\sqrt{\omega_c}\Gamma\left(\frac{1}{2} + \omega_c^{-1}\right)}. \tag{5.31}$$

In Table 5.9 we set $\alpha = 0.01$ and provide a comparison of the present energy values with those obtained from Eq. (5.31) for a series of magnetic field strength. A glance at the corresponding numerical values reveals that the agreement is almost perfect.

Table 5.9: Comparison between the energy with effective mass argument for α=0.01

ω_c	E_p	E
0.1	(-1)0.34422	(-1)0.340951
0.2	(-1)0.84399	(-1)0.83895
0.5	(0)0.23427	(0)0.23329
1	(0)0.48393	(0)0.48228
2	(0)0.98305	(0)0.48228
5	(1)0.24802	(1)0.24752
10	(1)0.49758	(1)0.49683
20	(1)0.99688	(1)0.99577
50	(2)0.24954	(2)0.24936

ii- $(\omega_c = 0)$ **case of zero magnetic field**

Ignoring phonon coupling, from Eq. (5.23) one readily notes that in the absence of a magnetic field ($\gamma = 0$), one obtains $E = -\beta^2$: the two dimensional Rydberg which is four times that for the bulk case.

With the inclusion of electron-phonon coupling one expects the binding to become stronger. Choosing $\alpha = 0.07$ and $\beta = 0.781$ for GaAs, for instance we obtain $E/\beta^2 \simeq -1.197$; the binding deepened by 20 per cent. The value obtained here is in very close agreement with that derived by Mason and Das Sarma [19] using the Feynmann path integral technique. In alternative interesting view to the problem in the small β^2 regime consist of approaching the problem using the effective mass argument based reasoning. In this regime one can visualize the electron as revolving about the donor center together with the concomitant lattice deformation. Thus replacing m^* by

$$m_p = \left(1 + \frac{\pi}{8}\alpha\right) m^*, \tag{5.32}$$

one has

$$R_{2D} = -\beta^2 \to -\beta^2 \left(1 + \frac{\pi}{8}\alpha\right), \tag{5.33}$$

and consequently

$$\begin{aligned} E &= E_p - R_{2D} \\ &\simeq -\beta^2 - \frac{\pi}{2}\alpha - \frac{\pi}{8}\alpha\beta^2 \end{aligned} \tag{5.34}$$

which is expected to have reasonable validity for small α and for small β^2 (i.e., $R_{2D} \ll \hbar\omega_0$). For completeness, in Figure 5.4 we compare our results with numeric values predicted by Eq. (5.31). We note a very close agreement between the two approaches in a limited domain in which β is not too large. The mismatch in the small β-limit is due to that a 1s-like wavefunction for the electronic charge density becomes rather inadequate to reflect a correct description of the case where a frail Coulombic structure is dominated by the polaronic aspect. (Clearly, in this extreme, a gaussian-based approach would have been more appropriate.)

At the other extreme of comparatively strong Coulomb potentials the deviation is essentially because the approximate effective mass formula Eq. (5.30) becomes no longer capable of yielding a satisfying description of the polaron state which undergoes a qualitative change from a nearly free to a relatively localized one.

5.3 Polaronic Donor in a Magnetic Field

In this section we study the problem in complete form where neither β nor ω_c is set equal to zero. We thus explore the polaron effect in the hydrogenic ground state together with the additional contribution coming from the magnetic field. Rather than displaying the energy we chose to study the phonon induced shift

$$\Delta E = |E - E(\alpha = 0)| \tag{5.35}$$

in the binding energy as a function of the parameters characterizing the problem.

With InSb selected as an example of compound semiconductor of general interest we display the polaron shift on the binding energy as a function of the magnetic field.

In our dimensionless units, a given value of γ corresponds to different magnetic field strengths depending on the material. For instance $\gamma = 1$ corresponds to 6kG for InSb. It should be noted that a magnetic field of intensity 60 kG can be regarded as strong for InSb.

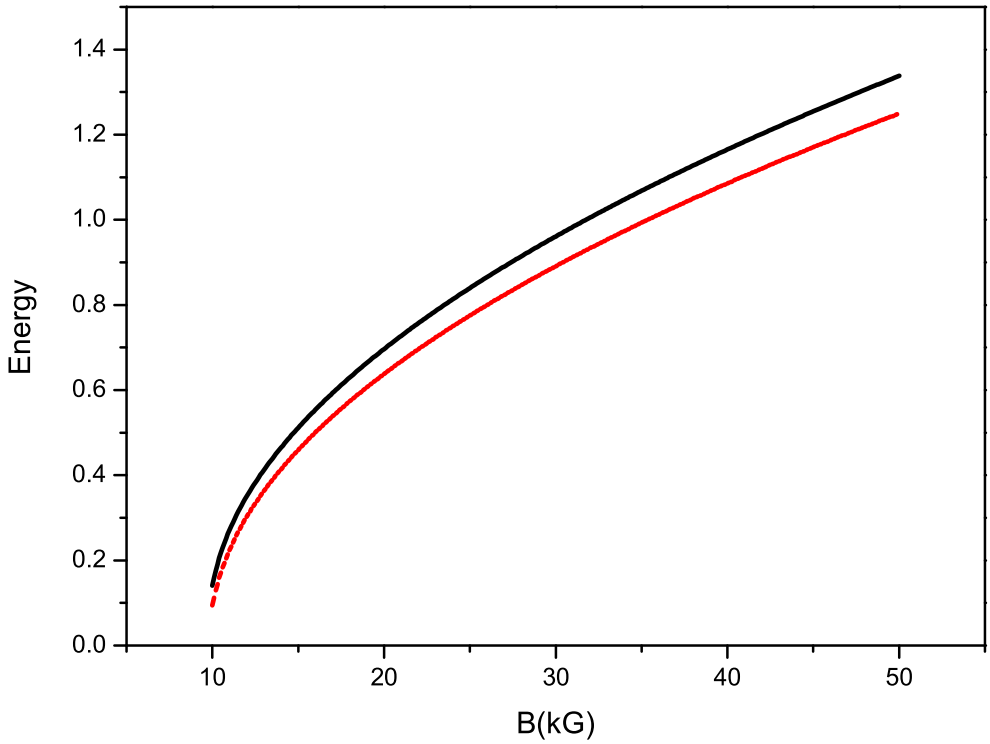

Figure 5.6: Energy versus B for α=0 and α=0.03 the theoretic value for InSb. The top line corresponds to α=0.03 where there is a polaronic contribution to the energy and the bottom line corresponds to α=0 case where there is no polaronic contribution.

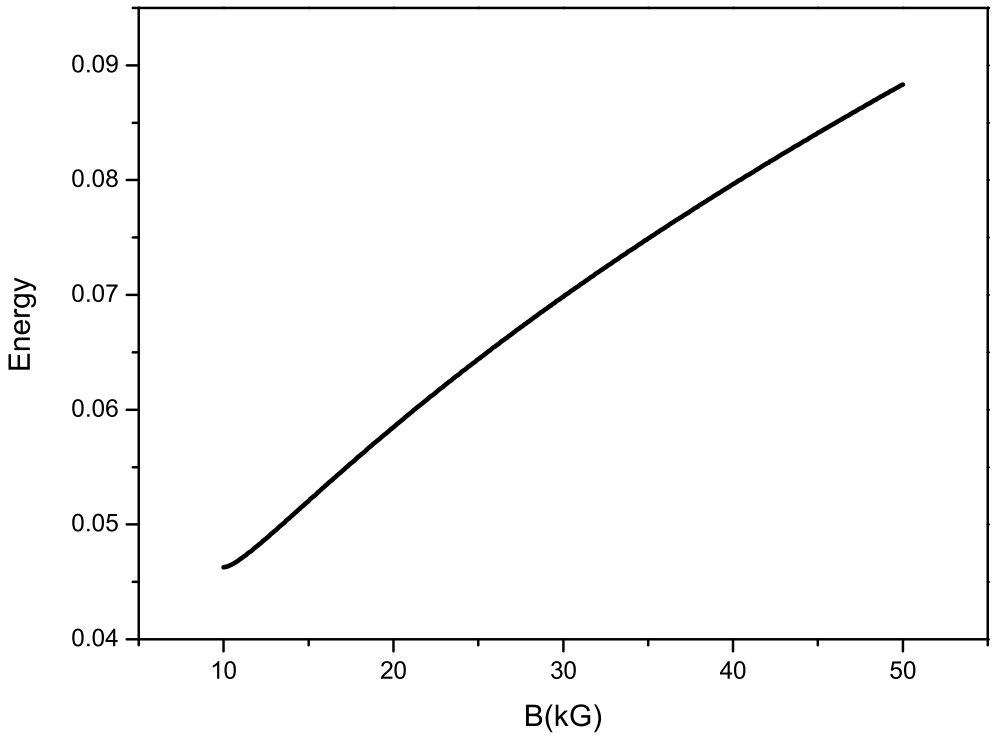

Figure 5.7: Energy versus B for the phonon-induced shift obtained by Eq. (5.35) for InSb.

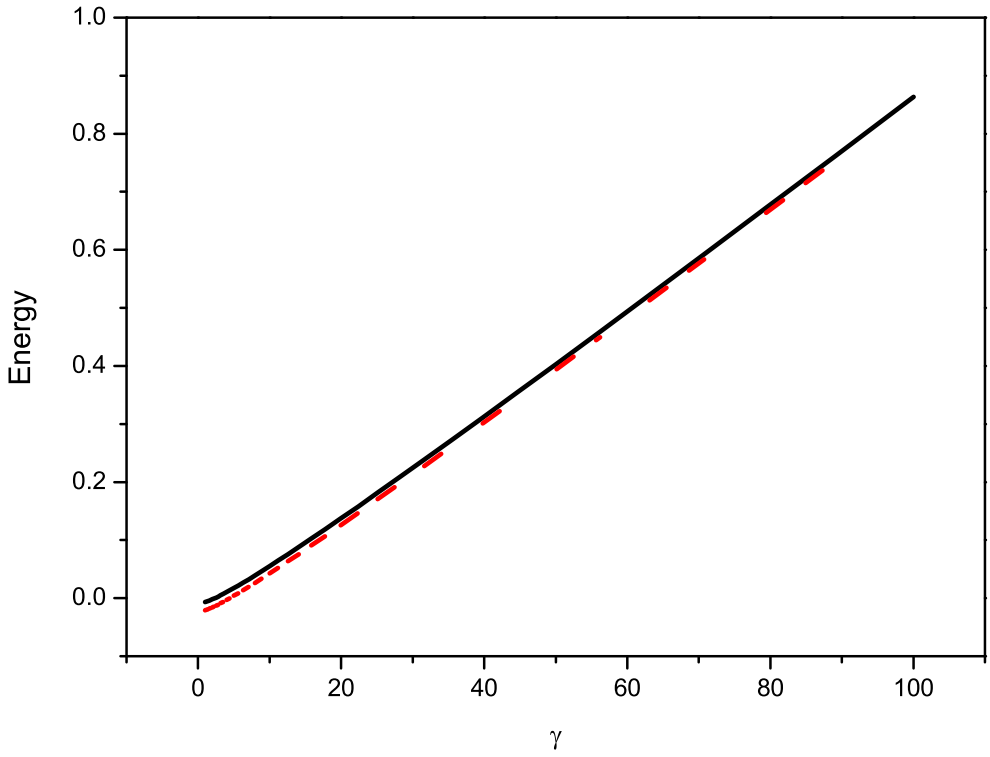

Figure 5.8: Energy versus γ for the interpolation between strong coupling and the extended theory. The solid line is for extended theory and the dashed line is for the strong coupling theory

In Figures 5.6 and 5.7, we plot the energy and phonon-induced shift in the binding energy as a function of the magnetic field intensity for InSb. In Figure 5.6 we plot energy as a function of B for α=0, and α=0.03. The top line corresponds to α=0.03 and the bottom line corresponds to α=0 case. From these lines one can see the difference of energy due to the electron-phonon coupling strength. The general trend is that ΔE displays a monotonically increasing profile as the magnetic field strength is made larger.

In Figure 5.8 one can compare the strong coupling theory and the extended theory result. The above line is for extended solution and the below one is for the strong coupling solution. And the contribution coming from the nonzero α has seen from this graph easily.

Chapter 6

Conclusion

In this thesis, we have presented two different approaches for calculating the two and three dimensional polaron ground state energy. We have shown the use of perturbation, strong coupling and variational perturbative theory and domain of validity of electron phonon coupling strength for these two theories. Moreover, we computed ground state energy of the hydrogenic impurity in both two- and three- dimensions. For the case of not sufficiently large electron-phonon coupling strength we have shown the weakness of the strong coupling theory. To eliminate this problem we combine strong coupling theory with variational perturbation theory. Furthermore, we apply the magnetic field to the medium and again calculate the ground state energy of the polaron. In this part, we see that for weak magnetic field the choice of wavefunction most suitable is hydrogenic, and for strong magnetic field this becomes gaussian wavefunction. We have compared our results with MacDonald and Ritchie's results [16], where they gave analytic calculation to the energies and we get strong agreement with their results. For the gaussian wavefunction under magnetic field it has been shown that when electron-phonon coupling strength is zero and the Coulombic interaction is zero, the ground state energy is $\omega_c/2$ which is Landau orbit energy.

In the general scope of this thesis work, we have presented an overview to the single polaron properties in two dimensions. Giving most emphasis to the formal structure of the problem, we have demonstrated the bulk phonon effects on the

free electron under magnetic field within the framework of variational calculation. In other words electron-phonon interaction and magnetic field effects on a two-dimensional electron bound to a Coulomb center is studied within the framework of a variational approximation consisting of an adiabatic polaronic wave function corrected by a first order perturbative extension by which it is possible to inter-relate the strong and weak coupling counterparts of the coupled electron-phonon system. Various aspects of the problem is considered depending on the Coulomb interaction, magnetic field, and electron-phonon coupling strength.

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