

GROUND STATE ENERGY OF THE FRÖHLICH POLARON AS A FUNCTION OF DIMENSIONALITY AND THE PHONON COUPLING STRENGTH

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Ground State Energy of the Fröhlich Polaron as a Function of Dimensionality and the Phonon Coupling Strength

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We certify that we have read this thesis and that in our opinion it is fully adequate, in scope and in quality, as a thesis for the degree of Master of Science.

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ABSTRACT

GROUND STATE ENERGY OF THE FRÖHLICH POLARON AS A FUNCTION OF DIMENSIONALITY AND THE PHONON COUPLING STRENGTH

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We use the trial polaron wave function introduced by Devreese et al. [1] to estimate the ground state energies of the Fröhlich polaron over a broad range of the phonon coupling strength by a variational approach. We calculate the binding energy of the polaron as a function of dimensionality interpolating between two and three dimensions. We compare these results with the outcomes obtained by the Strong and Weak Coupling Theories and conclude that in the strong coupling regime, the present work leads to a significantly improved upper bound for the ground state energy.

Keywords: Fröhlich, polaron, weak coupling, strong coupling .

ÖZET

BOYUTUN VE PHONON BAĞLANMA KUVVETİNİN FONKSİYONU OLARAK FRÖHLICH POLARONUN TEMEL DURUM ENERJİSİ

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Fröhlich polaronun temel durum enerjisini, Devresee ve diğerlerinin öne sürdüğü polaron deneme dalga fonksiyonunu kullanarak [1], phonon bağlanma kuvvetinin oldukça çeşitli değerleri için, varyasyonel bir yaklaşım ile tahmin ediyoruz. Boyutu iki ile üç arasında değişen bir polaronun bağlanma enerjisini hesaplıyoruz. Elde ettiğimiz sonuçları Kuvvetli ve Zayıf Bağlanma kuramları ile kıyaslıyoruz. Sonuç olarak, kuvvetli bağlanma rejiminde, mevcut çalışmanın temel durum enerjisinin üst sınırını dikkate değer bir biçimde geliştirdiğini gözlemliyoruz.

Anahtar sözcükler: Fröhlich, polaron, zayıf bağlanma, kuvvetli bağlanma .

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Chapter 1

Introduction

The first appearance of the polaron concept in the literature is often attributed to the paper proposed by Landau[2]. The basic rationale behind the polaron concept can be described as follows: When a charge carrier has a sufficiently slow motion in an ionic crystal, the equilibrium positions of the surrounding ions are shifted. This change in the positions of the ions creates a potential well for such carrier. If the energy required to remove the carrier from this well is greater than the phonons characteristic energy, the potential well can be considered almost static. Consequently, it is said that the carrier is self-trapped; that is, its existence induces a potential well so that it cannot escape beyond the well.

Such a structure described above (i.e. the carrier which is self-trapped and the surrounding ions) is called with a specific name: strong-coupling polaron. However, for every polaron formation, the self-trapping situation may not necessarily occur; that is, if the interaction between the charge carrier and the ions is weak, a potential well that traps the carrier is not established. Nevertheless, the carrier and the surrounding ions still have an appearance of a composite quasi-particle; and this structure is termed as a weak-coupling polaron.

Among these two types of polarons (i.e. strong and weak-coupling polarons), the strong-coupling polaron is considered under two titles: Large polaron and

small polaron. Large polaron wave functions and the corresponding lattice distortions exceed the characteristic inner-site separation of the lattice. Such polaron can be described as a free particle moving in an elastic continuum[3]. On the other hand, a small polaron is confined in a single structural unit. The carrier's motion in this polaron is generally described by the successive random phonon-assisted jumps between the adjacent sites[4].

Motivation behind working on the polaron problem can be summarized as follows: The interaction between electron and phonons leads to phase transformations such as superconductivity, and dominates the transport properties of many metals and semiconductors[3],[5],[6]. Second, despite of the simplicity of the formulation of the problem, the exact solution has not been formulated yet[7]; hence, such a problem becomes a reference problem to test the various methods of approximations[8].

To bring a solution to the polaron problem, there are many models that describe the interaction between the carrier and phonons. Among them, one of the most important models is the Fröhlich's interaction[9] (i.e. the interaction between the electron and the phonon reservoirs).

Based on the Fröhlich's polaron, it turns out that the strength of the interaction between the electron and the phonons determines the validity of the approximation methods. For example, for the weak coupling case, Fröhlich's himself employed the perturbation theory to estimate the ground state energy of the complex[9].

For the strong-coupling polaron, the perturbation theory is regarded not a reliable method to calculate the energy values of the polaron[10],[11]. In such a strong interaction situation, the adiabatic approximation is generally used; that is, it is assumed that there is no correlation between the instantaneous position of the electron and the induced polarization field[5]. With this approach, the energy of the polaron is calculated by the variational principle[2],[12],[10]. Without using the adiabatic approach, based on the variational principle, it is possible to find some other methods in the literature which is applied to the strong-coupling

regime[11].

In this thesis, we calculate the ground state energies of the Fröhlich polaron for all coupling regimes(i.e. weak, intermediate and strong couplings) for three cases: two and three dimensional polarons(2D and 3D polarons) and a polaron with one dimensional confinement (2-3 D polaron). Throughout our work, we use the variational principle to estimate the (ground state) energy values of the polarons and we employ the polaron trial wave function $|\psi\rangle$ introduced by Devreese et al. [1] having the form:

$$|\psi\rangle = c |0\rangle |\phi_n\rangle + \sum_{\mathbf{k}} g_{\mathbf{k}}^* V_{\mathbf{k}}^* (e^{-i\mathbf{k}\cdot\mathbf{r}} - \rho_{\mathbf{k}}^*) a_{\mathbf{k}}^+ |0\rangle |\phi_n\rangle .$$

To calculate the energy values of the nD polaron ($n = 2, 3$) and 2-3 D polaron, we adapt the generalized polaron Hamiltonian which was introduced by Peeters and Smondyrev [13] to our problem.

For this purpose, the rest of the thesis is organized as the following: In the next section, we derive the Fröhlich Hamiltonian and generalize this Hamiltonian according to the reference [13]. In the second chapter, we introduce two approximation methods, namely, the perturbation theory and the variational approximation. Using these techniques, we verify the validity of such a generalization. In Chapter three, based on the wave function given above, we present our analytical calculations and give the numerical results. Moreover, we compare these results with the outcomes obtained from the strong and weak coupling theories. In the last chapter, we give a brief summary and conclusions of our work.

1.1 The Fröhlich Polaron Hamiltonian

In this section, we derive an expression for the Hamiltonian of a Fröhlich polaron in which a single electron exists; it interacts with (longitudinal) optical bulk phonon modes and is confined by an external potential. In other words, we introduce three different Hamiltonians, namely Hamiltonians of the electron, the phonons and the interaction between the electron and the phonon modes where the last one is the so-called Fröhlich Hamiltonian, and their sum is equivalent to the polaron's Hamiltonian. Even though there are three major Hamiltonians, our main focus will be on the interaction Hamiltonian. For a more detailed derivation of Fröhlich Hamiltonian one can see the article [9] and the book [14].

1.1.1 Preliminaries

When a linear atomic chain consisting of N point particles with mass M is treated quantum mechanically, the Hamiltonian resulting from the vibrations of the atoms is expressed as:

$$H = \sum_k \hbar \omega_k a_k^\dagger a_k + \frac{1}{2} \sum_k \hbar \omega_k, \quad (1.1)$$

where $a_k^\dagger$ and a_k and ω_k are the creation and annihilation operators and the oscillation frequency of the particle with the wave number k , respectively. Note that the second term in the equation above stands for the energy of the zero point vibrations and with the appropriate choice of the zero energy, this term might be omitted. Thus, the Schrödinger equation for such a system becomes:

$$\left(\sum_k \hbar \omega_k a_k^\dagger a_k \right) \Phi = E \Phi \quad (1.2)$$

where Φ is the phonon wave function and E is the corresponding eigenvalue. Furthermore, these operators satisfy the following commutation relations:

$$[a_k, a_{k'}^\dagger] = \delta_{k,k'}, \quad (1.3)$$

$$[a_k, a_{k'}] = 0, \quad (1.4)$$

and

$$[a_k^+, a_{k'}^+] = 0. \quad (1.5)$$

Moreover, the displacement operator q_l for the l th atom is given in terms of the raising and lowering operators as:

$$q_l = \sum_k \sqrt{\frac{\hbar}{2MN\omega_k}} (a_{-k}^+ + a_k) e^{ikla}, \quad (1.6)$$

where a is the distance between two successive atoms.

Note that taking into consideration (1.2) and (1.6), it may be interpreted that in the stationary state the lattice waves with the wave number k are occupied by n_k quasi-particles, which are termed as phonons.

1.1.2 The Hamiltonian of the Polaron

In this subsection, we shall give an expression for the Hamiltonian of the specific case of the Fröhlich polaron, where a single electron is in a polar crystal and it interacts with vibrating dipoles. Before starting our derivation, we make some assumptions which simplify our system: The electron's Bloch function has a small k -vector; thus its wavelength is large compared with the lattice constant. Furthermore, the lattice vibrations are important only for the interaction with the electron. Then, with these assumptions, we can ignore the detailed lattice structure and consider our the lattice as a dielectric continuum. Besides, we take into consideration the effective mass approximation. Moreover, the frequency $\omega_{\mathbf{k}}$ of the phonon modes is independent of $\mathbf{k}$, i.e. $\omega_{\mathbf{k}} = \omega$, which is approximately the case for optical lattice vibrations.

Then the total Hamiltonian of the polaron is

$$H = H_e + H_p + H_{e-p}, \quad (1.7)$$

where H_e , H_p represent the Hamiltonians of the electron and phonons, respectively; and H_{e-p} stands for the *electron – phonon* interaction Hamiltonian that is called Fröhlich Hamiltonian.

The Hamiltonian of the electron is written as

$$H_e = \frac{p^2}{2m^*} + V_{conf}(\mathbf{r}), \quad (1.8)$$

where $\mathbf{p}$ and $\mathbf{r}$ are the momentum and position operators of the electron, m^* is the effective mass of the electron and V_{conf} represents the external potential within which electron is confined. Later, we will see that this term will be used in our work as either zero or an infinite potential barrier.

Next, we handle the Hamiltonian of the phonons. At this point, we introduce the Hamiltonian of phonons in continuum by the analogy with equation (1.1) as [14]:

$$H_p = \sum_{\mathbf{k}} \hbar \omega_{\mathbf{k}} a_{\mathbf{k}}^{\dagger} a_{\mathbf{k}} \quad (1.9)$$

The creation and annihilation operators in (1.9) satisfy the following commutation relations:

$$[a_{\mathbf{k}}, a_{\mathbf{k}'}^{\dagger}] = \delta_{\mathbf{k}, \mathbf{k}'}, \quad (1.10)$$

$$[a_{\mathbf{k}}, a_{\mathbf{k}'}] = [a_{\mathbf{k}}^{\dagger}, a_{\mathbf{k}'}^{\dagger}] = 0. \quad (1.11)$$

Furthermore, the number operator is given as:

$$n_{\mathbf{k}} = a_{\mathbf{k}}^{\dagger} a_{\mathbf{k}}. \quad (1.12)$$

Note that when the number operator in (1.12) is applied the phonon wave function Φ , the resulting eigenvalue is the number of phonons with the wave vector $\mathbf{k}$.

Moreover, the position operator $q(\mathbf{r})$ is expressed by the analogy with (1.6) in terms of the raising and lowering operators in the following form:

$$q(\mathbf{r}) = \sum_{\mathbf{k}} \frac{1}{\sqrt{V}} \sqrt{\frac{\hbar}{2\rho\omega}} (e^{i\mathbf{k}\cdot\mathbf{r}} a_{\mathbf{k}} + e^{-i\mathbf{k}\cdot\mathbf{r}} a_{\mathbf{k}}^{\dagger}) \quad (1.13)$$

where V is the volume of the lattice and ρ is the mass density.

Finally, we focus on the interaction Hamiltonian H_{e-p} . The total energy of an individual dipole resulting from the existence of the electron is given as:

$$\frac{m_l}{2} (\dot{\mathbf{q}}_l^2 + \omega^2 \mathbf{q}_l^2), \quad (1.14)$$

where m is the vibrating mass of the dipole ω is the characteristic frequency and $\mathbf{q}_l$ is the displacement vector. Here, we consider that the dipoles are located at the sites of the crystal and the dipoles are not coupled. To move on from this discrete case to the continuum, we replace dipole moments by dipole densities as:

$$e^* \mathbf{q}_l \longrightarrow \mathbf{P}(\mathbf{r}) \quad (1.15)$$

where e^* is the effective charge of the dipole moment and $\mathbf{P}(\mathbf{r})$ is the polarization of the medium. Moreover, one can express the mass m_l in terms of the mass density ρ :

$$m_l = \rho(\mathbf{r}) d^3 r \quad (1.16)$$

If we introduce the equation

$$\frac{m_l}{e^{*2}} = \gamma d^3 r \quad (1.17)$$

then we can express the kinetic energy K and potential energy U of a vibrating lattice as:

$$K = \int \frac{\gamma}{2} \dot{\mathbf{P}}^2(\mathbf{r}) d^3 r \quad (1.18)$$

and

$$U = \int \frac{\gamma \omega^2}{2} \mathbf{P}^2(\mathbf{r}) d^3 r, \quad (1.19)$$

where γ is a constant and ω is the frequency of the optical lattice vibrations as it is mentioned in the assumptions. Note that so far we have not described the vibration of the dipole densities as longitudinal. However, it will shortly turn out that the vibration is necessarily longitudinal.

It is a known fact, in classical electrodynamics, that the interaction energy between an electric charge e located at $\mathbf{r}$ and dipole density $\mathbf{P}(\mathbf{r}')$ at $\mathbf{r}'$ is:

$$\varepsilon_{int} = e \frac{\mathbf{r} - \mathbf{r}'}{|\mathbf{r} - \mathbf{r}'|^3} \mathbf{P}(\mathbf{r}') d^3 r'. \quad (1.20)$$

Therefore, total interaction energy E_{int} of the polarization field $\mathbf{P}$ and the charge e is obtained by integrating (1.20) over all volume as:

$$E_{int} = \int e \frac{\mathbf{r} - \mathbf{r}'}{|\mathbf{r} - \mathbf{r}'|^3} \mathbf{P}(\mathbf{r}') d^3 r'. \quad (1.21)$$

The Lagrangian for such a system is given as

$$L = K - U - E_{int} \quad (1.22)$$

and Lagrangian equations are:

$$\frac{d}{dt} \frac{\delta L}{\delta \dot{P}_i} - \frac{\delta L}{\delta P_i} = 0 \quad (1.23)$$

where $i = x, y, z$.

Using the relations $\frac{\delta q(x)}{\delta q(x')} = \delta(x - x')$ and $\frac{\delta \dot{q}(x)}{\delta \dot{q}(x')} = \delta(x - x')$, one can solve (1.23) and obtain the equation of motion as:

$$\gamma(\ddot{\mathbf{P}}(\mathbf{r}') + \omega^2 \mathbf{P}(\mathbf{r}')) = -e \frac{\mathbf{r} - \mathbf{r}'}{|\mathbf{r} - \mathbf{r}'|^3}. \quad (1.24)$$

Notice that the right-hand side in (1.24) is nothing but the dielectric displacement $\mathbf{D}(\mathbf{r}')$ that results from the electric charge e . When we consider the static case, equation (1.24) becomes

$$\gamma \omega^2 \mathbf{P}(\mathbf{r}') = \mathbf{D}(\mathbf{r}'). \quad (1.25)$$

Here, we employ the connection between the field strength and the electric displacement:

$$\mathbf{D} = \mathbf{E} + 4\pi \mathbf{P}_{tot} = \varepsilon_0 \mathbf{E}, \quad (1.26)$$

where ε_0 is the static dielectric constant.

Thus,

$$4\pi \mathbf{P}_{tot} = \left(1 - \frac{1}{\varepsilon_0}\right) \mathbf{D}. \quad (1.27)$$

Note that $\mathbf{P}_{tot}$ is expressed as $\mathbf{P}_{tot} = \mathbf{P}_e + \mathbf{P}$ where $\mathbf{P}_e$ is the polarization of the electrons in the ionic shells and $\mathbf{P}$ is the polarization of the ionic displacement. However, our main interest is on the polarization coming from the ionic displacement; so we need to express P_e in terms of the known variables. To do this, we expose the system to a quick appearance of an external field. Since only the electrons (not ions) can respond to such a sudden switch-on of the field, we have the relation:

$$4\pi \mathbf{P}_e = \left(1 - \frac{1}{\varepsilon_\infty}\right) \mathbf{D} \quad (1.28)$$

where ε_∞ is the high frequency dielectric constant. Therefore, by using (1.27) and (1.28), we obtain the polarization due to the ionic displacement

$$4\pi \mathbf{P} = \left(\frac{1}{\varepsilon_\infty} - \frac{1}{\varepsilon_0}\right) \mathbf{D}. \quad (1.29)$$

Hence, to find the value of the constant γ , it is sufficient to solve equations (1.25) and (1.29) together:

$$\gamma = \frac{4\pi}{\omega^2} \left(\frac{1}{\varepsilon_\infty} - \frac{1}{\varepsilon_0} \right)^{-1}. \quad (1.30)$$

Now, we are tempted E_{int} in the operator format to lead to H_{e-p} . Before this, we may express E_{int} in more convenient form if we make the following observation:

$$\begin{aligned} \frac{\mathbf{r}-\mathbf{r}'}{|\mathbf{r}-\mathbf{r}'|^3} \mathbf{P}(\mathbf{r}') &= -\nabla_r \left(\frac{1}{|\mathbf{r}-\mathbf{r}'|} \right) \cdot \mathbf{P}(\mathbf{r}') \\ &= \nabla_{r'} \cdot \left(\frac{\mathbf{P}(\mathbf{r}')}{|\mathbf{r}-\mathbf{r}'|} \right) - \left(\frac{1}{|\mathbf{r}-\mathbf{r}'|} \right) \nabla_{r'} \cdot \mathbf{P}(\mathbf{r}'). \end{aligned} \quad (1.31)$$

Therefore, equation (1.21) becomes:

$$E_{int} = - \int d^3r' \frac{e}{|\mathbf{r}-\mathbf{r}'|} \nabla_{r'} \cdot \mathbf{P}(\mathbf{r}') \quad (1.32)$$

Note that when the plane wave expansion of $\mathbf{P}$ is performed equation (1.32) allows only the longitudinal vibrations to contribute to the interaction energy. So, it can be assumed at the very beginning that the lattice vibrations are longitudinal. Using equations (1.13), (1.16) and (1.17), we can express the polarization $\mathbf{P}$ in terms of the creation and annihilation operators as:

$$\mathbf{P}(\mathbf{r}') = \frac{1}{\sqrt{V}} \sum_{\mathbf{k}} \sqrt{\frac{\hbar}{2\gamma\omega}} \frac{\mathbf{k}}{k} e^{i\mathbf{k}\cdot\mathbf{r}'} (a_{\mathbf{k}} - a_{-\mathbf{k}}^+). \quad (1.33)$$

If we substitute (1.33) into (1.32), we have the electron-phonon interaction Hamiltonian H_{e-p} :

$$H_{e-ph} = \sum_{\mathbf{k}} (V_{\mathbf{k}} a_{\mathbf{k}} e^{i\mathbf{k}\cdot\mathbf{r}} + V_{\mathbf{k}}^* a_{\mathbf{k}}^+ e^{-i\mathbf{k}\cdot\mathbf{r}}) \quad (1.34)$$

where the factor $V_{\mathbf{k}}$ is given as

$$V_{\mathbf{k}} = -4\pi i \left(\frac{e^2 \hbar}{2\gamma\omega V} \right)^{(1/2)} \frac{1}{k}, \quad (1.35)$$

and the magnitude of $V_{\mathbf{k}}$ with the explicit expression of γ is

$$|V_{\mathbf{k}}| = \frac{1}{\sqrt{V}} \frac{e}{k} \sqrt{2\pi\hbar\omega \left(\frac{1}{\varepsilon_\infty} - \frac{1}{\varepsilon_0} \right)}. \quad (1.36)$$

At this point, we introduce the unit of length as $u = \sqrt{\frac{\hbar}{2m^*\omega}}$ and making those scaling transformations:

$\mathbf{r} \longrightarrow \mathbf{r}u$, $V \longrightarrow Vu^3$ and $\mathbf{k} \longrightarrow \mathbf{k}/u$. Keeping these transformations in mind, we introduce a constant α , namely, dimensionless electron-phonon coupling constant as:

$$\alpha = \frac{1}{2} \left(\frac{1}{\varepsilon_\infty} - \frac{1}{\varepsilon_0} \right) \frac{e^2}{\hbar\omega u}. \quad (1.37)$$

Thus, equation (1.36) has the form:

$$|V_k| = \hbar\omega \sqrt{\frac{4\pi\alpha}{V}} \frac{1}{k}. \quad (1.38)$$

One remark is that some authors prefer to use $u' = \sqrt{\frac{\hbar}{m^*\omega}}$ for the unit of length. So if this unit is used and α is expressed as in equation (1.37), there occurs a relation between $V_{k,u}$ and $V_{k,u'}$ (i.e. the term $V_{k,u}$ represents the expression of V_k where the unit of length is chosen as u ; similarly, $V_{k,u'}$ stands for the expression of V_k where the unit of length is chosen as u') as

$$|V_{k,u}| = 2^{1/4} |V_{k,u'}|. \quad (1.39)$$

Note that, in this paper, we always use u for the unit of length.

So, the Hamiltonian of the polaron is given as:

$$H = \frac{p^2}{2m^*} + V_{conf}(\mathbf{r}) + \sum_{\mathbf{k}} \hbar\omega a_{\mathbf{k}}^+ a_{\mathbf{k}} + \sum_{\mathbf{k}} (V_k a_{\mathbf{k}} e^{i\mathbf{k}\cdot\mathbf{r}} + V_k^* a_{\mathbf{k}}^+ e^{-i\mathbf{k}\cdot\mathbf{r}}). \quad (1.40)$$

So far, we considered the three dimensional(3D) polaron and equation (1.40) represents the Hamiltonian for the 3D polaron. However, Peeters and Smondyrev [13] propose a general Hamiltonian for the n D polaron (i.e. by the n D polaron we mean electron is allowed to move in n dimensions where $n=1,2,3$ and interacts with n dimensional lattice). They do such a generalization by generalizing the interaction amplitude V_k and the dimensionless electron-phonon coupling constant α as the following:

$$|V_k|^2 = (\hbar\omega)^2 \Gamma\left[\frac{n}{2}\right] 2^n \pi^{\frac{n}{2}-1} \frac{\alpha'}{V_k^{n-1}} \quad (1.41)$$

where the generalized coupling constant α' is

$$\alpha' = \alpha \sqrt{\pi} \frac{\Gamma[\frac{n-1}{2}]}{2\Gamma[\frac{n}{2}]}. \quad (1.42)$$

So, for example, if one wishes to study the polaron in two dimensions, one has to insert $n=2$ into equation (1.41); and the result turns out in terms of the

generalized coupling constant α' . Furthermore, to express the outcome in terms of standard coupling constant α , one has to use the transformation given in (1.42) by choosing $n=2$.

The explicit expression for $|V_k|^2$ is:

$$|V_k|^2 = \begin{cases} \frac{4\pi\alpha'}{V} \frac{1}{k^2} & \text{if } n = 3. \\ \frac{4\alpha'}{A} \frac{1}{k} & \text{if } n = 2. \\ \frac{2\alpha'}{L} & \text{if } n = 1. \end{cases} \quad (1.43)$$

One important property of equation (1.43) is that for an arbitrary function f , the sum $\sum_{\mathbf{k}} |V_k|^2 f$ transforms to the same integral for all n ; that is:

$$\sum_{\mathbf{k}} |V_k|^2 f = \frac{2\alpha'}{\pi} \int_0^\infty f dk, \quad n=1,2,3. \quad (1.44)$$

Furthermore, we need to underline the fact that equation (1.42) is divergent at $n=1$. The reason for such a divergence is the Coulomb nature of the problem[13]. Accordingly, with this formalism of the Hamiltonian, we may calculate the polaron's energy in 1D in terms of the generalized coupling-constant α' ; however, we are not allowed to express the result in terms of the standard electron-phonon coupling constant α .

According to equation (1.42), the explicit form of the relation between α' and α is:

$$\alpha' = \begin{cases} \alpha & \text{if } n = 3, \\ \frac{\pi}{2}\alpha & \text{if } n = 2, \\ \text{not applicable} & \text{if } n = 1. \end{cases} \quad (1.45)$$

One remark about equation (1.41) is that the authors in their paper use u' for the unit of length[15]. So, we transformed their expression by using equation (1.39).

In the next chapter, we will consider the approximation methods for the polaron problem. Specifically, our focus will be on the perturbation theory and the variational principle. Note that in all calculations we shall use the generalized form of the Hamiltonian of the polaron.



Chapter 2

Approximation Methods

In this chapter, we shall take into consideration mainly two approximation methods: (1) Perturbation theory and (2) Variational approach. The first one among these methods is appropriate for the weak-coupling regimes (i.e. $\alpha \ll 1$) and in this method, the electron-phonon interaction is considered as the perturbed Hamiltonian.

The second method is, on the contrary, available to use in strong-coupling limit (i.e. $\alpha \gg 1$) and this method basically contains three steps: first finding a trial wave function with one (or more) variational parameters, second calculating the expectation value of the intended observable with respect to this wave function, third calculating the minimum value of this expectation value which is a function of the variational parameter(s). Therefore, this minimum value gives an upper bound for the observable.

The main purpose in this chapter is to verify that the generalized Fröhlich Hamiltonian introduced in the previous chapter is valid. To do this we shall calculate the ground state energy values of the polaron in asymptotic limits and show that these results are compatible with the values given in the literature.

In the rest of this chapter our strategy is to focus on the weak-coupling case by the perturbation theory; next we will handle the strong-coupling polaron with the

Material	α
KCl	5.6
NaCl	5.5
AgBr	1.56
CdTe	0.40
InP	0.11
GaAs	0.07
InAs	0.05

Table 2.1: Coupling constants of some (bulk) materials

variational principle. To simplify the expressions, we shall consider the polaron dimensionless by letting $2m^* = \hbar = \omega = 1$.

2.1 Perturbation Theory

The polaron's Hamiltonian can be expressed as (see equation (1.7))

$$H = H^0 + H^1, \quad (2.1)$$

where $H^0 = H_e + H_p$ and $H^1 = H_{e-p}$.

Then the time independent Schrödinger equation for the polaron is expressed as:

$$H |\psi_n\rangle = E_n |\psi_n\rangle, \quad (2.2)$$

where ψ_n is the wave function of the polaron in nth state and E_n is the corresponding energy value of the polaron.

If the coupling constant α is sufficiently small, one can consider the term H^0 as the unperturbed Hamiltonian and H^1 as the perturbed Hamiltonian. Then the unperturbed Hamiltonian H^0 satisfies the following relation:

$$H^0 |\psi_n^{(0)}\rangle = E_n^{(0)} |\psi_n^{(0)}\rangle. \quad (2.3)$$

If we expand the variables $|\psi_n\rangle$ and E_n as a perturbation series, we have

$$|\psi_n\rangle = |\psi_n^{(0)}\rangle + |\psi_n^{(1)}\rangle + |\psi_n^{(2)}\rangle + \dots \quad (2.4)$$

and

$$E_n = E_n^{(0)} + E_n^{(1)} + E_n^{(2)} + \dots \quad (2.5)$$

where $|\psi_n^{(1)}\rangle, E_n^{(1)}$ are first-order corrections to the nth eigenfunction and eigenvalue, $|\psi_n^{(2)}\rangle, E_n^{(2)}$ are second-order corrections to the nth eigenfunction and eigenvalue, respectively, and so on.

Now, we can start to calculate the corrections (up to 2nd order) to ground state energy eigenvalue for the nD polaron where n=1,2,3.

2.1.1 3D Polaron

For 3D polaron, the unperturbed Hamiltonian H^0 is given as

$$H^0 = \frac{p^2}{2m^*} + H_p. \quad (2.6)$$

Note that by definition of 3D polaron (actually nD polaron) $V_{conf} = 0$. However, we can use the following trick:

$$H^0 = \frac{p^2}{2m^*} + \frac{1}{2}m^*\Omega^2 r^2 + H_p \quad (2.7)$$

where $r^2 = (x^2 + y^2 + z^2)$ and $\Omega \rightarrow 0$. Notice that we have just added an harmonic oscillatory potential to equation (2.6) as a confining for the electron. The underlying reason to use a harmonic potential is to be able to apply the well-known operator formalism (for the electron) to our problem. Then, for such a Hamiltonian given in (2.7), the wave function $|\psi_n^0\rangle$ in the nth state is given as:

$$|\psi_n^0\rangle = |n_x, n_y, n_z\rangle |\vec{\ell}\rangle \quad (2.8)$$

where $|n_x, n_y, n_z\rangle$ is the wave function of the electron and $|\vec{\ell}\rangle$ is the phonon wave function. Accordingly, the ground state wave function $|\psi_0^0\rangle$ of the polaron is:

$$|\psi_0^0\rangle = |0, 0, 0\rangle |\vec{0}\rangle. \quad (2.9)$$

Therefore, clearly, first-order correction to the ground state eigenvalue $E_0^{(1)}$ is:

$$E_0^{(1)} = \langle \psi_0^0 | H^{(1)} | \psi_0^0 \rangle = 0. \quad (2.10)$$

So, the contribution coming from the first order correction for the ground state energy is zero. However, we shall see that this situation is not valid for the second order correction $E_0^{(2)}$ which is given as:

$$E_0^{(2)} = \sum_m \frac{|\langle \psi_0^0 | H^{(1)} | \psi_m^0 \rangle|^2}{E_0^{(0)} - E_m^{(0)}}. \quad (2.11)$$

In more explicit form:

$$E_0^{(2)} = \sum_{n_x, n_y, n_z, \vec{\ell}} \frac{|\langle \vec{\ell} | \langle n_x, n_y, n_z | H^{(1)} | 0, 0, 0 \rangle |\vec{0}\rangle|^2}{E_{0,0,0,\vec{0}}^{(0)} - E_{n_x, n_y, n_z, \vec{\ell}}^{(0)}}. \quad (2.12)$$

Note that

$$H^{(1)} |0, 0, 0\rangle |\vec{0}\rangle = H_{e-p} |0, 0, 0\rangle |\vec{0}\rangle = \sum_{\mathbf{k}} (V_k^* a_{\mathbf{k}}^\dagger e^{-i\mathbf{k}\cdot\mathbf{r}}) |0, 0, 0\rangle |\vec{0}\rangle. \quad (2.13)$$

At that point we choose the vector $\mathbf{k}$ in the $\hat{x}$ direction, i.e. $\mathbf{k} = k\hat{x}$. Therefore, the product $\mathbf{k} \cdot \mathbf{r}$ becomes $\mathbf{k} \cdot \mathbf{r} = kx$. Thus, (2.12) becomes

$$E_0^{(2)} = \sum_{n_x, \vec{\ell}} \frac{\left| \langle \vec{\ell} | \langle n_x | \sum_{\mathbf{k}} (V_k^* a_{\mathbf{k}}^+ e^{-ikx}) | 0 \rangle | \vec{0} \rangle \right|^2}{E_{0,0,0,\vec{0}}^{(0)} - E_{n_x,0,0,\vec{\ell}}^{(0)}}. \quad (2.14)$$

We may reexpress $|\vec{\ell}\rangle$ as $|\vec{\ell}\rangle = |\mathbf{v}\rangle |m_{\mathbf{k}}\rangle$. Then, $|\vec{0}\rangle = |\mathbf{0}\rangle |0_{\mathbf{k}}\rangle$. Accordingly,

$$\sum_{\mathbf{k}} (V_k^* a_{\mathbf{k}}^+ e^{-ikx}) |0\rangle |\vec{0}\rangle = \sum_{\mathbf{k}} (V_k^* e^{-ikx}) |0\rangle |1_{\mathbf{k}}\rangle |\mathbf{0}\rangle. \quad (2.15)$$

Hence, equation (2.14) has the following form:

$$E_0^{(2)} = \sum_{n_x, \mathbf{k}} |V_k|^2 \frac{\left| \langle n_x | e^{-ikx} | 0 \rangle \right|^2}{E_{0,0,0,\vec{0}}^{(0)} - E_{n_x,0,0,\mathbf{0},1_{\mathbf{k}}}^{(0)}}. \quad (2.16)$$

Note that $E_{n,0,0,\mathbf{0},1_{\mathbf{k}}}^{(0)}$ (i.e. we have just changed the notation as $n_x \rightarrow n$) satisfies the following relation:

$$H^{(0)} |n, 0, 0\rangle |\mathbf{0}\rangle |1_{\mathbf{k}}\rangle = E_{n,0,0,\mathbf{0},1_{\mathbf{k}}}^{(0)} |n, 0, 0\rangle |\mathbf{0}\rangle |1_{\mathbf{k}}\rangle. \quad (2.17)$$

Since

$$H^{(0)} |n, 0, 0\rangle |\mathbf{0}\rangle |1_{\mathbf{k}}\rangle = [(n + 3/2)\hbar\Omega + \hbar\omega] |n, 0, 0\rangle |\mathbf{0}\rangle |1_{\mathbf{k}}\rangle,$$

it follows that

$$E_{n,0,0,\mathbf{0},1_{\mathbf{k}}}^{(0)} = (n + 3/2)\hbar\Omega + \hbar\omega. \quad (2.18)$$

Similarly,

$$E_{n,0,0,\vec{0}}^{(0)} = \frac{3}{2}\hbar\Omega. \quad (2.19)$$

Now, we shall handle the numerator in (2.16). To do this, we use the formalism for the harmonic oscillatory potential. Then we can express x in terms of the creation and annihilation operators b and b_+ as:

$$x = \sqrt{\frac{\hbar}{2m^*\Omega}} (b^+ + b) \quad (2.20)$$

If we let $\hbar = 2m^* = 1$ the expression e^{-ikx} becomes

$$e^{-ikx} = e^{\beta(b^+ + b)} = e^{\beta^2/2} e^{\beta b^+} e^{\beta b} \quad (2.21)$$

where $\beta = -ik \frac{1}{\sqrt{\Omega}}$ and we use the identity

$$e^{A+B} = e^A e^B e^{\frac{1}{2}[B,A]}. \quad (2.22)$$

Notice that

$$\begin{aligned} e^{-ikx}|0\rangle &= e^{\beta^2/2} e^{\beta b^+}|0\rangle \\ &= e^{\beta^2/2} \left(1 + \beta b^+ + \frac{(\beta b^+)^2}{2!} + \dots\right)|0\rangle \\ &= e^{\beta^2/2} \left(1 + \beta|1\rangle + \frac{\beta^2\sqrt{2}}{2}|2\rangle + \dots + \frac{\beta^n\sqrt{n}}{n!}|n\rangle + \dots\right). \end{aligned} \quad (2.23)$$

Therefore,

$$|\langle n|e^{-ikx}|0\rangle|^2 = \frac{e^{\beta^2}}{n!} |\beta^n|^2 = \frac{e^{-k^2/\Omega}}{n!} \left(\frac{k^2}{\Omega}\right)^n. \quad (2.24)$$

Hence, equation (2.16) (with the dimensionless units i.e. $\hbar = 2m^* = \omega = 1$) becomes

$$E_0^{(2)} = - \sum_{\mathbf{k}} |V_{\mathbf{k}}|^2 e^{-k^2/\Omega} \sum_n \frac{1}{n!} \frac{(k^2/\Omega)^n}{1 + \Omega n}. \quad (2.25)$$

If we employ the following identity

$$\sum_n \frac{1}{n!} \frac{\beta^n}{(a + bn)^{m+1}} = \frac{1}{m!} \int_0^\infty x^m e^{-ax + \beta e^{-bx}} dx, \quad (2.26)$$

we have

$$E_0^{(2)} = - \sum_{\mathbf{k}} |V_{\mathbf{k}}|^2 \int_0^\infty e^{-x} e^{-k^2 \left(\frac{1 - \exp(-\Omega x)}{\Omega}\right)} dx. \quad (2.27)$$

Considering free electron case i.e. $V_{conf} = 0$ or $\Omega \rightarrow 0$, we have:

$$- \sum_{\mathbf{k}} |V_{\mathbf{k}}|^2 \int_0^\infty e^{-x(1+k^2)} dx = - \sum_{\mathbf{k}} |V_{\mathbf{k}}|^2 \frac{1}{1 + k^2}. \quad (2.28)$$

Finally, we apply the result we have observed in equation (1.44) to get the second order correction to the ground state energy $E_0^{(2)}$:

$$E_0^{(2)} = - \sum_{\mathbf{k}} |V_{\mathbf{k}}|^2 \frac{1}{1 + k^2} = - \frac{2\alpha'}{\pi} \int_0^\infty \frac{dk}{1 + k^2} = -\alpha'. \quad (2.29)$$

To express this result in terms of standard dimensionless coupling constant α , we use the transformation given in equation (1.42). Hence, we conclude that

$$E_0^{(2)} = -\alpha. \quad (2.30)$$

Note that this result exactly matches with the results in reference [10] and [6]. So, we draw the conclusion that the generalized Hamiltonian is valid for $n=3$.

2.1.2 2D Polaron

Similar to the 3D case, we consider the electron-phonon interaction Hamiltonian H_{e-p} as the perturbed Hamiltonian $H^{(1)}$. Furthermore, we consider the unperturbed Hamiltonian H^0 as the sum of H_e and H_p . One difference from the preceding case is the form of external potential V_{conf} . In 2D case, we introduce this potential as:

$$V_{conf} = \frac{1}{4}\Omega^2(x^2 + y^2). \quad (2.31)$$

Recalling that electronic wave function is defined in two dimensional space, the (unperturbed) polaron's wave function in n th state is given as:

$$|\psi_n^0\rangle = |n_x, n_y\rangle |\vec{\ell}\rangle. \quad (2.32)$$

The first-order correction given as (2.10) to the ground state energy in 2D case again vanishes; i.e.

$$E_0^{(1)} = 0. \quad (2.33)$$

If we choose the direction of the $\mathbf{k}$ vector as in the x direction i.e. $\mathbf{k} = k\hat{x}$ and follow the procedures within (2.12)-(2.16), we obtain the second-order correction to the ground state eigenvalue as:

$$E_0^{(2)} = \sum_{n,\mathbf{k}} |V_k|^2 \frac{|\langle n|e^{-ikx}|0\rangle|^2}{E_{0,0,\vec{0}}^{(0)} - E_{n,0,\mathbf{0},1\mathbf{k}}^{(0)}}. \quad (2.34)$$

Note that when we perform the similar operations in equations (2.17)-(2.19) the energies in the denominator of equation (2.34) turn out as:

$$E_{0,0,\vec{0}}^{(0)} = \Omega \quad (2.35)$$

and

$$E_{n,0,\mathbf{0},1\mathbf{k}}^{(0)} = (n+1)\Omega + 1. \quad (2.36)$$

Notice that the value of the denominator does not change; that is, we can follow exactly the same steps between (2.20)-(2.29) to calculate the second-order correction in 2D. Hence, we have

$$E_0^{(2)} = - \sum_{\mathbf{k}} |V_{\mathbf{k}}|^2 \frac{1}{1+k^2} = - \frac{2\alpha'}{\pi} \int_0^\infty \frac{dk}{1+k^2} = -\alpha'. \quad (2.37)$$

Note that in (2.37) we have used our observation given in the previous section in equation (1.44).

So, in 2D polaron case, we obtain exactly the same energy value with the one calculated in 3D case. Using the relation (1.42) we can express our result in terms of standard coupling constant α :

$$E_0^{(2)} = -\frac{\pi}{2}\alpha. \quad (2.38)$$

This result is also (as the previous one) identical with the values given in our references [10],[6],[16] and [17]. So, we conclude that the generalized Hamiltonian given in (1.40) together with the expressions (1.41) and (1.42) is valid for $n=2$ case.

2.1.3 1D Polaron

Just as the previous 2 cases, we introduce the variables as the following: The perturbed Hamiltonian is

$$H^1 = H_{e-p}.$$

The unperturbed Hamiltonian is:

$$H^0 = H_e + H_p.$$

At that point we define our external potential as a parabolic potential in one dimension:

$$V_{conf} = \frac{1}{4}\Omega^2 x^2.$$

Then, the polaron's wave function (associated with unperturbed Hamiltonian) in n th state is given as:

$$|\psi_n^0\rangle = |n_x\rangle |\vec{\ell}\rangle.$$

Accordingly, the first-order correction to the ground state energy is zero, i.e.

$$E_0^{(1)} = 0.$$

Again, if we choose $\mathbf{k} = k\hat{x}$, and follow the steps within (2.11)-(2.16), we have

$$E_0^{(2)} = \sum_{n,\mathbf{k}} |V_k|^2 \frac{|\langle n|e^{-ikx}|0\rangle|^2}{E_{0,\vec{0}}^{(0)} - E_{n,\mathbf{0},1\mathbf{k}}^{(0)}}. \quad (2.39)$$

Since

$$E_{0,\vec{0}}^{(0)} = \frac{1}{2}\Omega,$$

and

$$E_{n,\mathbf{0},1\mathbf{k}}^{(0)} = (n + \frac{1}{2})\Omega.$$

Notice that the denominator in (2.39) does not change; hence, performing the procedures (2.17-2.29), we calculate the second-order correction to the ground state eigenvalue (with the fact given in (1.44)) as:

$$E_0^{(2)} = - \sum_{\mathbf{k}} |V_k|^2 \frac{1}{1+k^2} = -\frac{2\alpha'}{\pi} \int_0^\infty \frac{dk}{1+k^2} = -\alpha'. \quad (2.40)$$

As mentioned in Chapter 1, even though we are not allowed to express the result in terms of α , we obtain an energy value for 1D polaron. One important observation, as a result of such a generalization, is that we obtain exactly the same energy in all three cases: $-\alpha'$.

2.2 Strong Coupling Theory

In this section, we consider the situation where the electron-phonon interaction is sufficiently strong. Then, the force due to presence of the electron can no longer be omitted from the equation of the lattice vibration. Because of this reason, we perform the displaced oscillatory transformation.

2.2.1 Displaced Oscillator Transformation

The transformed Hamiltonian H' is given as the following canonical transformation[18]:

$$H' = e^{-S} H e^S \quad (2.41)$$

where $S = \sum_k u_k (a_k - a_k^+)$ and the Hamiltonian H is given in (1.40). Note that u_k is the lattice variational (real) parameter. Furthermore for convenience we consider the Hamiltonian H_{e-p} as

$$H_{e-p} = \sum_{\mathbf{k}} |V_{\mathbf{k}}| (a_{\mathbf{k}} e^{i\mathbf{k}\cdot\mathbf{r}} + a_{\mathbf{k}}^+ e^{-i\mathbf{k}\cdot\mathbf{r}}). \quad (2.42)$$

Note that if H_{e-p} is taken as in equation (1.34), one has to consider $S = \sum_k (a_k^+ u_k - a_k u_k^*)$ where u_k is no longer a real parameter[11]. To calculate the transformed Hamiltonian H' , we employ the following identity:

$$e^A B e^{-A} = B + [A, B] + \frac{1}{2!} [A, [A, B]] + \frac{1}{3!} [A, [A, [A, B]]] + \dots \quad (2.43)$$

Thus, equation (2.41) becomes:

$$H' = H + [H, S] + \frac{1}{2!} [[H, S], S] + \dots \quad (2.44)$$

After certain series of computations, it turns out that only first three terms survive in the equation above; hence, the transformed Hamiltonian H' has its final form:

$$H' = H - \sum_k u_k (a_k + a_k^+) - \sum_k |V_k| u_k (e^{i\mathbf{k}\cdot\mathbf{r}} + e^{-i\mathbf{k}\cdot\mathbf{r}}) + \sum_k u_k^2. \quad (2.45)$$

2.2.2 Variational Principle

In this subsection, we apply the variational procedure to the Hamiltonian H' given in (2.45). We assume that the ground state polaron trial wave function $|\psi\rangle$ is separable i.e.

$$|\psi\rangle = |\phi\rangle |\vec{0}\rangle \quad (2.46)$$

where $|\phi\rangle$ and $|\vec{0}\rangle$ are the electron and phonon wave functions respectively. Furthermore, we assume that the electronic (trial) wave function $|\phi\rangle$ is of Gaussian type. Then, the expectation value of H' with respect to the trial wave function given in (2.46) is:

$$\langle\psi| H' |\psi\rangle = \langle\phi| H_e |\phi\rangle - \sum_k |V_k| u_k (\rho_k + \rho_k^*) + \sum_k u_k^2 \quad (2.47)$$

where $\rho_k = \langle\phi| e^{i\mathbf{k}\cdot\mathbf{r}} |\phi\rangle$.

Now, we start to calculate the energy values of the nD polaron by the variational approach.

2.2.2.1 3D Polaron

For the three dimensional case, we consider $V_{conf}=0$ and $\mathbf{k} = k\hat{x}$.

Moreover, we choose our trial wave function as

$$|\phi\rangle = A e^{-ar^2} = A_x e^{-ax^2} A_y e^{-ay^2} A_z e^{-az^2} \quad (2.48)$$

where a is the variational parameter, $A = A_x A_y A_z$ is the normalization constant with

$$A_x^2 = A_y^2 = A_z^2 = \sqrt{\frac{2a}{\pi}}. \quad (2.49)$$

Thus,

$$\rho_k = \rho_k^* = e^{-\frac{k^2}{8a}}. \quad (2.50)$$

First, we minimize equation (2.47) with respect the variable u_k ; that is

$$\frac{\partial \langle\psi| H' |\psi\rangle}{\partial u_k} = 0. \quad (2.51)$$

If one performs the operation in (2.51), it turns out that

$$u_k = |V_k| \rho_k. \quad (2.52)$$

Therefore, equation (2.47) becomes:

$$\langle \psi | H' | \psi \rangle = \langle \phi | H_e | \phi \rangle - \sum_k |V_k|^2 \rho_k^2. \quad (2.53)$$

The first term above the equation is simply $\langle \phi | H_e | \phi \rangle = -\langle \phi | \nabla^2 | \phi \rangle$ and one may calculate it as:

$$\langle \phi | H_e | \phi \rangle = 3a. \quad (2.54)$$

Using the fact given in equation (1.44), the second term is obtained as

$$\sum_k |V_k|^2 \rho_k^2 = 2\alpha' \sqrt{\frac{a}{\pi}}. \quad (2.55)$$

Therefore, minimizing equation (2.53) with respect to variational parameter a , we obtain the ground state energy of the polaron E_{3D} in terms of the generalized coupling constant α' as:

$$E_{3D} = -\frac{\alpha'^2}{3\pi}. \quad (2.56)$$

By using the relation between the standard and generalized coupling constant (see equation 1.45), we may express this result in terms of α :

$$E = -\frac{\alpha^2}{3\pi}. \quad (2.57)$$

Note that this result given in (2.57) is exactly the value found by Das Sarma and Mason [10].

2.2.2.2 2D Polaron

Similar to the previous case we determine $V_{conf} = 0$ and $\mathbf{k} = k\hat{x}$. Furthermore, we choose the trial wave function for electronic part as two dimensional Gaussian function:

$$|\phi\rangle = A_x e^{-ax^2} A_y e^{-ay^2}. \quad (2.58)$$

where

$$A_x^2 = A_y^2 = \sqrt{\frac{2a}{\pi}}. \quad (2.59)$$

Furthermore, the value of the expression $\langle \phi | e^{i\mathbf{k}\cdot\mathbf{r}} | \phi \rangle$ does not change, i.e.

$$\rho_k = \rho_k^* = e^{-\frac{k^2}{8a}}. \quad (2.60)$$

If we follow the same steps (2.51) and (2.52), we obtain equation (2.53). Since ρ_k is the same with the one calculated in 3D, by the property (1.44) the value of the second term is given as (2.55). However, we cannot propose the same reasoning for the first term since the wave function has changed. When the first term is calculated, its explicit expression turns out as:

$$\langle \phi | H_e | \phi \rangle = 2a. \quad (2.61)$$

If equation (2.53) is minimized with respect to the variational parameter a , (an upper bound for)the ground state energy of 2D polaron E_{2D} is given as:

$$E_{2D} = -\frac{\alpha'^2}{2\pi}. \quad (2.62)$$

Using the relation given in (1.45), one can express the energy in terms of the standard electron-phonon coupling constant α as:

$$E = -\frac{\pi}{8}\alpha^2. \quad (2.63)$$

Note that this result is also what the strong-coupling theory predicts in two dimensional case [10], [17].

2.2.2.3 1D Polaron

As in the previous two cases, we choose $V_{conf} = 0$ and $\mathbf{k} = k\hat{x}$. Furthermore, we assume that the trial wave function has the 1D Gaussian form, i.e.

$$|\phi\rangle = A_x e^{-ax^2} \quad (2.64)$$

where $A_x^2 = \sqrt{\frac{2a}{\pi}}$. If we follow the same procedures in 3D case, we obtain

$$\langle \psi | H' | \psi \rangle = \langle \phi | H_e | \phi \rangle - \sum_k |V_k|^2 \rho_k^2 \quad (2.65)$$

where the second term on the right hand side of the equation above is given as (2.53) and the first term is of the form:

$$\langle \phi | H_e | \phi \rangle = a. \quad (2.66)$$

Thus, minimization operation on (2.65) with respect to the variational parameter a leads to the following ground state energy value of 1D polaron in terms of the generalized coupling constant:

$$E_{1D} = -\frac{\alpha'^2}{\pi} \quad (2.67)$$

Note that because of the definition of α' , we are not allowed to transform α' into α .

Another point we emphasize about overall energies is that these three energies (i.e. E_{1D} , E_{2D} and E_{3D}) can be written in more general form in terms of α' as:

$$E_{nD} = -\frac{\alpha'^2}{n\pi}. \quad (2.68)$$

2.2.2.4 "2-3" D Polaron

In this subsection, we consider a polaron whose dimension is continuously varied to two dimensions from three dimensions where the electron interacts with the bulk phonon modes of the polar lattice, and we calculate the ground state energy of such a polaron. To do this, we consider the following confinement potential for the electron:

$$V_{conf} = \begin{cases} \infty, & |z| \geq \frac{L}{2} \\ 0, & \text{otherwise.} \end{cases}$$

Furthermore, we use following ground state trial wave function $|\phi\rangle$ for the electron:

$$|\phi\rangle = A_x e^{-ax^2} A_y e^{-ay^2} A_z e^{-az^2} \cos\left(\frac{\pi}{L}z\right), \quad (2.70)$$

where

$$A_x^2 = A_y^2 = \sqrt{\frac{2a}{\pi}} \quad (2.71)$$

and

$$A_z^2 = \left(\int_{-L/2}^{L/2} \cos^2\left(\frac{\pi}{L}z\right) e^{-2az^2} dz \right)^{-1}. \quad (2.72)$$

As usual, we determine $\mathbf{k} = k\hat{x}$. Thus,

$$\rho_k = \rho_k^* = e^{-\frac{k^2}{8a}}. \quad (2.73)$$

Applying equation (2.51) we have

$$\langle \psi | H' | \psi \rangle = \langle \phi | H_e | \phi \rangle - \sum_k |V_k|^2 \rho_k^2. \quad (2.74)$$

Now, we calculate the second term in the right hand side of equation (2.74). At this point we assume that for all values of L the electron-phonon interaction is described either by the electron-phonon interaction of (strict) 3D polaron or the interaction of (strict) 2D polaron. Then, the second term on the RHS of equation (2.74) becomes

$$\sum_k |V_k|^2 \rho_k^2 = 2\alpha' \sqrt{\frac{a}{\pi}}. \quad (2.75)$$

Notice that when L is sufficiently large, α' transforms α according to equation (1.45). Similarly, when L is sufficiently small α' maps to $\frac{\pi}{2}\alpha$. For the case that L is neither sufficiently large nor small, α' transforms to either α or $\frac{\pi}{2}\alpha$. However, since we do not have a rule that determines to which value α' transforms in that interval of L (i.e. the intermediate values of L), we express our results in terms of α' .

On the other hand, the first terms in equation (2.74) might be written as:

$$\langle \phi | H_e | \phi \rangle = 2a + \left(2a + \frac{\pi^2}{L^2}\right) - \frac{4\pi a}{L} \langle \phi | z \tan \frac{\pi z}{L} | \phi \rangle - 4a^2 \langle \phi | z^2 | \phi \rangle. \quad (2.76)$$

Therefore, by minimizing equation (2.74) with respect to the variational parameter a , one can obtain the ground state energy of the free polaron (i.e. the subband energy π^2/L^2 coming from the potential barrier must be subtracted from (2.76)) for an arbitrary squeezing length L (i.e. the distance between potential barriers). In our work, we handle this minimization process via numerical methods.

Our first observation from Fig. 2.1 that while the coupling constant α' increases the polaron's energy decreases, as expected, since simply the weaker coupling between the electron and phonons leads to the lower binding energy. Secondly, we

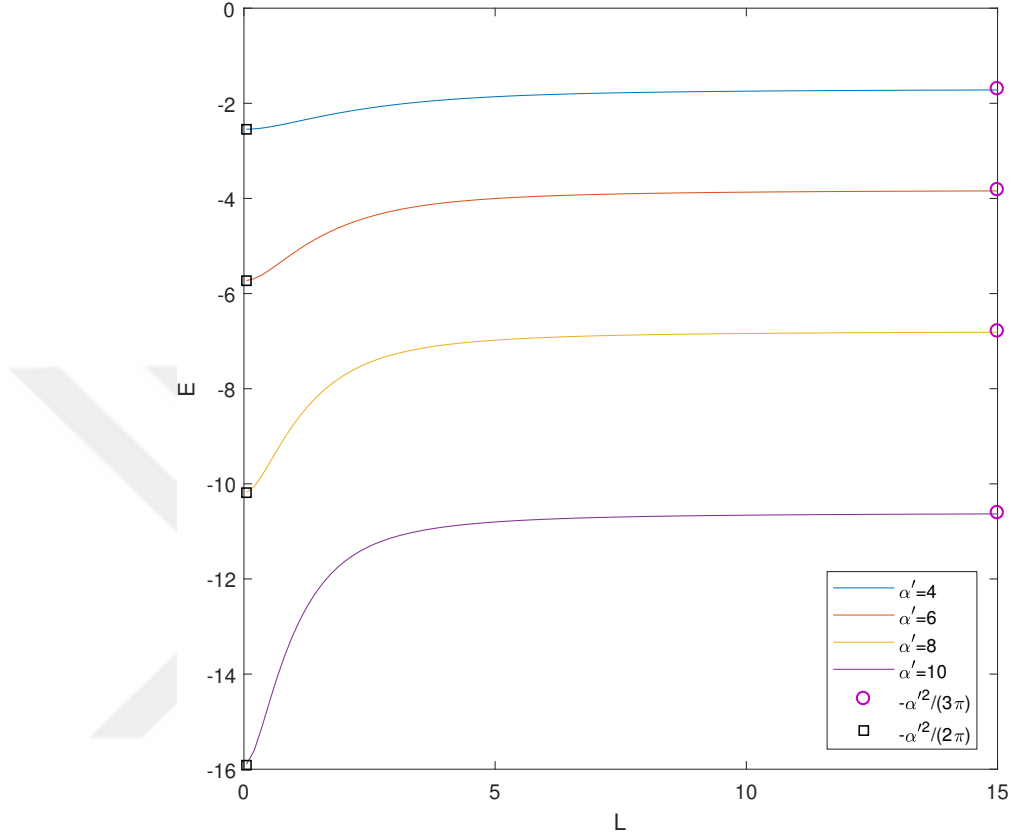
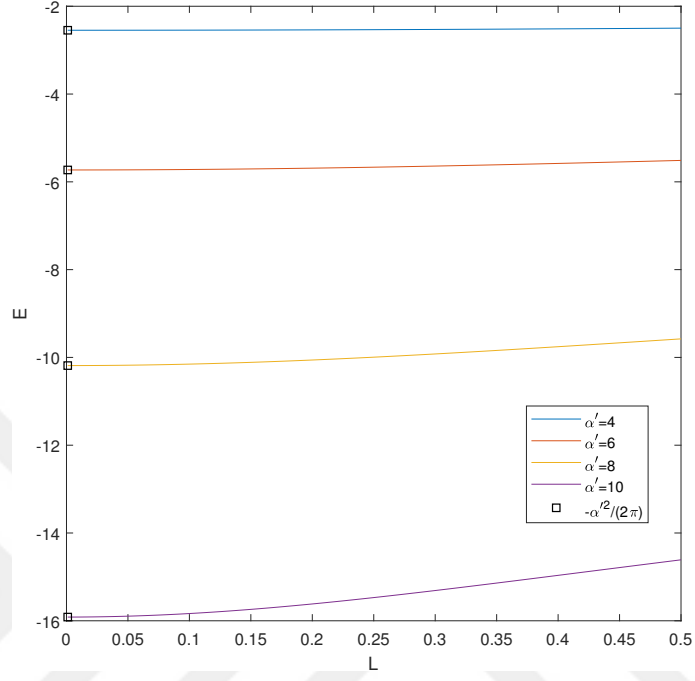


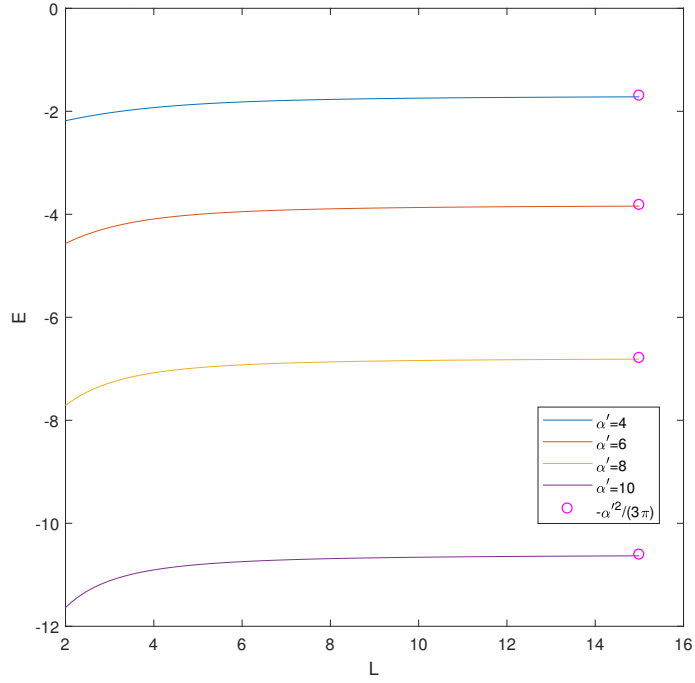
Figure 2.1: E vs L for various α' .

notice that while the squeezing length L increases, the polaron's energy converges to the energy of 3D polaron (i.e. $-\alpha'^2/(3\pi)$). This result is also expected because greater values of L implies the free electron case in all space dimensions. Furthermore, for the case $L \rightarrow 0$ we observe that the polaron's energy converges to the energy of 2D polaron (i.e. $-\alpha'^2/(2\pi)$).

Moreover, from Fig. 2.2 we see that for the values of L which are greater than a certain value of L , say critical length L_c , the ("2-3" D) polaron behaves like (strict) 3D polaron in terms of energy. Similarly, for those values of L which are less than a critical length L_c , the ("2-3" D) polaron might be considered as (strict) 2D polaron.



(a) Energy change for small L



(b) Energy change for large L

Figure 2.2: Energy change of the polaron for different L .

To be more precise, suppose the energy E_{neg} is the energy we may neglect in our system. Then, the critical length L_c is defined as:

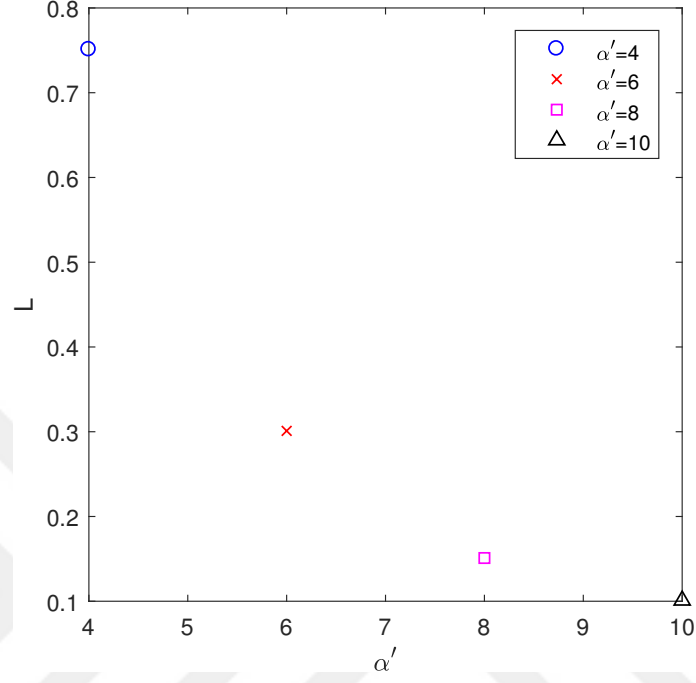
$$\text{If } 0 < L < L_c, \text{ then } |E_{2-3D} - E_{2D}| < E_{neg}. \quad (2.77)$$

Notice that the expression in (2.77) indicates that when L is less than the critical length L_c , the ("2-3" D) polaron acts like 2D polaron. Similar expression can be written for 3D case just by replacing E_{2D} with E_{3D} and the interval of L ; that is,

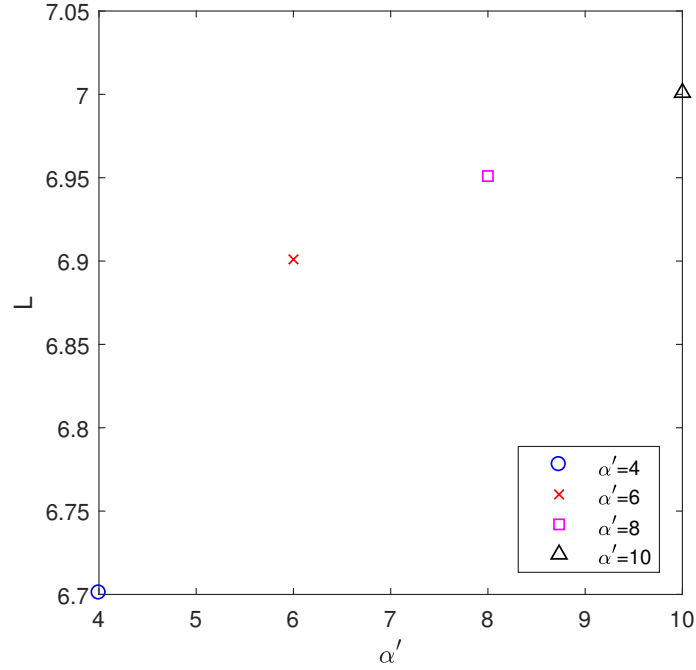
$$|E_{2-3D} - E_{3D}| < E_{neg} \text{ whenever } L_c < L < \infty. \quad (2.78)$$

Note that, similar to the previous case, equation (2.78) means that the polaron restricted by the plates where the distance between them is L behaves like (strict) 3D polaron when L is greater than a critical distance L_c .

Based on the definition of critical length L_c and considering Fig. 2.2, we propose that the length L_c is correlated to the coupling constant α' . In fact, this statement can be supported by regarding the specific case of the negligible energy E_{neg} : If we assume that $E_{neg} = 0.1(\hbar\omega)$, the critical lengths turn out as in Fig. 2.3. We observe from Fig. 2.3. (a) that for increasing values of coupling constant, we must consider the smaller values of L_c to be able to regard the ("2-3"D) polaron as 2D polaron. On the other hand, from Fig. 2.3 (b) we see that to consider the polaron as 3D polaron, we have to take greater values of L_c for increasing values of α' .



(a) Critical lengths L_c for various α' in the 2D limit. Circle, cross, square, and triangle represent the critical lengths for $\alpha' = 4, 6, 8$ and 10 , respectively.



(b) Critical lengths L_c for various α' in the 3D limit. The markers represent the (coupling constant, critical length) pairs respectively.

Figure 2.3: Critical lengths L_c for various coupling constants α' (with the negligible energy $E_{neg} = 0.1$).

Next chapter, we shall give the ground state energy of the nD ($n = 1, 2, 3$) and "2-3" D polaron for full range of couplings (i.e. $0 < \alpha' < 12$) and compare the results with the ones obtained by the weak-coupling and strong coupling theories.



Chapter 3

Improved Strong Coupling Theory

In this chapter, we calculate the ground state energy of the Fröhlich Polaron for all coupling constant values. Our work is based on the approach Devreese et al. [1] introduced. Their work is basically to improve Strong Coupling Theory by introducing a trial wave function which has been corrected by the perturbation theory having the form

$$|\psi\rangle = c |0\rangle |\phi_n\rangle + \sum_{\mathbf{k}} g_{\mathbf{k}}^* V_{\mathbf{k}}^* (e^{-i\mathbf{k}\cdot\mathbf{r}} - \rho_{\mathbf{k}}^*) a_{\mathbf{k}}^+ |0\rangle |\phi_n\rangle. \quad (3.1)$$

In this thesis, we will not discuss how to obtain such a wave function. Instead, we shall take into consideration the application of the trial wave function (3.1). For more detail, one can check the relevant paper.

3.1 Analytical Calculations

Considering the normalization condition of (3.1), if the expectation value of the polaron's Hamiltonian given in equation (1.40) with respect to the (ground state)trial wave function in (3.1) is calculated, the result turns out[1]

$$E = \langle \psi | H | \psi \rangle = \langle \phi | H_u | \phi \rangle + \frac{X}{2} \quad (3.2)$$

where

$$H_u = p^2 + V_{conf} + \sum_{\mathbf{k}} |V_{\mathbf{k}}|^2 |\rho_{\mathbf{k}}|^2 - \sum_{\mathbf{k}} |V_{\mathbf{k}}|^2 (\rho_{\mathbf{k}}^* e^{i\mathbf{k}\cdot\mathbf{r}} + \rho_{\mathbf{k}} e^{-i\mathbf{k}\cdot\mathbf{r}}) \quad (3.3)$$

and X satisfies the following integral equation:

$$\frac{X}{2} + \frac{2\alpha'}{\pi} \int_0^\infty \frac{(1 - |\rho_{\mathbf{k}}|^2)^2}{D_1(\mathbf{k}) + D_2(\mathbf{k}) - (1 - |\rho_{\mathbf{k}}|^2)^{\frac{X}{2}}} dk = 0 \quad (3.4)$$

with

$$D_1 = \langle \phi | (e^{i\mathbf{k}\cdot\mathbf{r}} - \rho_{\mathbf{k}}) H_u (e^{-i\mathbf{k}\cdot\mathbf{r}} - \rho_{\mathbf{k}}^*) | \phi \rangle \quad (3.5)$$

and

$$D_2 = (1 - |\rho_{\mathbf{k}}|^2)(1 - \langle \phi | H_u | \phi \rangle). \quad (3.6)$$

Note that we use the same definition for $\rho_{\mathbf{k}}$ which is given in strong coupling theory; that is, $\rho_k = \langle \phi | e^{i\mathbf{k}\cdot\mathbf{r}} | \phi \rangle$.

Notice that to obtain the ground state energy for the polaron, we have to minimize equation (3.2) with respect to the variational parameter, say a , which is embedded in the electronic wave function $|\phi\rangle$. However, our standard way (i.e. differentiating E with respect to the variational parameter, letting the resulting expression be zero, finding the parameter; so the minimum value of E) to find the minimum value of (3.2) is not readily available since X is a transcendental function of the variational parameter a (i.e. X cannot be expressed in terms of known functions of a) by equation (3.4). One candidate solution (and we use in our work) for this problem is to solve the integral equation for certain value of a numerically and to find the minimum value of E . Before doing this, we give the explicit form of the other variables (i.e. $\langle \phi | H_u | \phi \rangle$, D_1 and ρ_k).

3.1.1 3D Polaron

For the three dimensional polaron case, we consider $V_{conf} = 0$. Furthermore, we choose the electronic trial (ground state) wave function in the form of Gaussian i.e.

$$|\phi\rangle = A_x e^{-ax^2} A_y e^{-ay^2} A_z e^{-az^2} \quad (3.7)$$

where a is the variational parameter and the normalization constants are given by equation (2.49). Furthermore we determine $\mathbf{k} = k\hat{x}$. Thus,

$$\rho_k = \rho_k^* = e^{-\frac{k^2}{8a}}. \quad (3.8)$$

Now, we consider the term D_1 . Note that one can express D_1 as

$$D_1 = \langle \phi | e^{i\mathbf{k}\cdot\mathbf{r}} H_u e^{-i\mathbf{k}\cdot\mathbf{r}} | \phi \rangle - \rho_{\mathbf{k}} (\langle \phi | e^{i\mathbf{k}\cdot\mathbf{r}} H_u | \phi \rangle + \langle \phi | H_u e^{-i\mathbf{k}\cdot\mathbf{r}} | \phi \rangle) + \rho_{\mathbf{k}}^2 \langle \phi | H_u | \phi \rangle. \quad (3.9)$$

After certain amount of algebra one can show that

$$\langle \phi | e^{i\mathbf{k}\cdot\mathbf{r}} H_u e^{-i\mathbf{k}\cdot\mathbf{r}} | \phi \rangle = k^2 + \langle \phi | H_u | \phi \rangle. \quad (3.10)$$

Furthermore, the term $\langle \phi | H_u e^{-i\mathbf{k}\cdot\mathbf{r}} | \phi \rangle$ can be written as

$$\langle \phi | H_u e^{-i\mathbf{k}\cdot\mathbf{r}} | \phi \rangle = \langle \phi | \left(-\frac{\partial^2}{\partial y^2} - \frac{\partial^2}{\partial z^2} \right) e^{-ikx} | \phi \rangle + \langle \phi | \left(-\frac{\partial^2}{\partial x^2} \right) e^{-ikx} | \phi \rangle + \langle \phi | \xi e^{-ikx} | \phi \rangle. \quad (3.11)$$

where

$$\xi = \sum_{\mathbf{k}} |V_{\mathbf{k}}|^2 \rho_{\mathbf{k}}^2 - 2 \sum_{\mathbf{k}} |V_{\mathbf{k}}|^2 \rho_{\mathbf{k}} \cos kx. \quad (3.12)$$

Using equation (2.61), the first term can be calculated as:

$$\langle \phi | \left(-\frac{\partial^2}{\partial y^2} - \frac{\partial^2}{\partial z^2} \right) e^{-ikx} | \phi \rangle = \rho_k 2a. \quad (3.13)$$

Moreover, after some efforts one might show that the second term is

$$\langle \phi | \left(-\frac{\partial^2}{\partial x^2} \right) e^{-ikx} | \phi \rangle = \rho_k \left(a + \frac{k^2}{4} \right). \quad (3.14)$$

Also, the last term in (3.11) can be expressed as:

$$\langle \phi | \xi e^{-ikx} | \phi \rangle = 2\alpha' \sqrt{\frac{a}{\pi}} \rho_k - 4\alpha' \sqrt{\frac{a}{\pi}} \rho_k^{1/2}. \quad (3.15)$$

Finally, carrying out more or less similar (in fact comparably easier) integrals in (3.13)-(3.15), one can obtain

$$\langle \phi | H_u | \phi \rangle = 3a - 2\alpha' \sqrt{\frac{a}{\pi}}. \quad (3.16)$$

Thus, the energy expression E in (3.2) which has to be minimized becomes

$$E = 3a - 2\alpha' \sqrt{\frac{a}{\pi}} + \frac{X}{2} \quad (3.17)$$

where ρ_k is given by (3.8), X satisfies the integral equation (3.4), and the terms D_1 and D_2 are given as:

$$D_1 = k^2 + (1 + \rho_k^2) \left(3a - 2\alpha' \sqrt{\frac{a}{\pi}} \right) - 2\rho_k \left(\left(3a + \frac{k^2}{4} \right) \rho_k + 2\alpha' \sqrt{\frac{a}{\pi}} \rho_k - 4\alpha' \sqrt{\frac{a}{\pi}} \rho_k^{1/2} \right) \quad (3.18)$$

and

$$D_2 = (1 - \rho_k^2) \left(1 - [3a - 2\alpha' \sqrt{\frac{a}{\pi}}] \right). \quad (3.19)$$

3.1.2 nD Polaron

In fact, if one uses the two and one dimensional Gaussian trial wave functions (having the form of (2.58) and (2.64)) for the wave function of electron and carry out the procedures within (3.8)-(3.16), the results given in (3.17)-(3.19) can be generalized for the nD polaron ($n = 1, 2, 3$) as the following:

$$E_n = na - 2\alpha' \sqrt{\frac{a}{\pi}} + \frac{X}{2} \quad (3.20)$$

where ρ_k is given by (3.8), X satisfies the integral equation (3.4), and the terms D_1 and D_2 are given as:

$$D_1 = k^2 + (1 + \rho_k^2) \left(na - 2\alpha' \sqrt{\frac{a}{\pi}} \right) - 2\rho_k \left(\left(na + \frac{k^2}{4} \right) \rho_k + 2\alpha' \sqrt{\frac{a}{\pi}} \rho_k - 4\alpha' \sqrt{\frac{a}{\pi}} \rho_k^{1/2} \right) \quad (3.21)$$

and

$$D_2 = (1 - \rho_k^2) \left(1 - [na - 2\alpha' \sqrt{\frac{a}{\pi}}] \right). \quad (3.22)$$

3.1.3 "2-3" D Polaron

In this case, we consider exactly the same problem expressed in Strong-Coupling Theory in the third chapter. So, we choose the external potential as:

$$V_{conf} = \begin{cases} \infty, & |z| \geq \frac{L}{2} \\ 0, & \text{otherwise.} \end{cases}$$

Furthermore, we use following ground state trial wave function $|\phi\rangle$ for the electron:

$$|\phi\rangle = A_x e^{-ax^2} A_y e^{-ay^2} A_z e^{-az^2} \cos\left(\frac{\pi}{L}z\right). \quad (3.24)$$

Moreover, we consider $\mathbf{k} = k\hat{x}$. Then, the term D_1 may be expressed as:

$$D_1 = k^2 + (1 + \rho_k^2) \langle\phi| H_u |\phi\rangle - \rho_{\mathbf{k}} (\langle\phi| e^{ikx} H_u |\phi\rangle + \langle\phi| H_u e^{-ikx} |\phi\rangle). \quad (3.25)$$

Note that

$$\langle\phi| H_u e^{-ikx} |\phi\rangle = \rho_k a + \langle\phi| -\frac{\partial^2}{\partial z^2} e^{-ikx} |\phi\rangle + \langle\phi| \left(-\frac{\partial^2}{\partial x^2}\right) e^{-ikx} |\phi\rangle + \langle\phi| \xi e^{-ikx} |\phi\rangle \quad (3.26)$$

where ξ is defined by (3.12). The second term in (3.26) can be written by using (2.76) as

$$\langle\phi| -\frac{\partial^2}{\partial z^2} e^{-ikx} |\phi\rangle = \rho_k \left(\left(2a + \frac{\pi^2}{L^2}\right) - \frac{4\pi a}{L} \langle\phi| z \tan \frac{\pi z}{L} |\phi\rangle - 4a^2 \langle\phi| z^2 |\phi\rangle \right). \quad (3.27)$$

Notice that the third has already been calculated in equations (3.14). At that point we assume (as we did in Strong-Coupling Theory) that for an arbitrary squeezing length L the electron-phonon interaction can be considered as the same with the interaction of (strict) 3D polaron or the interaction of (strict) 2D polaron. With this assumption, then the fourth term in (3.26) is given by equation (3.15).

Finally, (using the same assumption made in the preceding paragraph) the term $\langle\phi| H_u |\phi\rangle$ is calculated as

$$\langle\phi| H_u |\phi\rangle = 2a + \left(2a + \frac{\pi^2}{L^2}\right) - \frac{4\pi a}{L} \langle\phi| z \tan \frac{\pi z}{L} |\phi\rangle - 4a^2 \langle\phi| z^2 |\phi\rangle - 2\alpha' \sqrt{\frac{a}{\pi}}. \quad (3.28)$$

Therefore, the ground state energy E which must be minimized with respect to the variational parameter a has the final form:

$$E = \langle \phi | H_u | \phi \rangle + \frac{X}{2} \quad (3.29)$$

where $\langle \phi | H_u | \phi \rangle$ is given by (3.28), X satisfies the integral equation (3.14) in which the terms D_1 and D_2 are

$$D_1 = k^2 + (1 + \rho_k^2) \langle \phi | H_u | \phi \rangle - 2\rho_{\mathbf{k}} \langle \phi | H_u e^{-ikx} | \phi \rangle \quad (3.30)$$

and

$$D_2 = (1 - \rho_k^2)(1 - \langle \phi | H_u | \phi \rangle) \quad (3.31)$$

where $\langle \phi | H_u e^{-ikx} | \phi \rangle$ is given by equation (3.26).

3.2 Numerical Results and Discussion

If we minimize equation (3.20) with respect to the variational parameter a for $n = 3$, the results turn out as the following:

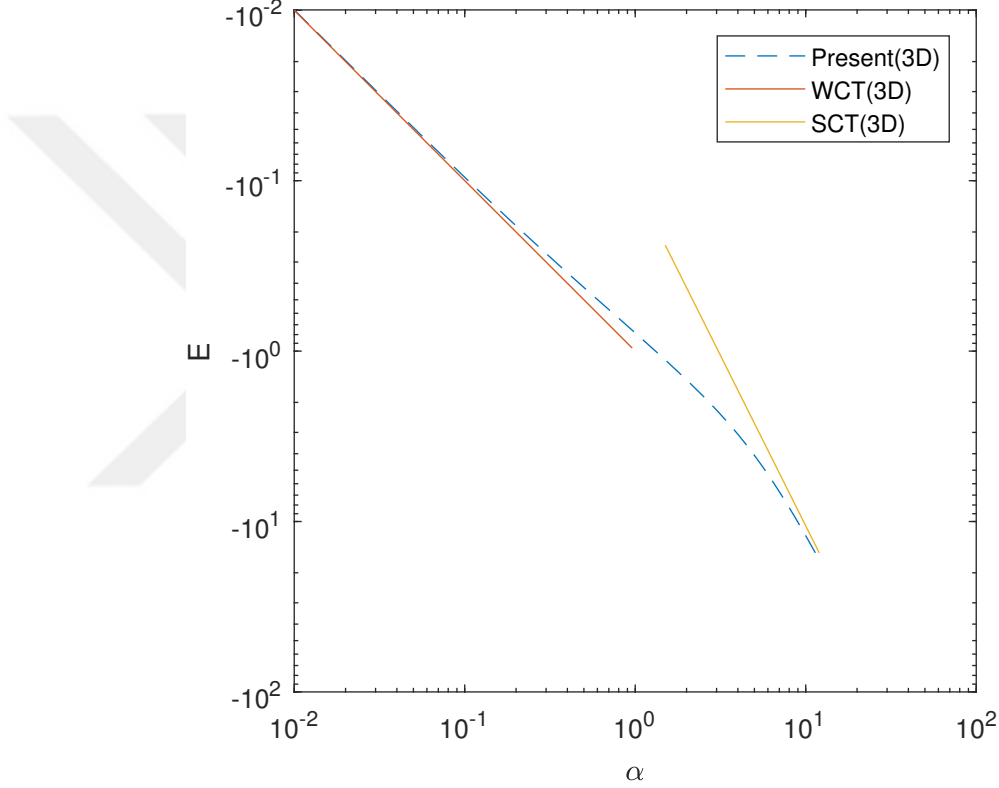


Figure 3.1: E vs α for the 3D polaron.

From Fig. 3.1 we observe that the present work (i.e. improved strong coupling theory (ISCT)) provides better energy estimations compared to Strong Coupling Theory (SCT) in strong coupling regime (i.e. $\alpha \gg 1$) for 3D polaron. Furthermore, the present work calculates the energies in the intermediate-coupling regime in which neither SCT nor Weak Coupling Theory (WCT) is valid. In the weak-coupling regime (i.e. $\alpha \ll 1$), we observe that the energy calculated by the present work converges to the energy obtained by WCT for small coupling constants. However, in such limit, the energy of WCT is smaller than the energy the present work estimates. One possible explanation for this situation could be

the fact that the Gaussian type trial wave function is not an appropriate wave function for weak coupling regime.

If we perform the minimization procedure in equation (3.20) with $n = 2$, we have the energies for all coupling regimes for the 2D polaron as seen in Fig. 3.2.

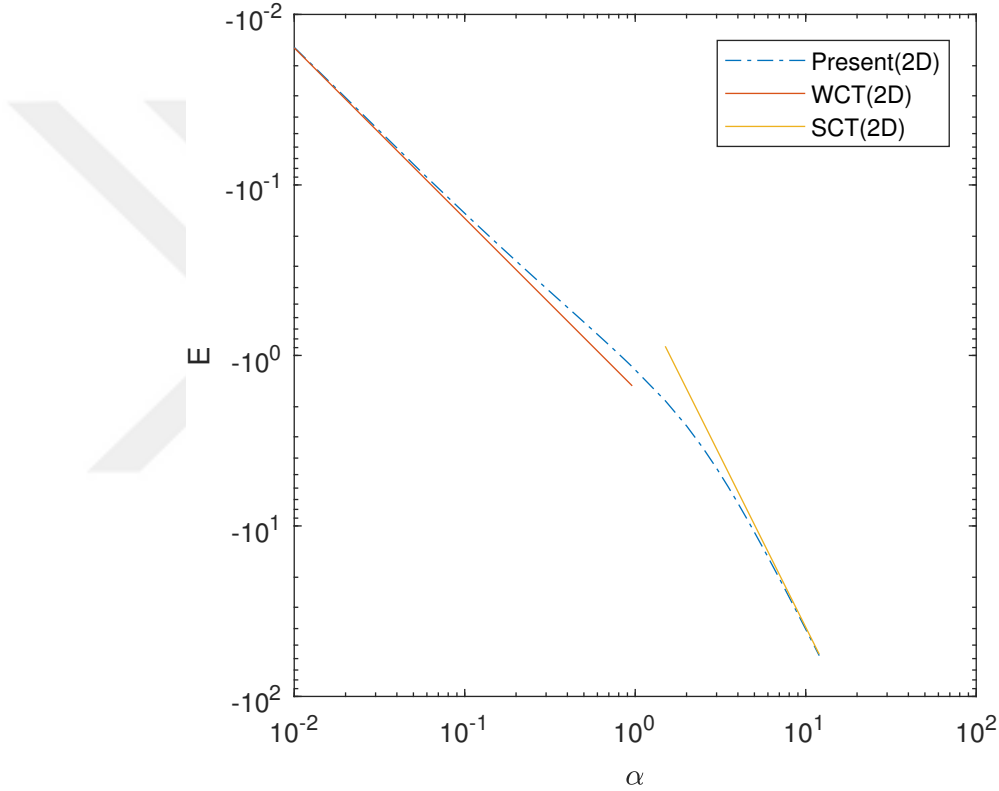
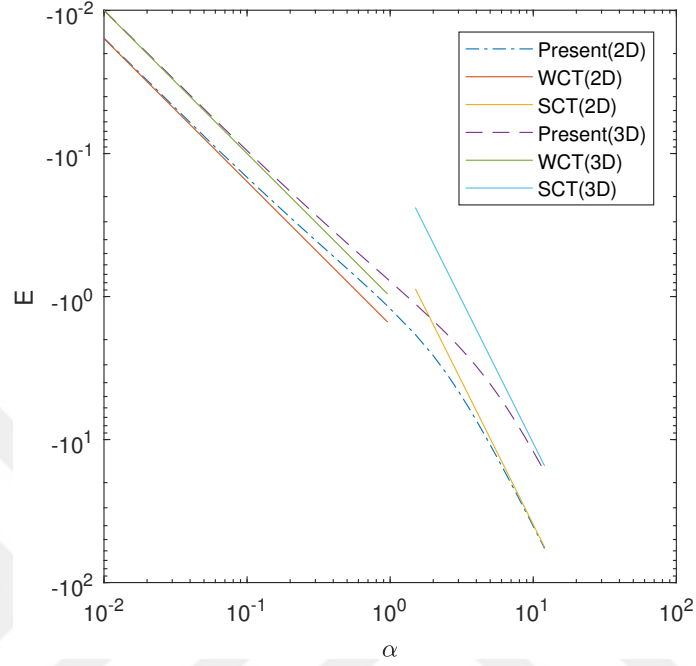
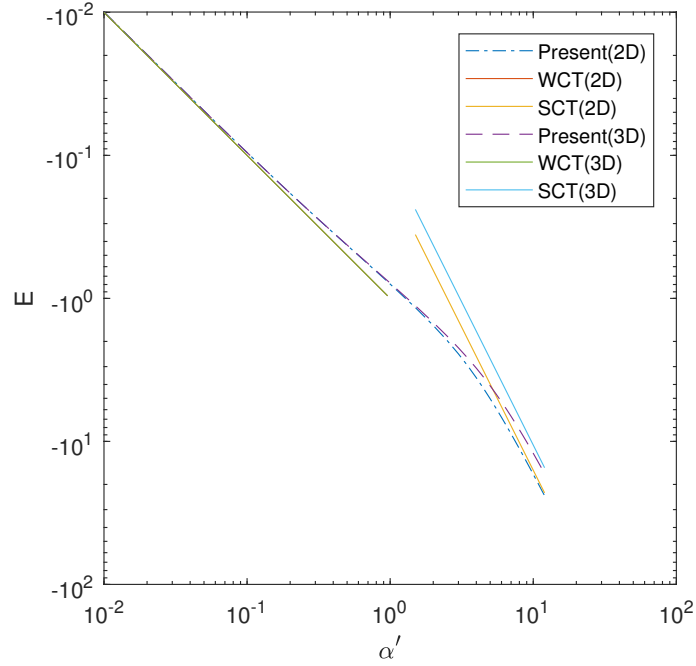


Figure 3.2: E vs α for the 2D polaron

From Fig. 3.2 we observe some facts similar to the 3D case. That is, in the strong coupling regime, the present work gives us an upper bound for the ground state energy of the 2D polaron which is smaller than the one obtained by SCT. Moreover, in the intermediate-coupling regime (i.e. $\alpha > 1$), present work gives some data for the energy of 2D polaron which are more valid compared to other two theories (i.e. WCT and SCT). On the other hand, in the weak-coupling regime, the energy of the present work converges to the energy of WCT but it is bounded below as opposite to the situation in the strong coupling regime.



(a) Energies obtained by the present work for both (strict) 2D and 3D polarons vs standard coupling constant α .



(b) Energies obtained by Present work, WCT and STC vs the generalized coupling constant α' for 2D and 3D polaron.

Figure 3.3: Energies of the 2D and 3D polaron.

One may observe some interesting properties when these two cases are plotted in one graph as in Fig. 3.3.

From this graph (i.e. Fig. 3.3 (a)), we observe that for an arbitrary value of α the energy of 2D polaron is less than the energy of 3D polaron; that is, when the dimension decreases, the energy also decreases. Moreover, the same figure shows that for a certain coupling constant value in the strong coupling regime, the difference between energies calculated by Present (2D) and SCT(2D) is smaller than the difference gained by Present (3D) and SCT(3D). However, the same situation cannot be proposed in the weak-coupling regime; the differences in this regime are approximately the same.

One can also express these results in terms of the generalized coupling constant α' as seen in Fig. 3.3 (b). From this figure we see that for both polarons, the corresponding energies obtained by the present work lesser than the ones calculated by SCT in the strong coupling regime. Moreover, in weak coupling regimes, both energies obtained by ISCT in 2D and 3D converge to the energy $-\alpha'$ that is exactly the energy obtained by WCT(2D) and WCT(3D) (see equations (2.30) and (2.37)). And these energies are greater than $-\alpha'$; that is, no energy improvement occurs in this regime as it has been observed in previous three graphs.

Now, we consider the confined polaron(i.e. "2-3" D polaron) case. If one minimizes equation (3.29), one may obtain a graph of the energy of the polaron vs L for various α' (see Fig. 3.4) . We observe that for increasing value of the distance between the slabs (i.e. L) the energy converges to the energy improved strong coupling(ISCT) predicts for (strict) 3D polaron(circles). Similary, on the opposite limit, i.e. $L \rightarrow 0$, the energy converges to the value ISCT provides for 2D polaron case (i.e. squares). Note that this situation might be considered that the formalism in (3.29) is correct. Furthermore, we observe that for increasing value of the (generalized) coupling constant α' , the energy of the polaron decreases, as expected, since stronger interaction leads to higher binding energy.

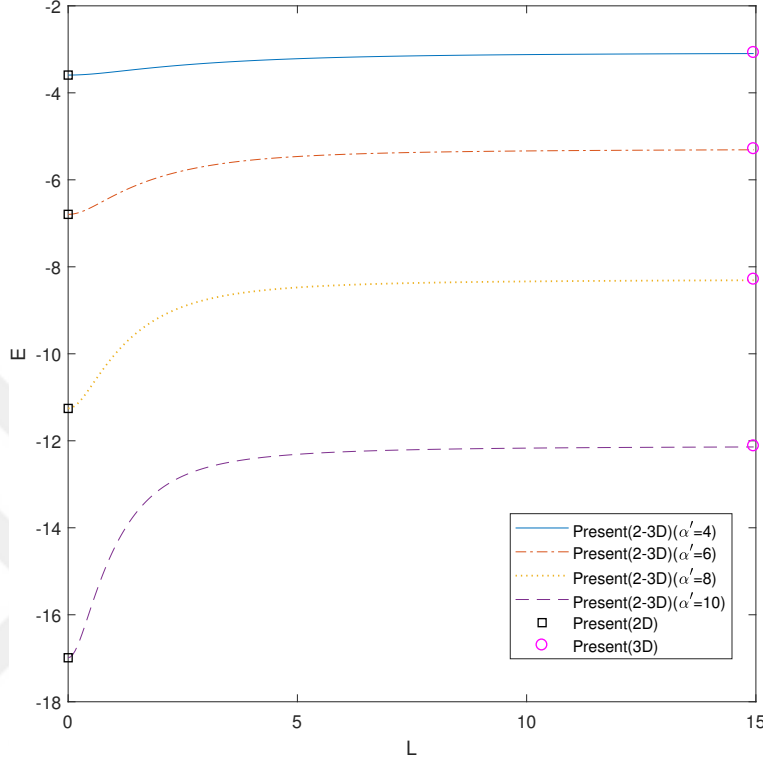
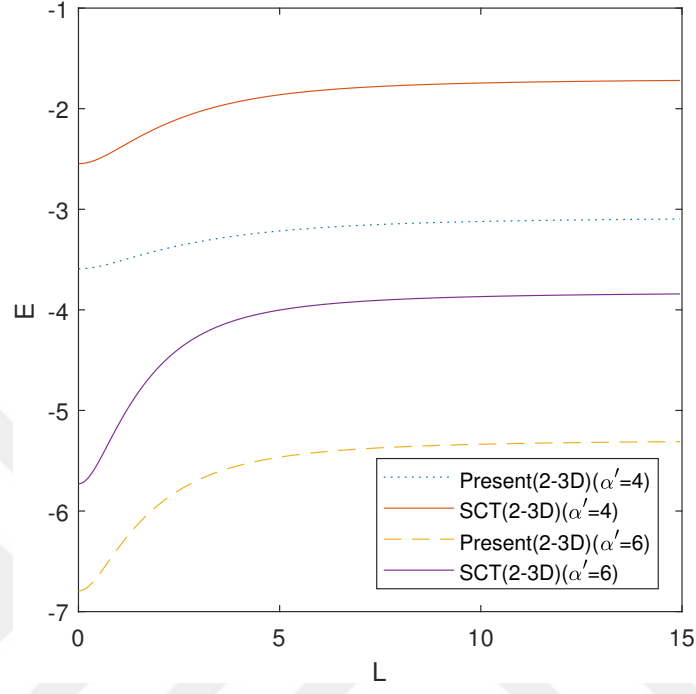


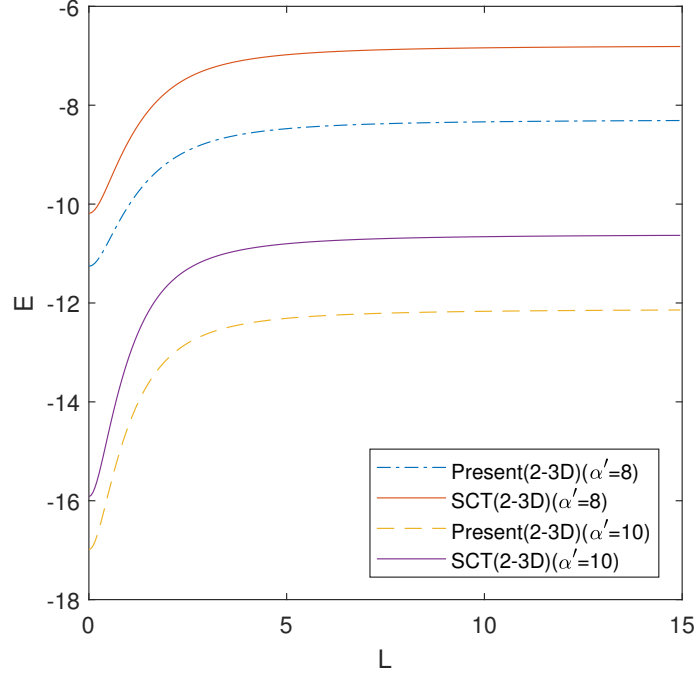
Figure 3.4: Energy E (ISCT predicts) vs L for various α' .

To compare the ("2-3"D) energies obtained by SCT to ones calculated by the present work (i.e. ISCT), one may plot the results in one graph (see Fig. 3.5). From Fig. 3.5 (a) and (b) we observe that for an arbitrary coupling constant α' the present work predicts lesser energy compared to the energy calculated via SCT for every possible slab distance L .

If we take into consideration the extreme cases of L (i.e. $L < 0.5$ and $L > 2$), we may suggest some values about the critical length L_c as performed in Strong-Coupling Theory. Based on the definitions of the critical length L_c given in (2.77) and (2.78), if we assume the negligible energy $E_{neg} = 0.1$, the critical lengths L_c resulting from the present work turn out as in Fig 3.6. We observe from Fig. 3.6 (a) that to consider the polaron as a strict 2D polaron, we must decrease the slab distance for increasing value of the coupling constant. On the other hand, from Fig. 3.6 (b) we see that for increasing α' , the greater values of L are need to be able to consider ("2-3"D) polaron as strict 3D polaron.

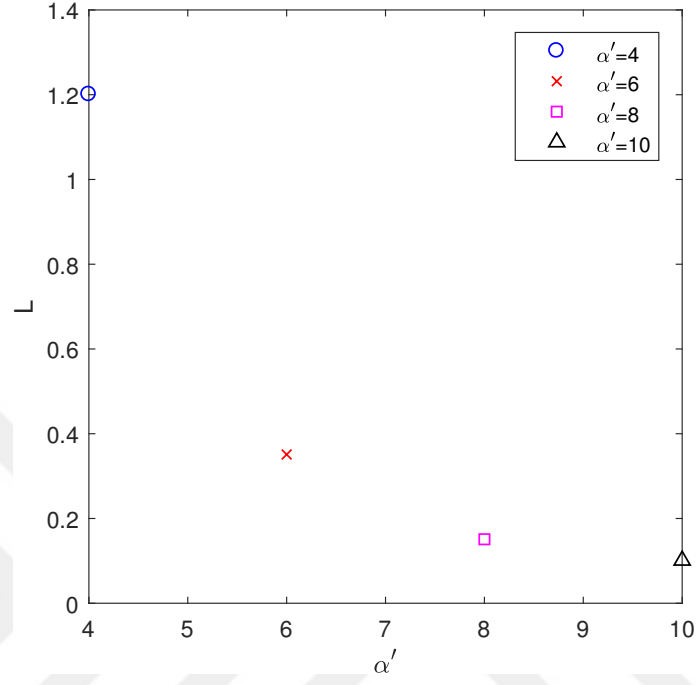


(a) E vs L for $\alpha' = 4, 6$.

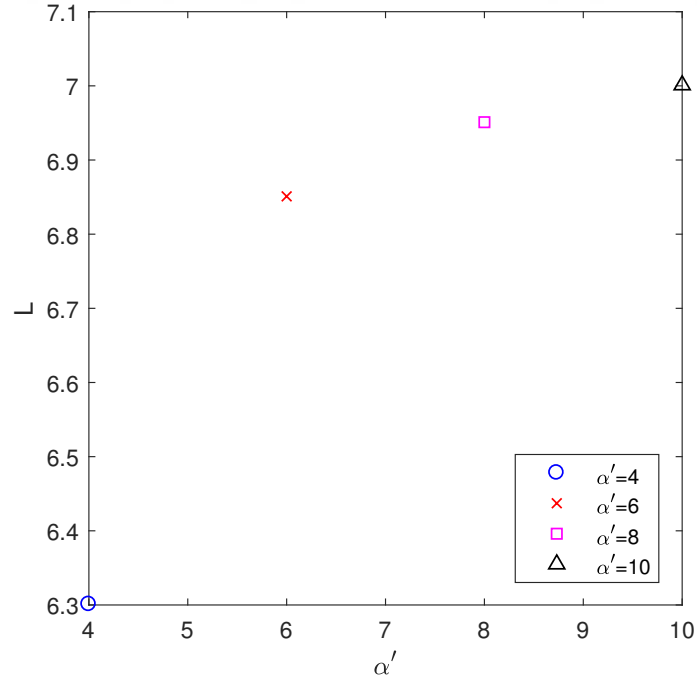


(b) E vs L for $\alpha' = 8, 10$.

Figure 3.5: E (calculated by ISCT and SCT) vs L .



(a) L_c vs α' in 2D limit ($E_{neg} = 0.1$).

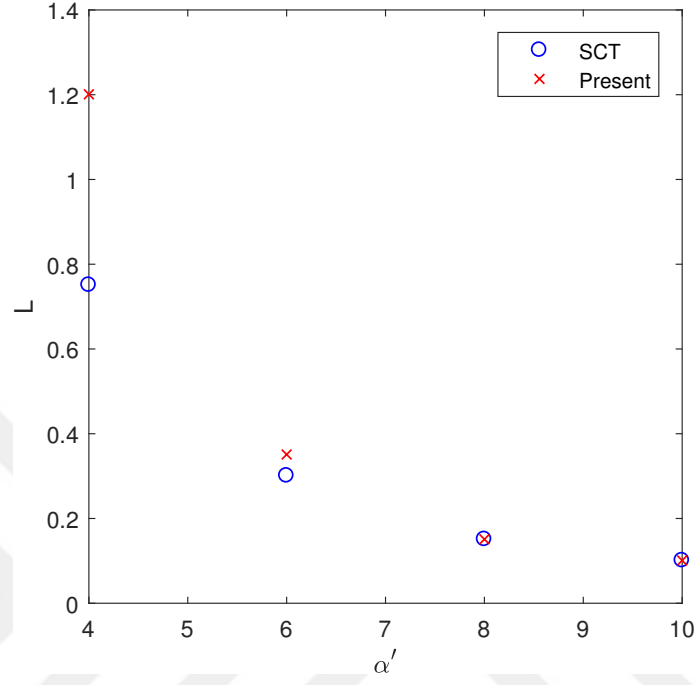


(b) L_c vs α' in 3D limit ($E_{neg} = 0.1$).

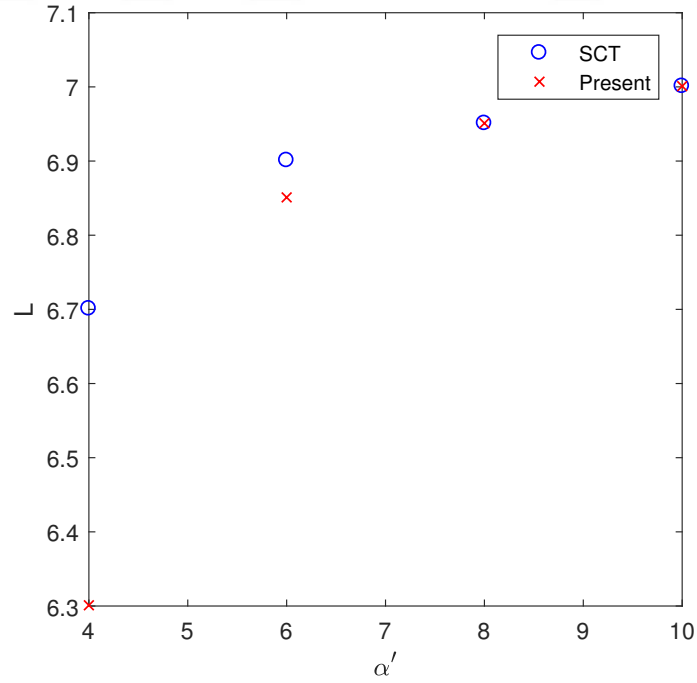
Figure 3.6: L_c (obtained by ISCT) vs α' .

One interesting question could be whether there is any difference between the critical lengths obtained by SCT and ISCT. To find out, we combine two data given in Fig. 2.3 and Fig. 3.6 (see Fig 3.7).

We observe from Fig. 3.7 (a) that for $\alpha' = 4$, the length L_c obtained by present calculation is greater than L_c SCT gives. For the coupling constant $\alpha' = 6$, L_c the present calculation gives is (with a small magnitude) greater compared to the L_c of SCT. For the other values of the coupling constant (i.e. $\alpha' = 8, 10$) both theories give the same critical length value. On the other hand, the subfigure (b) shows that for $\alpha' = 4$, to be able to consider the polaron as 3D polaron, it is sufficient to have a slab length L which is greater than 6.3 according to ISCT while this value is calculated as 6.7 by SCT. For $\alpha' = 6$, L_c obtained by the present work is smaller than the one SCT predicts but the magnitude of their difference is small. For $\alpha' = 8, 10$, we obtain the same critical lengths by the two theories.



(a) L_c vs α' in 2D limit.



(b) L_c vs α' in 3D limit.

Figure 3.7: L_c (obtained by the theories SCT and ISCT) vs α' (with $E_{neg} = 0.1$).

Chapter 4

Summary and Conclusion

In this thesis, first, using Weak-Coupling Theory, we calculated the ground state energies of the nD polaron in the weak-coupling regimes in terms of the generalized coupling constant α' , and found that the energy for all n is equal to α' .

Furthermore, using Strong Coupling Theory, we obtained the (ground state) energies of the nD polaron in strong-coupling regime in terms of α' and we found that there is a relation between the dimension n and the energy; which is, $E_n = -\alpha'^2/(n\pi)$. Moreover, using the same theory, we have taken into consideration a polaron which is confined in one dimension. In this case, we calculated the energy of the confined polaron ("2-3" D polaron) as a function of the slab length L for the certain values of α' . We observed that in the limits of the slab length L (i.e. $L \rightarrow 0$ and $L \rightarrow \infty$) the energy converges to the energy of strict polaron (i.e. E_{2D} or E_{3D}). Next, we introduced the critical length L_c concept and calculated the such lengths in both 2D and 3D limits. Furthermore, we showed that L_c is dependent on α' .

After completing the analysis of WCT and SCT, we introduced Improved Strong Coupling Theory (ISCT), which is based on the variational principle and the trial wave function Devreese et al [1] proposed. By using this theory, we

calculated the energies of the nD polaron in all coupling limits (weak, intermediate, strong coupling). And we demonstrated that in the strong-coupling limit, ISCT predicts better energy values than SCT. Furthermore, we proposed energies in intermediate-coupling limit where WCT and SCT are not very reliable. In the weak-coupling regime, we have observed that the energy calculated by ISCT converges to the energy of WCT while the coupling constant becomes smaller; however, the energy of ISCT was bounded below. Using ISCT, we also considered "2-3" D polaron and calculated the energies as a function of L for various α' . At the limits of L we observed that the energy converges to the energy of the 2D or 3D polaron that ISCT predicts. Furthermore, we also analyzed the critical length concept in ISCT and showed that L_c is dependent on coupling constant in this theory as well. Moreover, we compared the L_c 's obtained by two different theories (i.e. SCT and ISCT) and conclude that the difference in L_c 's coming from the different theories disappears when the coupling constant increases.

We note that although we gave the analytical expression for the 1D polaron in the thesis, we preferred not to demonstrate the result of 1D since the result is not convertible to standard coupling constant α .

As a final comment, we underline the fact that even though ISCT is superior to SCT in strong coupling regime, it may not necessarily mean that ISCT is the most powerful method to estimate the energy in such regime. In fact, in the reference [3] it is mentioned that Feynman's formalism is the one of the strongest estimator of the energy. However, since we restrict ourselves to only WCT and SCT to test the success of ISCT, we do not make any comment about the Feynman's method.

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