FRÖHLICH POLARON CALCULATIONS IN NON-INTEGER DIMENSIONAL SPACE AS A MODEL OF CONFINEMENT

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ABSTRACT

FRÖHLICH POLARON CALCULATIONS IN NON-INTEGER DIMENSIONAL SPACE AS A MODEL OF CONFINEMENT

Polaron is a quasiparticle describing an electron in interaction with phonons of a medium. A microscopic description of large polaron is given by the Fröhlich Hamiltonian which does not admit exact solutions. For calculating the ground state energy and effective mass of polaron there are several approximation methods, some of which are valid only for large or small values of the electron-phonon coupling constant. In low-dimensional systems, where the polaron is confined by an external potential such as in the form of slab or wire geometries, the polaronic energy and effective mass are known to get enhanced.

In this thesis we present an approach towards quantifying the degree of confinement on a large polaron provided by a parabolic potential. On that purpose, first, variation of polaronic ground state energy as a function of the parameters of the confinement potential for both slab- and wire-like geometries and using a methodology valid for all values of electron-phonon coupling constant is calculated. Then, applying a non-integer-dimensional-space algebra the polaron problem has been solved in an isotropic D-dimensional space using the same approch (D varies continuously from 3 to 2 for slab, and from 3 to 1 for wire geometry.)

Finally, by matching the polaron ground state energy values obtained from the two calculations in large electron-phonon coupling constant limit, we identify the effective dimensionality D, of the polaron for a given set of confinement and material parameters.

ÖZET

BİR SINIRLAMA MODELİ OLARAK TAMSAYI OLMAYAN BOYUTLU UZAYDA FRÖHLICH POLARON HESAPLAMALARI

Polaron bir ortamın fononlarıyla elektronun etkileşimini tarif eden tanımlayan sözde parçacıktır. Büyük polaronun mikroskopik açıklaması tam çözümleri kabul etmeyen Fröhlich Hamiltonyen tarafından verilir. Polaronun temel durum enerjisinin ve etkin kütlesinin hesaplanmasında bazılarının sadece büyük veya küçük elektron fonon çiftlenim sabiti için geçerli olduğu birkaç yaklaşım yöntemi kullanılır.

Polaronun levha veya tel geometrisi gibi bir dış potansiyel tarafından hapsedildiği düşük boyutlu sistemlerde polaronik enerji ve etkin kütlenin artış gösterdiği bilinmektedir. Bu tezde büyük polaron üzerindeki parabolik potansiyelin getirdiği sınırlama derecesinin miktarının belirlenmesi yönünde bir yaklaşım sunacağız. Bu amaç doğrultusunda öncelikle, elektron fonon çitflenim sabitinin tüm değerlerini kapsayan bir metodoloji kullanarak, levha ve tel benzeri geometriler biçimindeki sınırlandırma potansiyelinin parametrelerinin fonksiyonu olarak temel durum enerjisinin varyasyonu hesaplandı. Daha sonra aynı yaklaşım çevresinde tam sayı olmayan boyutlu uzay cebirini uygulayarak polaron problemi izotropik D boyutlu uzayda çözüldü. (Boyut parametresi D levha geometrisi için kesiksiz olarak 3ten 2ye, tel geometrisi için 3ten 1e kadar değişir.)

Son olarak elektron-fonon çiftlenim sabitinin büyük olduğu limitde, iki hesaplamadan elde edilen polaronun temel durum enerjilerini eşleştirerek verilen sınırlama ve malzeme parametreleri için polaronun etkin boyut parametresini tanımladık.

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CHAPTER 1

INTRODUCTION

The polaron concept, first proposed nearly 80 years ago by Landau [1]. Theoretical and experimental studies on the polarons are increasing gradually day by day. There are host of reasons why polarons carry on receiving much attention nowadays. One of the main reasons which constitutes great importance is offering a simplificative and nontrivial model consists of an electron interacting with a phonon field. And the other significant one is leading to implementation of many approximation methods which are extremely powerful tools in the absence of exact analytical solution. These methods are applied in order to overcome challenges come from mathematical structure of polarons and making them to be a test bed for the application of these techniques. The explicit connection of the issue to the electronic structure of the ionic or polar-semiconductor materials is required to investigation of the electron phonon interaction effects to find out the properties of materials in detail. Within the last few decades much attention has been paid to low dimensional semiconductor structures that play a central role in the areas of electronics, optoelectronics and theoretical condensed matter physics. Thanks to great advances in semiconductor fabrication techniques, low dimensional microstructures namely quantum wells, wires and dots have recently become available.

In these microstructures, charge carriers are restricted in one or more spatial directions. Two dimensional systems are member of the low dimensional systems confined in one dimension. In actual systems the polaron will not be exactly two dimensional; it is more justified to speak about quasi 2-D polarons. The thickness of the 2D electron layer perpendicular to the layer is nonzero [2]. Another member of the low dimensional structures are nanowires which are quasi-one dimensional semiconductor systems. The formation of a strictly one-dimensional systems requires strong confinement in the x-y direction. And finally quantum dots are mesoscopic devices in which the number of free charge carriers is strongly quantized.

There is an inverse relationship between the ground state properties and the structure geometry. It is found that ground state energy and the effective mass of the polaron are increase rapidly with decreasing the confinement lengths. Accordingly, it is understood that polaron and its characteristic ground state properties within the framework of lower dimensionality have been the subject of considerable views for a long time.

The theory of polaron arises from the motion of an electron in an ionic or polar semiconductor crystals. The long range Coulomb interaction of the electron with the ions of the crystal, displaces the positive and negative ions. A separation of ions from their equilibrium positions produces a polarization field and modifies the electron motion in classical frame. From the view of the quantum field theory, electron which couples to the phonon modes of the crystal is surrounded by the phonon field. The compound system of electron plus accompanying phonon field can be treated as a quasiparticle called a "polaron" . Polarons can be divided roughly into two groups. Polarons whose electronic chrage carriers are not self-trapped are labeled as *weak coupling polarons* because of the weak interaction. By contrast, polarons whose electronic carriers are self-trapped are termed *strong coupling polarons* due to the strong interaction [3]. Also, strong coupling polarons are treated as consisting of two sub-groups namely large and small polarons respectively. The polaron is considered as large when the spatial extent is large compared to the lattice constant a. A large polaron generally moves as a free particle with coherence in an elastic continuum except for weak scattering due to the phonons. Furthermore long range interaction causes a formation of large polaron in the strong coupling and weak coupling regimes. When the spatial extent becomes comparable to a lattice constant a, the polaron is treated as small.

The electron phonon interaction brings about modified properties of electron such as reducing the self energy and increasing the inertia of it by an amount according to the strength of coupling. It has been reported in the literature that the polaronic quantities (binding energy, effective mass etc.)get considerably larger in low dimensionally confined systems than their corresponding values for the bulk polaron.

During the thesis, we will concentrate merely on large polarons called Fröhlich polarons and bulk phonon approximation will be applied. We deal with dynamical characteristic of the electron's motion limited to the external potential , and let alone all the other effects like coupling of the electron to the confined phonon modes as well as interface surface-optical(SO)phonons. Thus our main purpose to gain a perspective of the bulk phonon effects purified with not taking into account other perturbing quantities. We neglect not only SO phonons but also other kinds of phonon modes' contributions, additionally we will also ignore any screening effects. There can be some complications owing to non-parabolicity corrections to the electron band or we encounter conditions such as those due to loss of validity either the effective-mass approximation or the Fröhlich continuum Hamiltonian in very small microstructures.

Although in low dimensional systems numerous results has been discovered in the

last years there are just few results concerning non-integer dimensional systems. Aside from investigating the movement of the polaron in low dimensional confined systems, recently it is crucial to understand how polaron behaves in D-dimensional space. F.M Peeters, Wu Xiaoguang, and J.T.Devreese pointed out that the Fröhlich Hamiltonian can be generalized to the case of an electron moving in n space dimensions by using Feynman path integral formalism [4]. Polaron under the influence of the confinement in low dimensional systems can not move freely but in non-integer dimensional space it moves loosely namely it does not feel any confinement. The calculations of ground state energy and effective mass are performed here based on conventional approximation methods except Feynman path integral formalism which is seemed to be most successful approach. Accordingly, we will have considered variational method and perturbation theory for large and small electron-phonon coupling constant values in NIDS. However in some cases electron-phonon interaction constant has intermediate values. For these cases we have to introduce an other approach covers all electron phonon coupling strengths. Variational perturbative approach will be quite appropriate for taking into account weak and strong coupling counterparts simultaneously in NIDS.

We need to reflect polaron problem in two separate cases; one is to reconsider the properties of the Fröhlich polaron confined in a parabolic quantum well with adjustable dimensions and the other one is determine the behaviour of the optical polaron in non-integer dimensional space as if, polaron does not sense any confinement. Both cases will be studied in detail with making a delicate comparasion between free polaron and confined polaron by reviewing the ground state properties. Our goal is presenting a theoretical model which establishes a relationship between dimensionality and confinement parameter. The overwhelming majority of the results obtained from calculations are used to set up functional dependence to each other. Such a correlation has been established for weak coupling polaron by [5].

After this general introduction we now present our work in four chapters. The remainder of this thesis will be organized as follows. We will give definition for the Fröhlich Hamiltonian in next section of this chapter and in the other two sections, as a warm up ,the ground state properties of weak and strong coupling polaron in confined media will be discussed without going into details. The derivation of ground state properties of arbitrary coupling polaron will be presented by using variational perturbative approach in the last section of this chapter. In chapter 2 we will give a brief information about mathematical structure of the NID space to introduce the notation. The explicit calculations and numerical results related to non-integer dimensional polaronic properties will be given

the 3rd chapter. And also functional dependence of effective dimensionality D on the confinement parameter Ω in large α limit for the slab- and wire-like geometries will be given in the last section of the 3rd chapter. Finally in the last chapter, we will conclude with summarizing the analytical and numerical results in NIDS for the completeness. We also discuss physics of the simple relation between D and Ω in conclusion.

1.1. Fröhlich Hamiltonian

In this section we introduce the Hamiltonian describing the large (Fröhlich) polarons. It should be emphasised that polaron consists of the single electron confined in an external potential and LO phonons of a medium. As we mentioned before certain requirements should be provided in expressing the Hamiltonian like avoiding the contributions that may come from all other kinds of phonon modes and also ignoring the screening effects and further details. We will not give the derivation of the Fröhlich Hamiltonian in here but one may refer to the original paper by Fröhlich et al., [6] and some relevant books [7–9] in order to get a detailed information about how quantized form of the Hamiltonian can be obtained from classical electrodynamics by using second quantization. The Hamiltonian of an electron confined in a various geometries interacting with the field of bulk LO-phonons is given as

$$H = \frac{p^2}{2m^*} + V_{conf}(\boldsymbol{r};\{\Omega_i\}) + \hbar\omega_{LO}\sum_Q a_Q^\dagger a_Q + \sum_Q (V_Q a_Q e^{i\boldsymbol{Q}.\boldsymbol{r}} + {V_Q}^* a_Q^\dagger e^{-i\boldsymbol{Q}.\boldsymbol{r}}) \quad (1.1)$$

This Hamiltonian will be the starting point of many investigations in the following chapters. Scaling energies by the phonon quantum $\hbar\omega_{LO}$ as a unit of energy and $(\hbar/2m^*\omega_{LO})^{1/2}$ as a unit of length, the Hamiltonian is rewritten in the following form

$$H = p^2 + V(\boldsymbol{r};\{\Omega_i\}) + \sum_Q a_Q^\dagger a_Q + \sum_Q V_Q(a_Q e^{i\boldsymbol{Q}.\boldsymbol{r}} + a_Q^\dagger e^{-i\boldsymbol{Q}.\boldsymbol{r}}) \quad (1.2)$$

with the appropriate polaron units ($\hbar = 2m^* = \omega_{LO} = 1$) are set in our calculations to simplify the notation. In the Fröhlich Hamiltonian the first two term

$$H_e = p^2 + V(\boldsymbol{r};\{\Omega_i\}) \quad (1.3)$$

is the electronic part with the confining potential $V(\boldsymbol{r};\{\Omega_i\}$ or due to the anisotropy it takes this form $V_{conf}(\boldsymbol{\rho},z;\Omega_1,\Omega_2)$ in cylindrical coordinates.
The following term is the phonon-related part of the Hamiltonian

$$H_{ph}=\sum_{Q}a_Q^{\dagger}a_Q \tag{1.4}$$

and the last term, is given below, expresses the non-local interaction Hamiltonian which defines the interaction between electron and a LO phonon branch

$$H_{e-ph}=\sum_{Q}V_Q(a_Qe^{i\boldsymbol{Q}.\boldsymbol{r}}+a_Q^{\dagger}e^{-i\boldsymbol{Q}.\boldsymbol{r}}) \tag{1.5}$$

where $a_Q^{\dagger}(a_Q)$ is the creation (annihilation) operators respectively for bulk LO phonons with wavevector $\boldsymbol{Q}$. In the above, $\boldsymbol{r}$ denotes the electron position in spherical coordinates and Ω_i denotes tunable parameter which is useful to gain a comprehensive understanding about effect of confining potential on the ground state property of polaron with manipulating the degree of confinement. Amplitude of the electron phonon interaction which is assumed to be real and spherically symmetric function [10] is given in this form,

$$V_Q \;=\; \sqrt{\frac{4\pi\alpha}{\vartheta_3}}\frac{1}{\boldsymbol{Q}} \tag{1.6}$$

where

$$V_Q \;=\; {V_Q}^{*}=V(|Q|) \tag{1.7}$$

with unitless coupling constant α is considered as strength of the interaction for the Fröhlich polaron model. The explicit form of α is expressed by

$$\alpha=\frac{e^2}{2\hbar\omega_{LO}}\left(\frac{2m^*\omega_{LO}}{\hbar}\right)^{1/2}\left(\frac{1}{\varepsilon_\infty}-\frac{1}{\varepsilon_0}\right) \tag{1.8}$$

ε_∞ and ε_0 are high-frequency and static dielectric constants of the material, respectively. The LO phonons are usually represented by an Einstein model in the study of single polarons. In the Einstein model, optical phonon frequency is independent of phonon wave vector, namely , i.e. $\omega_{\boldsymbol{Q}} \equiv \omega_{LO}$.

1.2. Weak Coupling Formalism

The scope of this section we concentrate on the case where the kinetic energy of the electron is much smaller than the phonon modes of a medium. In other words we consider availability of electron-phonon interaction constant is quite small, $\alpha \ll 1$. Since, electron-phonon interaction is rather weak, lattice deformation tends to follow the electron moving in the crystal. In order to clearly display such a case, it is appropriate to treat the electron phonon interaction as a perturbation in weak interaction domain. In summary the main theme of the weak coupling formalism is perturbation theory comprises with the effect of small disturbances. We present a revised version of weakly coupled polarons within second order perturbation theory that is studied previously [11].
Derivations of the expressions for ground state energy and the effective mass of the polaron start with recalling the Fröhlich Hamiltonian. In the following calculations we shall restrict our consideration to the slab and wire-like geometries by setting the confining potential in a flexible way.

First, let us concentrate quasi-2D slab-like configuration for the confinement of the electron. Confining potential has the form $V_{conf}(\rho, z) = \frac{1}{4}\Omega^2 z^2$ to reflect the ground state energy and the effective mass which are considered as most obvious features of Fröhlich polaron for bulk (3D), slab-like (quasi-2D), and slab (strictly 2D) polaron properties. One might ask a question what could be the impact of the dimensionless frequency (Ω) on the confining potential? In the absence of an confinement, $V_{conf}(\rho, z) = 0$. In this case we deal with the bulk (3D) optical polaron. In the presence of confining potential, by varying Ω from zero to infinity, a continuous transition from bulk geometry to the strict two dimensional geometry is achieved. It is possible to set the trial total wave function in a product form as following

$$\Psi_{total} = \psi_{\boldsymbol{k},n}\phi_{ph} \tag{1.9}$$

where $\psi_{\boldsymbol{k},n}$ is the part of the total wavefunction describing position of the electron and

ϕ_{ph} is the part that describes phonon state.
One has to solve eigenvalue equation provided by electronic part

$$H_e\psi_{\boldsymbol{k},n}(\boldsymbol{\rho},z) = E_{n,\boldsymbol{k}}\psi_{\boldsymbol{k},n}(\boldsymbol{\rho},z) \qquad n = 0,1,2,... \tag{1.10}$$

Electronic wave function is separable in transverse and longitudinal coordinates in the form

$$\psi_{\boldsymbol{k},n}(\boldsymbol{\rho},z) = \frac{1}{\sqrt{2^n n!}}\left(\frac{\omega}{2\pi}\right)^{1/4} H_n\left(\sqrt{\frac{\omega}{2}}z\right)\exp\left(-\frac{1}{4}\omega z^2\right)\phi_{\boldsymbol{k}}(\boldsymbol{\rho}) \tag{1.11}$$

where in the plane wave representation sets the system in motion along the transverse direction to the z-axis and harmonic oscillator states with Hermite polynomials of degree n represents the confined electron along the z direction.
Corresponding energy eigenvalues of Eq.(1.10) can be readily obtained as given

$$E_n(\boldsymbol{k}) = (n+\frac{1}{2})\omega + k^2 \tag{1.12}$$

We begin by considering the system, consists of three term including zeroth order, first order and second order contributions to the energy of the ground state

$$E = E^0_{\boldsymbol{k}} + E^1_{\boldsymbol{k}} + E^2_{\boldsymbol{k}} \tag{1.13}$$

and these contributions are listed in a compact form, respectively as

$$E^{(0)}_k = \langle\psi_{\boldsymbol{k},0}|\hat{H}_0|\psi_{\boldsymbol{k},0}\rangle \tag{1.14}$$
$$E^{(1)}_k = \langle\psi_{\boldsymbol{k},0}|\hat{H}_{e-ph}|\psi_{\boldsymbol{k},0}\rangle \tag{1.15}$$
$$E^{(2)}_k = \sum_i \frac{\langle\psi_{\boldsymbol{k},i}|\hat{H}_{e-ph}|\psi_{\boldsymbol{k},0}\rangle}{E_0 - E_i} \tag{1.16}$$

Let us consider the explicit forms of contributions to the energy of the ground state, start-

ing with the derivation of the zeroth order term

$$\begin{aligned} & \langle\psi_{\boldsymbol{k},0}|\langle 0_{\boldsymbol{Q}}\hat{H}_0||0_{\boldsymbol{Q}}\rangle\psi_{\boldsymbol{k},0}\rangle \\ = \; & \langle\psi_{\boldsymbol{k},0}|\langle 0_{\boldsymbol{Q}}|\hat{H}_0|0_{\boldsymbol{Q}}\rangle|\psi_{\boldsymbol{k},0}\rangle \\ = \; & \langle\psi_{\boldsymbol{k},0}|\langle 0_{\boldsymbol{Q}}|\left(\nabla^2 + V(\boldsymbol{\rho},z) + \sum_Q a_Q^\dagger a_Q\right)|0_{\boldsymbol{Q}}\rangle|\psi_{\boldsymbol{k},0}\rangle \\ = \; & k^2 + \frac{1}{2}\omega \end{aligned} \tag{1.17}$$

We immediately see that, in Eq.(1.17) the phonon-related term of the unperturbed Hamiltonian does not give any contribution to the ground state energy. Then, the first order term is given as

$$\begin{aligned} & \langle\psi_{\boldsymbol{k},0}|\langle 0_{\boldsymbol{Q}}|\hat{H}_{e-ph}||0_{\boldsymbol{Q}}\rangle\psi_{\boldsymbol{k},0}\rangle \\ = \; & \langle\psi_{\boldsymbol{k},0}|\langle 0_{\boldsymbol{Q}}|\sum_Q V_Q(a_Q e^{i\boldsymbol{q}\cdot\boldsymbol{\rho}}e^{iq_z z} + a_Q^\dagger e^{-i\boldsymbol{q}\cdot\boldsymbol{\rho}}e^{-iq_z z})|0_{\boldsymbol{Q}}\rangle\psi_{\boldsymbol{k},0}\rangle \end{aligned} \tag{1.18}$$

It is clear that, contribution coming from the first order term is zero.
Finally, the second order term

$$\begin{aligned} E_k^{(2)} &= \sum_Q \sum_{\boldsymbol{k}'} \sum_n \frac{|\langle\psi_{\boldsymbol{k}',n}|\langle 1_{\boldsymbol{Q}}|H_{e-ph}|0_{\boldsymbol{Q}}\rangle|\psi_{\boldsymbol{k},0}\rangle|^2}{E_0(\boldsymbol{k}) - E_n(\boldsymbol{k}')} \\ &= \sum_Q \sum_{\boldsymbol{k}'} \sum_n \frac{|\langle\psi_{\boldsymbol{k}',n}|\langle 1_{\boldsymbol{Q}}|\sum_Q V_Q(a_Q e^{i\boldsymbol{q}\cdot\boldsymbol{\rho}}e^{iq_z z} + HC)|0_{\boldsymbol{Q}}\rangle|\psi_{\boldsymbol{k},0}\rangle|^2}{E_0(\boldsymbol{k}) - E_n(\boldsymbol{k}')} \end{aligned} \tag{1.19}$$

with the substitution of the energy expressions in the denominator and using shorthand notation for the q_z dependent term, it takes the following form

$$E_k^{(2)} = -\sum_Q V_Q^2 \sum_{\boldsymbol{k}'} \sum_n \frac{|\langle\psi_{\boldsymbol{k}'}|e^{-i\boldsymbol{q}\cdot\boldsymbol{\rho}}|\psi_{\boldsymbol{k}}\rangle|^2}{\omega n + 1 + k'^2 - k^2}|h_n(q_z)|^2 \tag{1.20}$$

where the energies of ground state and intermediate states, respectively

$$E_0(\boldsymbol{k}) = \frac{1}{2}\omega + k^2 \tag{1.21}$$

$$E_n(\boldsymbol{k}^{'}) = k^2 - n\omega - k^{'2} - 1 \tag{1.22}$$

we take the electron immersed in the lowest subband ($n = 0$) and because, the current temperature is fairly lower than the LO phonons, there will be no effective phonon. Therefore it is convenient that choosing ϕ_{ph} as the phonon vacuum $|0\rangle$ for the ground state of the polaron. In Eq.(1.20), the q_z dependent term can be given as explicitly

$$\begin{aligned} h_n(q_z) &= \langle\psi_{\boldsymbol{k},n}|e^{-iq_z z}|\psi_{\boldsymbol{k},0}\rangle \\ &= \frac{(-i)^n}{\sqrt{n!}}\left(\frac{q_z^2}{\omega}\right)^{n/2}\exp\left(-\frac{q_z^2}{2\omega}\right) \end{aligned} \tag{1.23}$$

Projecting out the $\boldsymbol{k}^{'}$ summation, we obtain

$$E_k^{(2)} = -\sum_Q V_Q^2 \sum_n \frac{1}{n!}\frac{1}{\omega n + 1 + q^2 - 2\boldsymbol{k}.\boldsymbol{q}}\left(\frac{q_z^2}{\omega}\right)^n \exp\left(-\frac{q_z^2}{\omega}\right) \tag{1.24}$$

Before proceeding with calculations firstly, it is worth noting that when phonon energy is considerably small compared to the term q^2, a contribution does not make sense arising from the virtual phonons because the Q summation fall of rather rapidly. It is required that q is not extremely large to give remarkable contribution to the polaron energy. The remarkable contribution coming from the virtual phonons is obtained in case q is not too large. Secondly, in order to calculate the effective mass of the polaron, we assume that an electron moves with virtual momentum $\boldsymbol{k}$ along the x-y axis. In this respect for small electron momentum, $\boldsymbol{k}.\boldsymbol{q}$ term will be extremely small. When we make a comparison between the terms q^2 and $\boldsymbol{k}.\boldsymbol{q}$ in the denominator we can make an expansion up to second order in $\boldsymbol{k}.\boldsymbol{q}$. Then we obtain the following form from power series expansion

$$E_k^{(2)} = -\sum_Q V_Q^2\left(-\frac{q_z^2}{\omega}\right)\sum_n \frac{1}{n!}\left(\frac{q_z^2}{\omega}\right)^n\left(\frac{1}{\omega n + 1 + q^2} + \frac{(2\boldsymbol{k}.\boldsymbol{q})^2}{(\omega n + 1 + q^2)^3}\right) \tag{1.25}$$

using the identity

$$\sum_{n=0}^{\infty} \frac{1}{n!} \frac{\beta^n}{(an+b)^{m+1}} = \frac{1}{m!} \int_0^{\infty} d\eta \eta^m e^{-b\eta} \exp\left(\beta e^{-a\eta}\right) \qquad m = 0, 1, 2, ... \tag{1.26}$$

second order correction takes the form

$$\begin{aligned} E_k^{(2)} &= -\sum_Q V_Q^2 \int_0^{\infty} d\eta e^{-\eta} \exp\left[-\eta\left(q^2 + \frac{q_z^2}{\sigma}\right)\right] \\ &- \sum_Q V_Q^2 \int_0^{\infty} d\eta \eta^2 e^{-\eta} \exp\left[-\eta\left(q^2 + \frac{q_z^2}{\sigma}\right)\right] \end{aligned} \tag{1.27}$$

where

$$\sigma = \frac{\omega\eta}{1 - e^{-\omega\eta}} \tag{1.28}$$

We have managed to calculate the second order correction by solving the integrations analytically

$$\begin{aligned} E_k^2 &= -\sum_Q V_Q^2 \int_0^{\infty} d\eta e^{-\eta} \rho_Q^2 - k^2 \sum_Q V_Q^2 q^2 \int_0^{\infty} d\eta e^{-\eta} \eta^2 \rho_Q^2 \\ &= -\varepsilon_p - k^2 \mu \end{aligned} \tag{1.29}$$

where the binding energy and the phonon-related correction are given as

$$\varepsilon_p = -\sum_Q V_Q^2 \int_0^{\infty} d\eta e^{-\eta} \rho_Q^2, \qquad \mu = \sum_Q V_Q^2 q^2 \int_0^{\infty} d\eta e^{-\eta} \eta^2 \rho_Q^2 \tag{1.30}$$

We can obtain compact form of the effective mass by admitting the correction is rather small

$$m_p/m^* = (1 - \mu)^{-1} \simeq 1 + \mu \tag{1.31}$$

For the wire-like (quasi-1D) geometry one can make a modification by replacing the q_z^2 with q^2 Finally arrive at bulk polaron results which demands $\omega = 0$ and corresponding term $\sigma = 1$

$$\varepsilon_p^{3D} = \sum_Q V_Q^2 \int_0^\infty d\eta e^{1+Q^2\eta} = \sum_Q V_Q^2 \frac{1}{1+Q^2} = \alpha \tag{1.32}$$

$$\mu^{3D} = \sum_Q V_Q^2 q^2 \int_0^\infty d\eta \eta^2 e^{1+Q^2\eta} = \frac{\alpha}{6} \tag{1.33}$$

For the slab geometry (strict 2D limit) as required $\omega \to \infty$ and $\sigma^{-1} \to 0$

$$\varepsilon_p^{2D} = \sum_Q \frac{V_Q^2}{1+q^2} = \frac{\pi}{2}\alpha \tag{1.34}$$

$$\mu^{3D} = \sum_Q V_Q^2 q^2 \frac{2}{(1+q^2)^3} = \frac{\pi}{8}\alpha \tag{1.35}$$

Fig.1.1 depicts the binding energy and the phononic contribution to the effective mass as

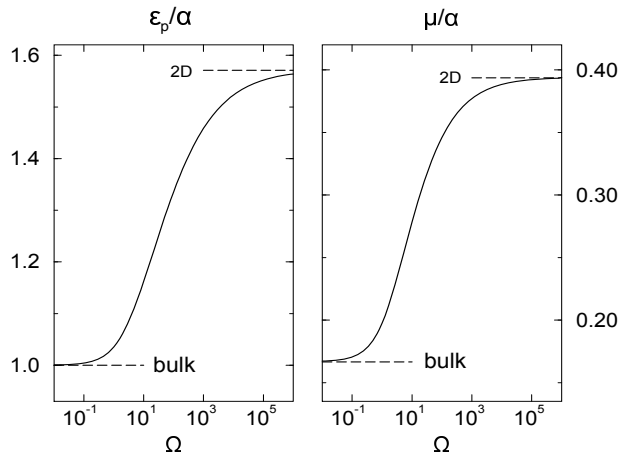

Figure 1.1. Perturbation theory results for quasi-2-dimensional polaron . The binding energy ε_p and the phonon correction to the effective mass μ as functons of the degree of confinement Ω.

a function of the degree of confinement. Dashed lines indicate that limit values of the bulk and strictly 2D geometries. It is clearly seen that, with the increasing value of the degree of confinement, both binding energy and the effective mass of the polaron are increasing.

As well as Ω and ε converges smoothly to their strict 2D values.

1.3. Strong Coupling Formalism

In strongly interacting regime where electron-phonon coupling constant is larger enough, there is a phonon field effect encloses the electron with generating a deep deformation potential. It is clear that strong coupling theory being reasonable for large α values. Looking at the earlier works were done diligently by Pekar (and others) the state of the system is denoted by product of the electronic wave function and a phonon part. The Pekar ansatz states that in the presence of large coupling, the phonons can not reach the fast-moving electrons, therefore they interact only with mean-field owing to the electronic density which is also called adiabatic approximation.
By using variational method strongly coupled confined polaron self-energy and effective mass are reviewed briefly which are considered in [12]and for Q-1D system in [13] previously. This will further give us a key insights to understand the behaviour of strongly coupled polaron in NID space. The Hamiltonian of the system is Fröhlich Hamiltonian as usual. It has been shown in Eq.(1.1) and trapping potential is in the form of $V(\boldsymbol{q}, z) = \frac{1}{4}(\beta^2\rho^2 + \mu^2 z^2)$. Ground state wave function of the polaron is written in the form of non-entangled product state by imposing product ansatz

$$\Psi_g = \Phi_e(\boldsymbol{\rho}, z)|\Phi_{ph}\rangle \tag{1.36}$$

product states of an electron states is defined as oscillator particle wavefunction as given

$$\Phi_e(\boldsymbol{\rho}, z) = N \exp\left\{\frac{1}{2}(\beta\rho^2 + \mu z^2)\right\} \exp\{i\boldsymbol{k}.\boldsymbol{r}\} \tag{1.37}$$

where $\boldsymbol{k}$ is a variational parameter sets the system in motion at the direction in which we want to calculate effective mass of the polaron will be determined later.
Here, N is the normalization constant $N = \langle\phi_e|\phi_e\rangle = (\frac{\beta}{\pi})^{1/2}\left(\frac{\mu}{\pi}\right)^{1/4}$ and β, μ are variational parameters.

Phonon ground state to be chosen as

$$|\Phi_{ph}\rangle = U|0\rangle = \exp \sum_{Q} u_Q (a_Q - a_Q^{\dagger})|0\rangle \tag{1.38}$$

rather than the bare phonon vacuum $|0\rangle$. The well known canonical transformation of the Hamiltonian is performed by the unitary operator as following

$$\tilde{H} = U^{-1} H U = e^{-S} H e^{S} \tag{1.39}$$

Modified hamiltonian through canonical transformation is obtained as

$$\tilde{H} = \nabla^2 + \sum_{Q} a_Q^{\dagger} a_Q - \sum_{Q} u_Q (a_Q^{\dagger} + a_Q) + \sum_{Q} {u_Q}^2 \tag{1.40}$$

$$+ \sum_{Q} V_Q [a_Q e^{i\boldsymbol{Q}.\boldsymbol{r}} + {a_Q}^{\dagger} e^{-i\boldsymbol{Q}.\boldsymbol{r}}] \tag{1.41}$$

The interaction amplitude is related to the electron-phonon coupling constant is defined by following expression

$$V_Q = \left(\frac{4\pi\alpha}{\vartheta_3}\right)^{1/2} \frac{1}{\sqrt{q^2 + q_z^2}} \tag{1.42}$$

$$\tag{1.43}$$

Since the Hamiltonian is invariant to translations of the electron together with accompanying phonon cloud arises from lattice deformation, the total momentum operator along the direction which is allowed free motion of polaron

$$\boldsymbol{\Pi_z} = -i\boldsymbol{\nabla} + \sum_{q_z} q_z a_{q_z}^{\dagger} a_{q_z} \tag{1.44}$$

commutes with the Hamiltonian if electron is moving freely along the z-direction. $\mathbf{\Pi_z}$ is a conserved quantity, $[\hat{\Pi}_z, \hat{H}] = 0$

$$\mathbf{\Pi_\mu} = -i\boldsymbol{\nabla} + \sum_q \boldsymbol{q} a_q^\dagger a_q \tag{1.45}$$

commutes with the Hamiltonian if electron is moving freely along the transverse direction perpendicular to the z-axis.
Under unitary transformation new form of the total momentum operator is generated as given

$$\tilde{\Pi} \rightarrow -i\boldsymbol{\nabla} + \sum_Q \boldsymbol{Q} a_Q^\dagger a_Q + \sum_Q Q u_Q^2(\phi_e) - \sum_Q Q u_Q(\phi_e)(a_Q + a_Q^\dagger) \tag{1.46}$$

After the canonical transformation, functional can be written as following form

$$\begin{aligned}
\partial F(\sigma, \upsilon; \boldsymbol{k}, u_Q) &= \langle \Psi_g | (H - \upsilon.\Pi) | \Psi_g \rangle & (1.47)\\
&= \langle \Phi_e(\boldsymbol{\rho}, z) | \langle 0 | U^{-1}(H - \upsilon.\Pi) U | 0 \rangle | \Phi_e(\boldsymbol{\rho}, z) \rangle \\
&= \langle \Phi_e | \langle 0 | - \nabla^2 + \sum_Q a_Q^\dagger a_Q + \sum_Q u_Q(a_Q + a_Q^\dagger) \\
&+ \sum_Q u_Q^2 + \sum_Q V_Q[a_Q e^{i\boldsymbol{Q}.\boldsymbol{r}} + a_Q^\dagger e^{-i\boldsymbol{Q}.\boldsymbol{r}}] \\
&- \sum_Q u_Q V_Q(e^{i\boldsymbol{Q}.\boldsymbol{r}} + e^{-i\boldsymbol{Q}.\boldsymbol{r}}) - \boldsymbol{\upsilon}.\boldsymbol{p} - \sum_Q \boldsymbol{\upsilon}.\boldsymbol{Q} a_Q^\dagger a_Q \\
&+ \sum_Q \boldsymbol{\upsilon}.\boldsymbol{Q} u_Q(a_Q + a_Q^\dagger) - \sum_Q \boldsymbol{\upsilon}.\boldsymbol{Q} u_Q^2 |0\rangle | \Phi_e \rangle & (1.48)
\end{aligned}$$

Variational procedure requires an optimization of the polaron state Ψ_g which minimizes $\langle \Psi_g | H | \Psi_g \rangle$ subject to the constraint that $\langle \Psi_g | \mathbf{\Pi} | \Psi_g \rangle$ is a constant of motion. Complete form of the Hamiltonian is determined by minimizing Eq.(1.47) by setting

$$\frac{\partial F(\sigma, \upsilon; \boldsymbol{k}, u_Q)}{u_Q} = 0, \qquad \frac{\partial F(\sigma, \upsilon; \boldsymbol{k}, u_Q)}{k} = 0 \tag{1.49}$$

with the minimization conditions we obtain the following optimal fits for $\boldsymbol{k}$ and u_Q,

$$\boldsymbol{k} = \frac{\boldsymbol{v}}{\sqrt{\sigma}}, \qquad u_Q(\Phi_e) = V_Q s_Q \rho_Q \tag{1.50}$$

where shorthand notations are introduced as

$$\rho_Q = (1 - \boldsymbol{v}.\boldsymbol{Q})^{-1}, \qquad s_Q = \langle \phi_e | \exp \pm (i\boldsymbol{q}.\boldsymbol{\rho} + iq_z z) | \phi_e \rangle \tag{1.51}$$

explicit form of the s_Q is given as

$$s_Q = e^{-q^2/2\beta} e^{-q_z^2/2\mu} \tag{1.52}$$

substituting the optimal fits $\boldsymbol{k}$ and u_Q back into (1.47) leads to arrive at final form of the Hamiltonian $\tilde{H}$ and total momentum Π

$$\begin{aligned} \tilde{H} &= \nabla^2 + \sum_Q a_Q^\dagger a_Q + \sum_Q V_Q^2 s_Q^2 \rho_Q^2 - \sum_Q V_Q^2 s_Q \rho_Q (e^{i\boldsymbol{Q}.\boldsymbol{r}} + e^{-i\boldsymbol{Q}.\boldsymbol{r}}) \\ &+ \sum_Q V_Q (\eta_Q a_Q + \eta_Q^* a_Q^\dagger) \end{aligned} \tag{1.53}$$

in which

$$\eta_Q = e^{i\boldsymbol{Q}.\boldsymbol{r}} - s_Q \rho_Q \tag{1.54}$$

modified total momentum takes the form

$$\begin{aligned} \tilde{\boldsymbol{\Pi}} &= i\boldsymbol{\nabla} + \sum_Q \boldsymbol{Q} a_Q^\dagger a_Q + \sum_Q \boldsymbol{Q} V_Q^2 s_Q^2 \rho_Q^2 \\ &- \sum_Q \boldsymbol{Q} V_Q s_Q \rho_Q (a_Q + a_Q^\dagger) \end{aligned} \tag{1.55}$$

$$E_g = \varepsilon_k - \sum_Q V_Q^2 s_Q^2 \tag{1.56}$$

A simple calculation gives kinetic energy of the electron

$$\varepsilon_k = \frac{1}{2}\left(\frac{\omega_1}{\beta}\right)^2 + \frac{1}{4}\left(\frac{\omega_2}{\mu}\right)^2 + \frac{\beta^2}{2} + \frac{\mu^2}{4} \tag{1.57}$$

and the second term in eq (1.56) gives

$$\begin{aligned} & \sum_Q V_Q^2 s_Q^2 \\ = \; & \frac{\vartheta_3}{(2\pi)^3}\int_0^\infty \int_{-\infty}^\infty \int_0^{2\pi} q dq dq_z d\phi V_Q^2 s_Q^2 \\ = \; & \frac{\alpha}{\sqrt{\pi}}\sqrt{\frac{\beta\mu}{\mu-\beta}}\arctan\sqrt{\frac{\mu}{\beta}-1} \end{aligned} \tag{1.58}$$

as a result we obtain the ground state energy of polaron

$$\begin{aligned} E_g \; = \; & \frac{1}{2}\left(\frac{\omega_1}{\beta}\right)^2 + \frac{1}{4}\left(\frac{\omega_2}{\mu}\right)^2 + \frac{\beta^2}{2} + \frac{\mu^2}{4} \\ - \; & \frac{\alpha}{\sqrt{\pi}}\sqrt{\frac{\beta\mu}{\mu-\beta}}\arctan\sqrt{\frac{\mu}{\beta}-1} \end{aligned} \tag{1.59}$$

and the binding energy

$$\varepsilon_p = \omega_1 + \frac{1}{2}\omega_2 - E_g \tag{1.60}$$

As mentioned before if there is no confinement namely $\omega_1 = \omega_2 = 0$, we will reach the bulk value (3D) of the binding energy. It should be noted that, bulk value limit brings about equality $E_g^{3D} = \varepsilon_p^{3D} = \alpha^2/3\pi$. Starting to adjust ω_1 and ω_2 leads to draw a character of the polaron in low dimensional systems. Fixing the $\omega_1 = 0$ which represents the confinement along z-axis and increasing the ω_2, allows us to find out binding energy of quasi-2D (Q2D) slab-like system. When ω_2 goes to infinity strictly 2D structure is obtained. The value for the binding energy of Q2D polaron is $\varepsilon_p^{(2D)} = \alpha^2/8\pi$. Applying

reverse of the condition that we mentioned, binding energy of the quasi one dimensional (Q1D) systems is obtained. Seting the $\omega_2 = 0$ means that there is no confinement in the x-y axis and varying the ω_1 from zero to infinity embeds the polaron into the Q1D systems. We are not talking about the strictly 1D system because when ω_1 goes to the infinity the binding energy diverges.

- **Effective Mass of Polaron ($m_p^{(3D)}, m_p^{(\rho)}, m_p^{(z)}$)**
  Here, we show the expression of the polaron effective mass for different geometries. For spherical or bulk geometry value of the effective mass is given as

$$1 + \chi_0 = 1 + \frac{2\alpha}{3\sqrt{\pi}}\sigma^{3/2} \simeq \frac{16}{81\pi^2}\alpha^4 \tag{1.61}$$

  where we take the dimensionality D=3 for the 3D mass and the quantity $\chi_0 = \frac{4}{D}\sum_Q Q^2 V_Q^2 s_Q^2$.

$$\begin{aligned}\frac{4}{D}\sum_Q V_Q^2 s_Q^2 q_z^2 &= \frac{4\alpha}{\pi}\int_0^\infty q exp\left(\frac{-q^2}{\beta}\right)dq \int_{-\infty}^\infty \frac{q_z^2}{q^2+q_z^2} exp\left(\frac{-q_z^2}{\mu}\right)dq_z \\ &= 2\alpha\left(\frac{\beta^2\mu^3}{\pi}\right)^{1/2} \\ &\quad \times\frac{1}{\mu-\beta}\left[1-\left(\frac{\mu}{\beta}-1\right)^{1/2}\arctan\left(\frac{\mu}{\beta}-1\right)^{1/2}\right]\end{aligned} \tag{1.62}$$

  Assuming that polaron moves freely through the z-axis, we can evaluate the $m_p^{(z)}/m$

$$\begin{aligned}m_p^{(z)}/m &= 1 + 2\alpha\left(\frac{\beta^2\mu^3}{\pi}\right)^{1/2} \\ &\quad \times\frac{1}{\mu-\beta}\left[1-\left(\frac{\mu}{\beta}-1\right)^{1/2}\arctan\left(\frac{\mu}{\beta}-1\right)^{1/2}\right]\end{aligned} \tag{1.63}$$

Since, polaron acts freely in one dimension we take D=1. For the polaron moving in along perpendicular axes to the z-coordinate m_p^{xy}

$$\begin{aligned} 2\sum_Q V_Q^2 s_Q^2 q^2 &= \frac{2\alpha}{\pi}\int_0^\infty q^3 exp\left(-\frac{q^2}{\beta}\right)dq \int_{-\infty}^\infty \frac{1}{q^2+q_z^2} exp\left(-\frac{q_z^2}{\mu}\right)dq_z \\ &= \alpha\left(\frac{\beta^2\mu^3}{\pi}\right)^{1/2} \\ &\quad \times\frac{1}{\mu-\beta}\left[\left(\frac{\beta}{\mu}-\beta\right)^{-1/2}\arctan\left(\frac{\mu}{\beta}-1\right)^{-1/2}-\frac{\beta}{\mu}\right] \quad (1.64) \end{aligned}$$

for the polaron moves freely along the xy-axis, we obtain the values of $m_p^{(xy)}/m$ as given below

$$\begin{aligned} m_p^{(xy)}/m &= 1+\alpha\left(\frac{\beta^2\mu^3}{\pi}\right)^{1/2} \\ &\quad \times\frac{1}{\mu-\beta}\left[\left(\frac{\beta}{\mu}-\beta\right)^{-1/2}\arctan\left(\frac{\mu}{\beta}-1\right)^{-1/2}-\frac{\beta}{\mu}\right] \quad (1.65) \end{aligned}$$

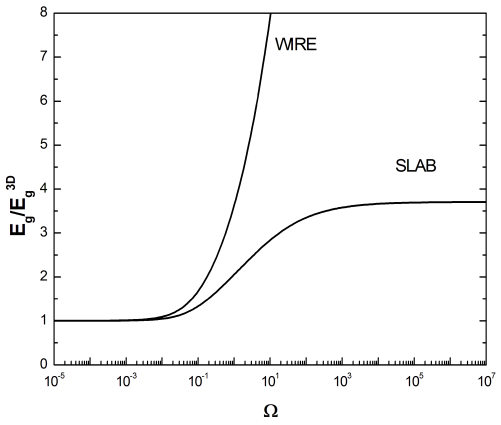

Figure 1.2. The ground energy against the degree of confinement for the slab-like ($\Omega_1 = 0$) and the wire-like ($\Omega_2 = 0$) configurations.

In fig.1.2 we show the results of the ground energy as a function of the degree of confinement taking into account both wire and slab-like configurations respectively. We find that with increase of the anisotropy, binding energy shows a sharp increase in wire ge-

ometry compared to the slab-like geometry. The reason of the difference in strength of the electron phonon coupling stems from the fact that in the wire geometry the polaron cloud is confined along the wire axis in all transverse directions. Confinement applied to the polaron cloud in wire geometry leads to not only much stronger electron phonon interaction but also much larger value of the binding energy than in the 2D geometry.

1.4. Arbitrary Coupling Formalism

Ground state properties of weak and strongly coupled polaron in confined geometry, have been summarized briefly in the last two sections. Strong coupling polaron theory is inadequate to describe the behaviour of the confined polaron at small α values. Likewise a pure perturbation treatment is not found to be suitable for reflecting characterization of the confined polaron at large α values. Therefore we need to a well-developed approach to solve the bulk polaron problem as taking consideration of its weak and strong coupling counterparts simultaneously. From now on one can follow a different method to get polaronic properties.

In this part we are tempted to formulate an all-coupling variational calculation based on Lee-Low-Pines (LLP) transformation [14] is performed to study the ground state in an anisotropic harmonic oscillator-type confining potential that is valid for the whole range of the electron phonon coupling constant. In order to achieve extended formalism, variational method should be used in conjunction with perturbation theory called perturbative variational approach used previously by Devreese *et al*.[15]. Variational perturbative method has been applied to in modelling 3D and 2D free polarons [16], quasi-1D polarons[17], 2D model of a magnetopolaron[18] and 3D and 2D bipolarons[19]. This methodology which interrelates the strong and weak coupling approaches, is based on extension of the adiabatic polaron state includes modified variational wavefunction by approximate first order perturbative correction. Taking into account simplifications that as mentioned before we focus on the derivation of analytical expressions for ground state energy and effective mass where electron completely confined within a quasi one dimensional(Q1D) and quasi two dimensional (Q2D) geometries.

If we are only dealing with strong coupling case, it is capable for going to do optimization (1.47) with respect to σ. But we want to get a generalized expression that covering all α values. Therefore, there will be a contribution to the energy and mass of the ground state which arises from small α domain. In order to make required calculations,

we are inspired by the studies [17, 20, 21]. Here, we focus on how to obtain the definition of an altered adiabatic polaron trial state related to variational scheme so as to cover the overall range of the coupling strength. Perturbative variational approach allows us to reconstruct shape of the trial state

$$\begin{aligned} |\tilde{\Psi}_g\rangle &= c|\Psi_g\rangle + \sum_Q V_Q \sum_i |i\rangle \frac{\langle i|(\exp(-i\boldsymbol{Q}.\boldsymbol{r}) - s_Q)a_Q^\dagger|0\rangle}{\Delta_{\varepsilon_{i-g}}} \\ &= c|0\rangle + \sum_Q V_Q g_Q (\exp(-i\boldsymbol{Q}.\boldsymbol{r}) - s_Q)a_Q^\dagger|\Psi_g\rangle \end{aligned} \tag{1.66}$$

where variational quantity $g_Q = \left\langle \frac{1}{\Delta_{\varepsilon_{i-g}}} \right\rangle_i$. It is rather difficult to calculate all the contributions coming from the intermediate states. Here we avoid such difficulty by replacing the denominator with average quantity. The new wave function which is determined by using perturbation theory, requires normalization. Normalized wave function corresponds to another constraint, interconnecting the parameters c and g_Q over the following normalization procedure

$$\begin{aligned} \langle\tilde{\Psi}_g|\tilde{\Psi}_g\rangle &= \langle\Psi_g|c + \langle\Psi_g| \sum_Q V_Q g_Q (e^{i\boldsymbol{Q}.\boldsymbol{r}} a_Q - s_Q) \sum_Q V_Q g_Q (e^{-i\boldsymbol{Q}.\boldsymbol{r}} - s_Q)a_Q^\dagger|0\rangle + c|\Psi_g\rangle \\ &= c^2\langle\Psi_g|\Psi_g\rangle + \sum_Q V_Q g_Q \sum_{Q'} V_{Q'} g_{Q'} \langle\Psi_g|(e^{i\boldsymbol{Q}.\boldsymbol{r}} - s_Q)(e^{-i\boldsymbol{Q'}.\boldsymbol{r}} - s_{Q'})a_Q a_{Q'}^\dagger|\Psi_g\rangle \\ &= c^2 + \sum_Q V_Q^2 g_Q^2 h_Q = 1 \end{aligned} \tag{1.67}$$

where h_Q denotes

$$h_Q = \langle 0|(e^{i\boldsymbol{Q}.\boldsymbol{r}} - s_Q)(e^{-i\boldsymbol{Q}.\boldsymbol{r}} - s_Q)|0\rangle \tag{1.68}$$

$$= 1 - s_Q^2 \tag{1.69}$$

Note that phonon operators obey the usual commutation relation $[a_Q, a_{Q'}^\dagger] = \delta_{QQ'}$. The result of the normalization displays the dependence on the terms g_Q and c accordingly we

may utilize the constraint as

$$f(c, g_Q) = c^2 + \sum_Q V_Q^2 g_Q^2 h_Q - 1 = 0 \tag{1.70}$$

The expectation value

$$\langle\tilde{\Psi}_g|\tilde{H} - \boldsymbol{\upsilon}.\tilde{\boldsymbol{\Pi}}|\tilde{\Psi}_g\rangle \;\; = \;\; \langle\tilde{\Psi}_g|\tilde{H}|\tilde{\Psi}_g\rangle - \langle\tilde{\Psi}_g|\boldsymbol{\upsilon}.\tilde{\boldsymbol{\Pi}}|\tilde{\Psi}_g\rangle \tag{1.71}$$

in the trial state Eq.(1.66). The first term in the equation is nothing more than binding energy energy and second term is the additional kinetic contribution, helps us to derive the expression of the effective mass. Let's calculate the expectation value of the$\langle\tilde{\Psi}_g|\tilde{H}|\tilde{\Psi}_g\rangle$step by step.
First determine the kinetic energy of the bare electron in in the new trial state $\langle\tilde{\Psi}_g|\tilde{H}|\tilde{\Psi}_g\rangle$ by using Eq.(1.53)

$$\langle\tilde{\Psi}_g|p^2|\tilde{\Psi}_g\rangle = c^2\langle 0|p^2|0\rangle + \sum_Q V_Q^2 g_Q^2 e_Q \tag{1.72}$$

where the momentum is given as $\vec{p} = \vec{\nabla} + \frac{1}{2}\vec{v}$ and the expectation values of p^2 in extended variational wavefunction is obtained as the following

$$\langle\tilde{\Psi}_g|p^2|\tilde{\Psi}_g\rangle \;\; = \;\; c^2\Big(e_0 + \frac{\upsilon^2}{4}\Big) + c^2\langle\Psi_g|\vec{v}.\vec{\nabla}|\Psi_g\rangle + \sum_Q V_Q^2 g_Q^2 e_Q \tag{1.73}$$

Furthermore, the expectation value of the phononic term in the $\tilde{\Psi_g}$ gives

$$\langle\tilde{\Psi}_g|\sum_Q a_Q^\dagger a_Q|\tilde{\Psi}_g\rangle = \sum_Q V_Q^2 g_Q^2 h_Q \tag{1.74}$$

Expectation values of the remaining terms are calculated in the same way

$$\langle\tilde{\Psi}_g|\sum_Q V_Q[(e^{i\boldsymbol{Q}.\boldsymbol{r}}-s_Q\rho_Q)a_Q+(e^{-i\boldsymbol{Q}.\boldsymbol{r}}-s_Q\rho_Q)a_Q^\dagger]|\tilde{\Psi}_g\rangle=2c\sum_Q V_Q^2 g_Q h_Q \quad (1.75)$$

and the next term is calculated as the following

$$\langle\tilde{\Psi}_g|\sum_Q V_Q^2 s_Q^2\rho_Q^2|\tilde{\Psi}_g\rangle=c^2\sum_Q V_Q^2 s_Q^2\rho_Q^2+\sum_Q V_Q^2 g_Q^2 h_Q\sum_{Q'} V_{Q'}^2 s_{Q'}^2\rho_{Q'}^2 \quad (1.76)$$

finally, the last term is obtained as follows

$$\begin{aligned}
&\langle\tilde{\Psi}_g|\sum_Q V_Q^2 s_Q^2\rho_Q(e^{i\boldsymbol{Q}.\boldsymbol{r}}+e^{-i\boldsymbol{Q}.\boldsymbol{r}})|\tilde{\Psi}_g\rangle\\
=\;& 2c^2\sum_Q V_Q^2 s_Q^2\rho_Q+\sum_Q V_Q^2 g_Q^2\sum_{Q'} V_{Q'}^2 s_{Q'}\rho_{Q'}\Delta_{QQ'}\\
=\;& 2c^2\sum_Q V_Q^2 s_Q^2\rho_Q+\sum_Q V_Q^2 g_Q^2\delta_{QQ'} \qquad (1.77)
\end{aligned}$$

Remaining terms displays corrections brought about by the extended formalism to the effective mass of the polaron. Additional kinetic contribution is calculated step by step as making for binding energy. The explicit form of $\langle\tilde{\Psi}_g|\boldsymbol{v}.\tilde{\boldsymbol{\Pi}}|\tilde{\Psi}_g\rangle$ can be written

$$\begin{aligned}
&\langle\tilde{\Psi}_g|\boldsymbol{v}.\tilde{\boldsymbol{\Pi}}|\tilde{\Psi}_g\rangle\\
=\;&\langle\tilde{\Psi}_g|\boldsymbol{v}.\boldsymbol{p}|\tilde{\Psi}_g\rangle\\
+\;&\langle\tilde{\Psi}_g|\sum_Q \boldsymbol{v}.\boldsymbol{Q}a_Q^\dagger a_Q|\tilde{\Psi}_g\rangle\\
+\;&\langle\tilde{\Psi}_g|\sum_Q \boldsymbol{v}.\boldsymbol{Q}V_Q^2 s_Q^2\rho_Q^2|\tilde{\Psi}_g\rangle\\
-\;&\langle\tilde{\Psi}_g|\sum_Q \boldsymbol{v}.\boldsymbol{Q}V_Q s_Q\rho_Q(a_Q+a_Q^\dagger)|\tilde{\Psi}_g\rangle \qquad (1.78)
\end{aligned}$$

First term of the Eq.(1.78) gives

$$\begin{aligned} & \langle\tilde{\Psi}_g|\boldsymbol{v}.\boldsymbol{p}|\tilde{\Psi}_g\rangle \\ = \; & c^2\langle\Psi_g|\boldsymbol{v}.\boldsymbol{\nabla}|\Psi_g\rangle + \frac{1}{2}c^2v^2 \\ + \; & \sum_Q V_Q^2 g_Q^2 \langle 0|(e^{i\boldsymbol{Q}.\boldsymbol{r}} - s_Q)\boldsymbol{v}.\boldsymbol{\nabla}(e^{-i\boldsymbol{Q}.\boldsymbol{r}} - s_Q)|0\rangle \\ + \; & \frac{1}{2}v^2 \sum_Q V_Q^2 g_Q^2 h_Q \end{aligned} \tag{1.79}$$

and the second term

$$\langle\tilde{\Psi}_g|\sum_Q \boldsymbol{v}.\boldsymbol{Q}a_Q^\dagger a_Q|\tilde{\Psi}_g\rangle = \sum_Q \boldsymbol{v}.\boldsymbol{Q}V_Q^2 g_Q^2 h_Q \tag{1.80}$$

the third term

$$\begin{aligned} & \langle\tilde{\Psi}_g|\sum_Q \boldsymbol{v}.\boldsymbol{Q}V_Q^2 s_Q^2 \rho_Q^2|\tilde{\Psi}_g\rangle \\ = \; & c^2 \sum_Q \boldsymbol{v}.\boldsymbol{Q}V_Q^2 s_Q^2 \rho_Q^2 \\ + \; & \sum_Q V_Q^2(D) g_Q^2 h_Q \sum_{Q'} \boldsymbol{v}.\boldsymbol{Q'}V_{Q'}^2 s_{Q'}^2 \rho_{Q'}^2 \end{aligned} \tag{1.81}$$

The last term in Eq.(1.82) gives no contribution to the functional

$$\langle\tilde{\Psi}_g|\sum_Q \boldsymbol{v}.\boldsymbol{Q}V_Q s_Q \rho_Q (a_Q + a_Q^\dagger)|\tilde{\Psi}_g\rangle = 0 \tag{1.82}$$

By combining the results of these equations expectation value of $\langle\tilde{\Psi}_g|\tilde{H} - \boldsymbol{v}.\tilde{\boldsymbol{\Pi}}|\tilde{\Psi}_g\rangle$ in modified trial state called functional, takes the complete form as a result of our calculations, is given below

$$\begin{aligned}\Phi(\sigma,\upsilon;c,g_Q) &= c^2(e_0+\frac{1}{4}\upsilon^2)-\frac{1}{2}\upsilon^2+\sum_Q V_Q^2 g_Q^2(e_Q-\delta_{QQ'}+h_Q)\\ &+ \chi(1-2c^2)+2c\sum_Q V_Q^2 g_Q h_Q \end{aligned} \tag{1.83}$$

where

$$\begin{aligned} e_Q &= \langle\phi_e|(e^{i\boldsymbol{Q}.\boldsymbol{r}}-s_Q)(-\nabla^2)(e^{-i\boldsymbol{Q}.\boldsymbol{r}}-s_Q)|\phi_e\rangle \\ &= \frac{1}{2}Q^2+(e_0+\frac{1}{2}Q^2)h_Q \end{aligned} \tag{1.84}$$

with

$$\begin{aligned} e_0 &= \langle\Phi_e|-\nabla^2+V(\boldsymbol{\rho},z)|\Phi_e\rangle \\ e_0 &= \frac{1}{2}\left(\frac{\omega_1}{\beta}\right)^2+\frac{1}{4}\left(\frac{\omega_2}{\mu}\right)^2+\frac{\beta^2}{2}+\frac{\mu^2}{4} \end{aligned} \tag{1.85}$$

and furthermore,

$$\chi = \sum_Q V_Q^2 s_Q^2 \rho_Q \tag{1.86}$$

$$\delta_Q = \sum_{Q'} V_{Q'}^2 s_{Q'} \Delta_{QQ'} \rho_{Q'} \tag{1.87}$$

wherein

$$\Delta_{QQ'} = \langle 0|(e^{i\boldsymbol{Q}.\boldsymbol{r}}-s_Q)(e^{i\boldsymbol{Q'}.\boldsymbol{r}}+e^{-i\boldsymbol{Q'}.\boldsymbol{r}})(e^{-i\boldsymbol{Q}.\boldsymbol{r}}-s_Q)|0\rangle \tag{1.88}$$

By following the variational procedure, minimization of the expectation value $\langle\tilde{\Psi}_g|\tilde{H}-\boldsymbol{\upsilon}.\tilde{\boldsymbol{\Pi}}|\tilde{\Psi}_g\rangle$ in the trial state is required to find optimal fit to g_Q and to the normalization constant c subject to the constraint (1.70) .

The variational fit to g_Q and to the normalization constant c actualized by providing the

condition below

$$\frac{\partial}{\partial g_Q}\{\Phi(\sigma,\upsilon;c,g_Q)-\Lambda f(c,g_Q)\}=0 \qquad \frac{\partial}{\partial c}\{\Phi(\sigma,\upsilon;c,g_Q)-\Lambda f(c,g_Q)\}=0 \tag{1.89}$$

where we use Lagrange multiplier method.
We obtain

$$g_Q=\frac{ch_Q}{\Lambda h_Q-(e_Q-\delta_Q+h_Q)} \tag{1.90}$$

$$c=\frac{\sum_Q V_Q^2 g_Q h_Q}{\Lambda-e_0-\frac{1}{4}\upsilon^2+2\chi} \tag{1.91}$$

Lagrange multiplier Λ is derived through the transcendental equation

$$\begin{aligned}\Lambda &= \sum_Q V_Q^2\left(\frac{g_Q}{c}\right)h_Q \\ &= -\sum_Q \frac{V_Q^2 {h_Q}^2}{(1-\Lambda+2\chi-e_0-\frac{1}{4}\upsilon^2)h_Q+e_Q-\delta_Q} \\ &= -\sum_Q \frac{V_Q^2 {h_Q}^2}{D_Q}\end{aligned} \tag{1.92}$$

in which

$$\frac{g_Q}{c}=-\frac{h_Q}{D_Q} \tag{1.93}$$

and the term D_Q is given as below

$$D_Q=(1-\Lambda+2\chi-e_0-\frac{1}{4}\upsilon^2)h_Q+e_Q-\delta_Q \tag{1.94}$$

further the functional form of quantities e_0, s_Q and $\chi^{(0)}$ are given in (1.94) which are

identical with the expressions of quantities obtained from strong coupling theory

Furthermore, we obtain

$$\Phi(\sigma,\upsilon) = E_g(\sigma) - \frac{1}{4}\upsilon^2 m_p \tag{1.95}$$

where

$$E_g \;=\; e_0 - \chi^{(0)} + \Lambda \tag{1.96}$$

refers to the ground state energy which is derived before via strong coupling theory with only one difference is lambda. We are going to get more approximate value is valid for whole alpha values with contribution comes from lambda. Ground state energy is written by substituting the explicit form of the Λ is derived through the transcendental equation.

$$\begin{aligned} E_g &= \frac{1}{2}\left(\frac{\omega_1}{\beta}\right)^2 + \frac{1}{4}\left(\frac{\omega_2}{\mu}\right)^2 + \frac{\beta^2}{2} + \frac{\mu^2}{4} \\ &- \frac{\alpha}{\sqrt{\pi}}\sqrt{\frac{\beta\mu}{\mu-\beta}}\arctan\sqrt{\frac{\mu}{\beta}-1} - \frac{\alpha}{\pi}\int_0^\infty\int_{-\infty}^\infty \frac{1}{q^2+q_z^2}\frac{h_Q^2}{D_Q^{(0)}} qdqdqz \end{aligned} \tag{1.97}$$

In here, the functional form of the quantity $\chi^{(0)}$ is

$$\chi^{(0)} = \frac{\alpha}{\sqrt{\pi}}\sqrt{\frac{\beta\mu}{\mu-\beta}}\arctan\sqrt{\frac{\mu}{\beta}-1} \tag{1.98}$$

same with the strong coupling result. The velocity independent terms are collected in Eq.(1.94) as follows

$$D_Q^{(0)} = e_Q^{(0)} - \delta_Q^{(0)} + (1 - e_0 + 2\chi^{(0)} - \Lambda)h_Q \tag{1.99}$$

with the explicit form of the $\delta_Q^{(0)}$

$$\begin{aligned}
\delta_Q^{(0)} &= 2\chi^0(1+s_Q^2) - 2s_Q \sum_{Q'} V_{Q'}^2 s_{Q'}(s_{Q\pm Q'}) \\
&= 2\chi^0(1+s_Q^2) - 2s_Q \frac{2\alpha}{\pi} s_Q \int_0^\infty \exp\left(\frac{-q^{'2}}{\beta}\right) I_0\left(\frac{qq^{'}}{\beta^2}\right) q^{'} dq^{'} \\
&\quad \times \int_{-\infty}^{\infty} \exp\left(\frac{-q_z^{'2}}{\nu}\right) \exp\left(\frac{q_z q_z^{'}}{\nu}\right) \frac{1}{q^{'2}+q_z^{'}} dq_z^{'} \\
&= 2\chi^0(1+s_Q^2) - s_Q^2 \frac{4\alpha}{\pi} \int_0^\infty \exp\left(\frac{-q^{'2}}{\beta}\right) I_0\left(\frac{qq^{'}}{\beta^2}\right) q^{'} dq^{'} \\
&\quad \times \int_{-\infty}^{\infty} \exp\left(\frac{-q_z^{'2}}{\nu}\right) \exp\left(\frac{q_z q_z^{'}}{\nu}\right) \frac{1}{q^{'2}+q_z^{'}} dq_z^{'}
\end{aligned} \tag{1.100}$$

- **Effective Mass of Polaron ($m_p^{(z)}$, $m_p^{(\rho)}$)**

  General formulation of the effective mass

$$m_p = 1 + \chi^{(1)} + \sum_Q \frac{V_Q^2 h_Q^2}{D_Q^{(0)}} \left[\frac{4}{D} Q^2 \left(\frac{h_Q}{D_Q^{(0)}} \right)^2 + \frac{\delta_Q^{(1)} - 2\chi^{(1)} h_Q}{D_Q^{(0)}} \right] \tag{1.101}$$

  effective mass equation for the polaron moves along the z-axis

$$m_p^{(z)} = 1 + \chi_z^{(1)} + \sum_Q \frac{V_Q^2 h_Q^2}{D_{q_z}^{(0)}} \left[\frac{4}{D} q_z^2 \left(\frac{h_Q}{D_{q_z}^{(0)}} \right)^2 + \frac{\delta_{q_z}^{(1)} - 2\chi_z^{(1)} h_Q}{D_{q_z}^{(0)}} \right] \tag{1.102}$$

  where

$$\begin{aligned}
\delta_{q_z}^{(1)} &= 2\chi_z^{(1)}(1+s_Q^2) \\
&- \frac{8\alpha}{\pi} s_Q^2 \int_0^\infty \exp\left(\frac{-q^{'2}}{\beta}\right) \mathrm{I}_0\left(\frac{qq^{'}}{\beta^2}\right) q^{'} dq^{'} \\
&\quad \times \int_{-\infty}^{\infty} \exp\left(\frac{-q_z^{'2}}{\mu}\right) \exp\left(\frac{q_z q_z^{'}}{\mu}\right) \frac{q_z^{'2}}{q^{'2}+q_z^{'2}}
\end{aligned} \tag{1.103}$$

and effective mass equation for the polaron lies through the xy-axis

$$m_p^{(xy)} = 1 + \chi_{xy}^{(1)} + \sum_Q \frac{V_Q^2 h_Q^2}{D_q^{(0)}} \left[\frac{4}{D} q^2 \left(\frac{h_Q}{D_q^{(0)}} \right)^2 + \frac{\delta_q^{(1)} - 2\chi_{xy}^{(1)} h_Q}{D_q^{(0)}} \right] \quad (1.104)$$

where

$$\begin{aligned} \delta_q^{(1)} &= 2\chi_{xy}^{(1)}(1 + s_Q^2) \\ &- \frac{8\alpha}{\pi} s_Q^2 \int_0^\infty \exp\left(\frac{-q^{'2}}{\beta} \right) \mathrm{I}_0 \left(\frac{qq^{'}}{\beta} \right) q^{'3} dq^{'} \\ &\times \int_{-\infty}^\infty \exp\left(\frac{-q_z^{'2}}{\mu} \right) \exp\left(\frac{q_z q_z^{'}}{\mu} \right) \frac{1}{q^{'2} + q_z^{'2}} \end{aligned} \quad (1.105)$$

CHAPTER 2

NON-INTEGER DIMENSIONAL SPACE (NIDS)

In this chapter, we will analyse algebra of non-integer dimensional space.

2.1. Calculus in NIDS

In principle it is possible to construct different mathematical formalisms for non-integer dimensional (NID) spaces, all of which behaving like a conventional Euclidean vector space when D is a positive integer. There are no other criteria to distinguish between the validity of alternative approaches except for the ability to combine simplicity and utility in a self-compatible formalism. Such a mathematically concrete realization of NID spaces is presented by Stillenger [22]. Several studies about confinement effects on electron-phonon interaction [23], excitonic polarons [24], polaronic exciton [25], polaron effects [5, 26] and magnetic polarons [27] have used the formulation of Stillenger for NIDS. We will stand on a structure of NID space a little bit and then give a short review of which is required to the notation and for the sake of completeness.
S indicates the space of interest and contains points x,y,... where the distance between x and y is written as r(x,y). Particularly

$$r(x) \equiv r(x, 0) \tag{2.1}$$

denotes the distance of x to some origin 0. S_D being a metric space, r(x,y) ensures the conventional criteria required of metrics. It is shown that S_D normally is not a vector space. Vector addition is allowed in ordinary Euclidean spaces as

$$\boldsymbol{u} = \boldsymbol{x} + b\boldsymbol{y} \tag{2.2}$$

and the resultant vector takes place in Euclidean space. Since any vector space must have a finite integer, or infinite number of basis vectors, it has to be rejected for non-integer D.

Therefore it not possible to define vectors and vector algebra on S_D. But however, still it is possible to introduce the angle θ between two line segments, by the use of 'cosine law'

$$cos\theta(\boldsymbol{x},\boldsymbol{y}) = \frac{r^2(\boldsymbol{x}) + r^2(\boldsymbol{y}) - r^2(\boldsymbol{x},\boldsymbol{y})}{2r(\boldsymbol{x})r(\boldsymbol{y})} \tag{2.3}$$

Then the projection of $\boldsymbol{x}$ along $(\boldsymbol{y},\boldsymbol{0}), p(\boldsymbol{x},\boldsymbol{y})$ and the orthogonal component $l(\boldsymbol{x},\boldsymbol{y})$are defined through

$$p(\boldsymbol{x},\boldsymbol{y}) = r(\boldsymbol{x})cos\theta(\boldsymbol{x},\boldsymbol{y}) \tag{2.4}$$

$$l(\boldsymbol{x},\boldsymbol{y}) = \sqrt{r^2(\boldsymbol{x}) - p^2(\boldsymbol{x},\boldsymbol{y}) = r(\boldsymbol{x})sin\theta(\boldsymbol{x},\boldsymbol{y})} \tag{2.5}$$

At this point, the way dealing with the vectorial terms which are contained in Fröhlich Hamiltonian namely $\boldsymbol{Q.r}$ in S_D arises naturally. Dot product operation simply meaning the projection of a vector on another, we will let;

$$\vec{Q}.\vec{r} = Q.r.cos\theta \rightarrow \boldsymbol{qr} = p(\boldsymbol{q},\boldsymbol{r})r(\boldsymbol{r}) = r(\boldsymbol{q})r(\boldsymbol{r})cos\theta(\boldsymbol{q},\boldsymbol{r}) \tag{2.6}$$

and the representation of the Hamiltonian be modified correspondingly, where now both $\boldsymbol{q}$ and $\boldsymbol{r}$ are D-dimensional.
It is necessary for us to define integration in S_D. For radially symmetric functions it turns out to be

$$\int d^D\boldsymbol{x} f[r(\boldsymbol{x})] = \int_0^\infty dr W_D(r) f(r) \tag{2.7}$$

where $W_D(r)$ is the D-dimensional weight function given by

$$W_D(r) = \sigma(D) r^{D-1} \sigma(D) = \frac{2\pi^{D/2}}{\Gamma(D/2)} \tag{2.8}$$

Γ being the gamma function. For coherent modeling it is necessary to define derivatives and integrals of fractional order. Besides it is straightforward using fractional integration to comprehend features of the fractal medium.
In our calculations we also require integrals of the kind

$$I(k) = \int d^D \boldsymbol{x} \exp(-\alpha r^2(\boldsymbol{x}) + i\boldsymbol{k}\boldsymbol{r}) \tag{2.9}$$

which is the Fourier transform of a Gaussian function in S_D. The result is also barrowed from [22]

$$I(k) = \left(\frac{\Pi}{a}\right)^{D/2} \exp\left(\frac{-k^2}{4a}\right)$$

with k standing for $r(\boldsymbol{k})$as from now on we will denote $r(\boldsymbol{x})$ simply by x.
Finally we will conclude this section by stating the Laplacian operator in S_D .

$$\nabla_D^2 f(r,\theta) = \left[\frac{\partial^2}{\partial r^2} + \frac{D-1}{r}\frac{\partial}{\partial r} + \frac{1}{r^2 \sin^{D-2}\theta}\frac{\partial}{\partial\theta}\sin^{D-2}\theta\frac{\partial}{\partial\theta}\right] f(r,\theta) \tag{2.10}$$

2.2. Fröhlich Hamiltonian in Non-Integer Dimensional Space

When the electron is artificially restricted to move in an abstract D-dimensional space ($D \leq 3$), the interaction with the phonons occurs in a subspace of 3-dimensions which is also D-dimensional. The reduction in the effective dimensionality of phonons is due to the $\exp(\pm i\boldsymbol{Q}.\boldsymbol{r})$ terms in the interaction Hamiltonian Eq.(1.5), through which the electron couples to LO phonon modes.
To clarify the modification procedure, we will follow the complete analogy with deriva-

tive of the Hamiltonian for 2-dimensional polaron from the one for the bulk.
Consider the bulk polaron Hamiltonian Eq.(1.1) with $\Omega(w) = 0$, and electron being confined to x-y plane. The electron position is then represented by $\boldsymbol{\rho}$. Since $\boldsymbol{Q.r} = \boldsymbol{q.r}$, the effective Hamiltonian can be written in terms of 2-dimensional phonon wave vector $\boldsymbol{q}$,

$$H = -\nabla_2^2 + \sum_q a_q^\dagger a_q + \sum_q V_q(D)(a_q e^{i\boldsymbol{q.\rho}} + hc) \tag{2.11}$$

where the effective 2-dimensional interaction amplitude V_q is obtained by integrating out the remaining component q_z. With $Q^2 = q^2 + q_z^2$;

$$|V_q|^2 = \sum_{q_z} |V_Q|^2 = \frac{\upsilon}{2\pi} \int_{-\infty}^{\infty} dq_z \frac{4\pi\alpha}{\upsilon_3} \frac{1}{q^2 + q_z^2} = \frac{2\pi\alpha}{\upsilon_2} \frac{1}{q} \tag{2.12}$$

where $\upsilon_2 = \frac{\upsilon_3}{\upsilon_1}$ is the 2-dimensional normalization volume.
Similarly, when the configuration space of electron is D-dimensional, adopting the fore mentioned convention, the effective Hamiltonian conforms to;

$$H = -\nabla_D^2 + \sum_q a_q^\dagger a_q + \sum_q V_q(a_q e^{i\boldsymbol{q.r}} + a_q^\dagger e^{-i\boldsymbol{q.r}}) \tag{2.13}$$

where now the space of phonon wave vector is divided into two complimentary subspaces represented by $\boldsymbol{q}$ and $\boldsymbol{q}^{'}$ which are D- and (3-D)-dimensional respectively. Preserving the relation$Q^2 = q^2 + q^{'2}$, the interaction amplitude is obtained by integrating V_Q over $\boldsymbol{q}^{'}$ in (3-D)-dimensions

$$\begin{aligned} |V_q|^2 &= \sum_{q'} |V_Q|^2 = \frac{\upsilon_{3-D}}{(2\pi)^{3-D}} \int_0^\infty dq^{'} W_{3-D}(q^{'}) \frac{4\pi\alpha}{\upsilon_3} \frac{1}{q^2 + q^{'2}} \\ &= \frac{\Gamma\left(\frac{D-1}{2}\right)(4\pi)^{\frac{D-1}{2}}\alpha}{\upsilon_D} \frac{1}{q^{D-1}} \end{aligned} \tag{2.14}$$

describes the electron-phonon interaction amplitude in non-integer dimensional space with D-dimensional normalization volume of the crystal with periodic boundary conditions.

The above analysis makes it clear that we have generalized structure of the electron-phonon interaction amplitude with corresponding integration Eq.(2.7) for various geometries. This form of V_q reproduces the well known results Eq.(2.12) and Eq.(1.6) when D is 2 and 3, while it diverges D$\rightarrow 1$ as it is expected. Although the domain of validity for Eq.(2.14) is $1 < D \leq 3$ within the presented "deduction from 3-dimensions" approach , it is interesting to note that Peeters et al [4] has obtained exactly the same form for the interaction amplitude, which is valid for any integer n-dimensions, aside from the notational mismatch of dimensionless units. Therefore it is possible to claim that Eq.(2.14) is valid for any real value of D. Nevertheless, any confinement effect in our 3-dimensional universe should naturally be modelled in a lower dimensional space, if it can ever be possible. So in our present context, we are concerned with D in the range 1 to 3.

We can also derive the expressions of interaction amplitude for slab and wire geometries by following the same procedure. When the configuration space of electron is divided into two complementary subspaces represented by $\boldsymbol{q}$ and $\boldsymbol{q}^{'}$ which are D- and (3-D)-dimensional respectively. Expressions within the calculations reproduces the well known results obtained previously when D is 2 and 3, while it diverges when $D \rightarrow 1$. Besides we proposed a model which contains confinement effect in NID space as distinct from our three dimensional universe.

As well as we need to mention that for the slab and wire geometry, we shall divide the non-integer dimensional space into two subspace. Slab geometry is required that 2+D effective dimensional space which consists of 2-dimensional subspace where the charge carriers are free to move and D-dimensional subspace where the charge carriers confined. Likewise wire geometry supposed to be 1+2D dimensional space which contains 1-Dimensional subspace where the charge carriers move as unconfined way and 2-dimensional subspace where the motion of the charge carriers are restricted. We can make a transition from wire or slab geometry to bulk structure by changing the tunable dimensionality parameter (D) in the range from 0 to 1 denotes dimensionality. Let's space of phonon wave vector is divided into two complimentary subspaces represented by

$$\boldsymbol{Q} = (\boldsymbol{q_{2+D}}, \boldsymbol{q_{1-D}}) \tag{2.15}$$

the (2+D)-dimensional interaction amplitude is obtained by integrating V_Q over $\boldsymbol{q}^{'}$ in (1-D)-dimensions;

$$\begin{aligned} |V_q(2+D)|^2 &= \sum_{q^{'}} |V_Q|^2 \\ &= \frac{\upsilon_{1-D}}{(2\pi)^{1-D}} \int_0^\infty dq_{1-D} \frac{4\pi\alpha}{\upsilon_3} W_{1-D} \frac{1}{q_2^2 + q_D^2 + q_{1-D}^2} \\ &= \frac{\Gamma\left(\frac{1+D}{2}\right)(4\pi)^{\frac{1+D}{2}}}{\upsilon_{D+2}} \alpha \frac{1}{(q_2^2 + q_D^2)^{\frac{1+D}{2}}} \end{aligned} \tag{2.16}$$

Above result is compatible with preceding expressions of 2 and 3 dimensional interaction amplitude with determining the dimensionality parameter as 0 and 1. It is worth noting that when parameter D is changed between 0 and 1 continuously, one determines interaction amplitude for quasi two dimensional geometry (Q2D).
Space of phonon wavevector is divided into two complimentary subspaces represented by

$$\boldsymbol{Q} = (\boldsymbol{q_{1+2D}}, \boldsymbol{q_{2-2D}})$$

the (1+2D)-dimensional electron phonon interaction amplitude is derived by integrating V_Q over $\boldsymbol{q}^{'}$ in (1+2D)-dimensions

$$\begin{aligned} |V_q(1+2D)|^2 &= \sum_{q_{2-2D}} |V_Q|^2 \\ &= \frac{4\pi\alpha}{\upsilon_3} \frac{\upsilon_{2-2D}}{(2\pi)^{2-2D}} \int_0^\infty dq_{2-D} W_{2-2D} \frac{1}{q_2^2 + q_{2-2D}^2 + q_{2D}^2} \\ &= \frac{\Gamma(D)(4\pi)^D}{\upsilon_{1+2D}} \alpha \frac{1}{q_z^2 + q_{2D}^2} \end{aligned} \tag{2.17}$$

Above result is compatible with preceding expressions of 1 and 3 dimensional interaction amplitude with determining the dimensionality parameter as 0 and 1. It is worth noting that when parameter D is changed between 0 and 1 continuously, one determines interaction amplitude for quasi two dimensional geometry (Q1D). We have demonstrated that electron-phonon interaction amplitude related to geometry of the system as given below

respectively,

$$|V_Q(D)|^2 = \begin{cases} \frac{\Gamma(\frac{D-1}{2})(4\pi)^{\frac{D-1}{2}}}{\upsilon_D}\alpha\frac{1}{q^{D-1}} & \text{for the spherical geometry} \\ \frac{\Gamma(\frac{D+1}{2})(4\pi)^{\frac{D+1}{2}}}{\upsilon_{D+2}}\alpha\frac{1}{(q_2^2+q_D^2)^{\frac{1+D}{2}}} & \text{for the slab geometry} \\ \frac{\Gamma(D)(4\pi)^D}{\upsilon_{1+2D}}\alpha\frac{1}{(q_z^2+q_D^2)^D} & \text{for the wire geometry} \end{cases}$$

CHAPTER 3

APPROXIMATION METHODS IN NIDS

In this chapter we will give our study based on approximation methods in NIDS to derive generalized forms of polaronic ground state energy and the effective mass. It should be pointed out that Fröhlich polaron will be treated as an unconfined effective non-integer dimensional polaron. Polarons behave as if they are free particles. This isotropic geometry provides us obtaining simplified and generalized expressions for the properties of the NID polaron. In [2] scaling relations which connects the 2D and 3D results in actual space, are formally generalized to the n-dimensional optical polaron problem. Furthermore, n-dimensional ground state energy is obtained in [4]. Based on these studies, first for the small electron-phonon coupling constant limit, second order perturbation theory is the highly applicable approximation method to calculate more accurate corrections to the ground state energy and the effective mass. After studying the perturbation theory, we continue with the variational method which is valid in strong coupling limit for the large α values . However these two approximation methods that we mentioned before, are not enough for describing the intermediate electron-phonon coupling strength. Therefore we need to introduce an another approach that capable interpolating between the variational method and perturbation theory called as variational perturbative approach. Focusing on this approach in the last section, we will get expressions for non-integer dimensional polaronic properties with a much more accuracy.

3.1. Perturbation in NIDS

We now discuss a generalization of the previous calculations to the non-integer dimensional space using relevant algebra. Of particular interest to this section is the studies performed to until now. The original approach proposed by He [28, 29]. In the past few years, the non-integer dimensional space approach has been successfully used in modelling polaron [5, 26, 30, 31], exciton [32–40], and impurity states [41] in semiconductor systems. Considering the α values are small, we limit our calculations to the

weak-coupling case. The energy of a D-dimensional polaron in the ground state

$$E = E_k^{(0)} + E_k^{(1)} + E_k^{(2)} \tag{3.1}$$

where

$$\begin{aligned} E_k^{(0)} &= \langle \phi_0 | H_0 | \phi_0 \rangle & (3.2)\\ E_k^{(1)} &= \langle \phi_0 | H_{e-ph} | \phi_0 \rangle & (3.3)\\ E_k^{(2)} &= \sum_i \frac{\langle \phi_i | H_{e-ph} | \phi_0 \rangle}{E_0 - E_i} & (3.4) \end{aligned}$$

Initial $|\phi_0\rangle$ and intermediate states $|\phi_i\rangle$ are determined by the following form respectively,

$$|\phi_0\rangle = |0_{\boldsymbol{k}'}, 1_{\boldsymbol{k}}, 0_{\boldsymbol{q}}\rangle \tag{3.5}$$

$$|\phi_i\rangle = |1_{\boldsymbol{k}'}, 0_{\boldsymbol{k}}, 1_{\boldsymbol{q}}\rangle \tag{3.6}$$

in the initial state there is an electron with pseudo-wave vector $\boldsymbol{k}$, there is no electron with pseudo-wave vector $\boldsymbol{k}'$ and there is no phonon with the pseudo-wave vector $\boldsymbol{q}$. On the other hand in the intermediate state there is no electron with pseudo-wave vector $\boldsymbol{k}$, there is an electron with pseudo-wave vector $\boldsymbol{k}'$ and there is a one phonon with the pseudo-wave vector $\boldsymbol{q}$.

Zeroth order correction to the ground state energy

$$\langle 0_{\boldsymbol{k}'}, 1_{\boldsymbol{k}}, 0_{\boldsymbol{q}} | H_0 | 0_{\boldsymbol{k}'}, 1_{\boldsymbol{k}}, 0_{\boldsymbol{q}} \rangle \tag{3.7}$$

where unperturbed hamiltonian $H_0 = -\nabla_D^2 + \sum_q a_q^\dagger a_q$ noting that $a_q|0_{\boldsymbol{q}}\rangle$

$$\begin{aligned} E_k^{(0)} &= \langle 0_{\boldsymbol{k}'}, 1_{\boldsymbol{k}}, 0_{\boldsymbol{q}} | (-\nabla_D^2 + \sum_q a_q^\dagger a_q) | 0_{\boldsymbol{k}'}, 1_{\boldsymbol{k}}, 0_{\boldsymbol{q}} \rangle & (3.8)\\ &= \langle 0_{\boldsymbol{k}'}, 1_{\boldsymbol{k}}, 0_{\boldsymbol{q}} | - \nabla_D^2 | 0_{\boldsymbol{k}'}, 1_{\boldsymbol{k}}, 0_{\boldsymbol{q}} \rangle \\ &= -k^2 & (3.9) \end{aligned}$$

only related to electron pseudo-wavevector. Inserting the interaction Hamiltonian into the Eq.(3.3), first order term is calculated as the following,

$$\begin{aligned} E_k^{(1)} &= \langle\phi_0|H_{e-ph}|\phi_0\rangle \\ &= \langle 0_{\boldsymbol{k}'}, 1_{\boldsymbol{k}}, 0_{\boldsymbol{q}}| \sum_q V_q(D)(a_q e^{i\boldsymbol{q}.\boldsymbol{r}} + a_q^\dagger e^{-i\boldsymbol{q}.\boldsymbol{r}})|0_{\boldsymbol{k}'}, 1_{\boldsymbol{k}}, 0_{\boldsymbol{q}}\rangle \\ &= 0 \end{aligned} \tag{3.10}$$

According to the result, there is no contribution to the ground state energy coming from the first order term. by using the form of the fractional dimensional fröhlich interaction, the above equation can be written as

$$E_k^{(2)} = \sum_q |V_q(D)|^2 \sum_{k'} \frac{|\delta_{\boldsymbol{k}'-\boldsymbol{k}+\boldsymbol{q}}|^2}{\bar{E}_k - \bar{E}_{k'}} \tag{3.11}$$

where

$$\bar{E}_k = \langle 0_{\boldsymbol{k}'}, 1_{\boldsymbol{k}}, 0_{\boldsymbol{q}}|H_0|0_{\boldsymbol{q}}, 1_{\boldsymbol{k}}, 0_{\boldsymbol{k}'}\rangle = E_k^{(0)} \tag{3.12}$$

$$\begin{aligned} \bar{E}_{k'} &= \langle 1_{\boldsymbol{k}'}, 0_{\boldsymbol{k}}, 1_{\boldsymbol{q}}|H_0|1_{\boldsymbol{q}}, 0_{\boldsymbol{k}}, 1_{\boldsymbol{k}'}\rangle \\ &= \langle 1_{\boldsymbol{k}'}, 0_{\boldsymbol{k}}, 1_{\boldsymbol{q}}| - \nabla_D^2 + \sum_q a_q^\dagger a_q |1_{\boldsymbol{q}}, 0_{\boldsymbol{k}}, 1_{\boldsymbol{k}'}\rangle \\ &= \sum_q (k^{'})^2 + 1 \end{aligned} \tag{3.13}$$

when unperturbed energy values are substituted in the denominator, alternatively, second order term can be referred to as

$$\begin{aligned} E_k^{(2)} &= \sum_q |V_q(D)|^2 \sum_{k'} \frac{|\delta_{\boldsymbol{k}'-\boldsymbol{k}+\boldsymbol{q}}|^2}{1 + \boldsymbol{k}^{'2} - \boldsymbol{k}^2} \\ &= \sum_q \frac{|V_q(D)|^2}{1 + q^2 - 2\boldsymbol{k}.\boldsymbol{q}} \end{aligned} \tag{3.14}$$

δ_{ij} denotes the Kronecker-Delta function

$$\delta_{ij} = \begin{cases} 1, & \text{if } i = j \\ 0, & \text{if } i \neq j \end{cases}$$

If the psuedovector $\boldsymbol{q}$ is quite large compared to phonon energy the q summation fall of rapidly. So the virtual phonons just contribute to the phonon energy in the case of a psuedovector $\boldsymbol{q}$ has not a huge values. The term $\boldsymbol{k.q}$ will be less than q^2 in the denominator due to the small value of $\boldsymbol{q}$. Expansion of the q summand in a power series up to second order in $\boldsymbol{k.q}$ gives following form which only depends on pseudo-vector $\boldsymbol{q}$

$$\begin{aligned} E_k^{(2)} &= -\sum_q |V_q(D)|^2 \left(\frac{1}{1+q^2} + \frac{4k^2q^2}{(1+q^2)^3} \right) \\ &= \frac{\upsilon_D}{(2\pi)^D} \int_0^\infty W_D(q) |V_{(D)}|^2 \left(\frac{1}{1+q^2} + \frac{4k^2q^2}{(1+q^2)^3} \right) \\ &= \frac{\sqrt{\pi}}{2} \frac{\Gamma(\frac{D-1}{2})}{\Gamma(\frac{D}{2})} \alpha + k^2 \frac{\sqrt{\pi}}{4} \frac{(\frac{D-1}{2})}{(\frac{D}{2})} \alpha \end{aligned} \tag{3.15}$$

the result can be divided into two parts in a physical sense. The first part that the term dos not contain electron pseudo wave-vector $\boldsymbol{k}$, will contribute to the ground state energy of the polaron. And the second part which depends on electron pseudo wave-vector $\boldsymbol{k}$ will contribute to the effective mass of the polaron. Briefly we obtain the following expression for ground state energy and the effective mass of the polaron

$$\begin{aligned} E &= E_k^{(0)} + E_k^{(1)} + E_k^{(2)} \\ &= k^2 - \beta_1(D)\alpha - k^2\beta_2(D) \\ &= -\beta_1(D)\alpha + k^2(1 - \beta_2(D)\alpha) \end{aligned} \tag{3.16}$$

In equation (3.16) the D-dependent functions $\beta_1(D)$ and $\beta_2(D)$ are given respectively, by

$$\beta_1(D) = \frac{\sqrt{\pi}}{2} \frac{\Gamma(\frac{D-1}{2})}{\Gamma(\frac{D}{2})} \qquad \beta_2(D) = \frac{1}{D} \frac{\sqrt{\pi}}{4} \frac{(\frac{D-1}{2})}{(\frac{D}{2})} \tag{3.17}$$

The set of equations indicate contribution from the electron-phonon interaction. The results can be used to directly obtain E_g and m_p of the Fröhlich polaron in NIDS.

$$m_p^D/m^* = (1 - \beta_2(D)\alpha)^{-1} \simeq 1 + \beta_2(D)\alpha \tag{3.18}$$

Fig.3.1 clearly shows that, with decreasing dimensionality parameter D the polaron bind-

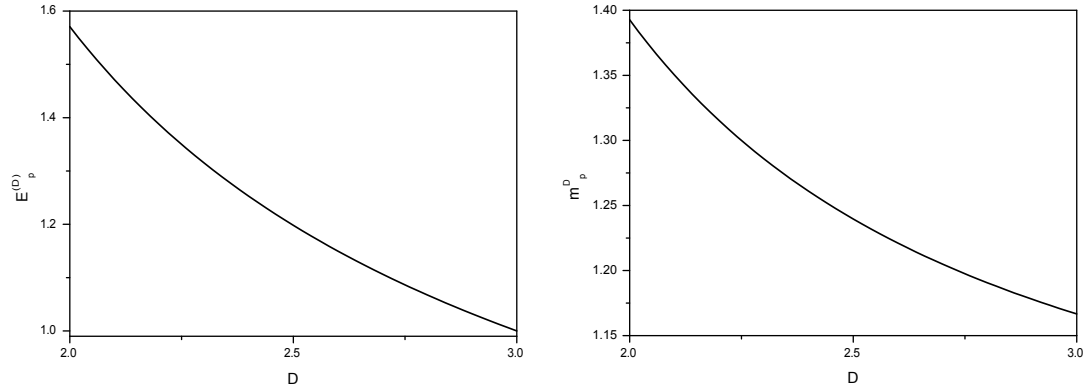

Figure 3.1. Perturbation theory results of the confined polaron in NIDS. (a) The binding energy $E_p^{(D)}$, and (b) effective mass $m_p^{(D)}$ of confined polaron as function of the effective dimensionality ($D = 3 \rightarrow 2$)for the slab-like geometries

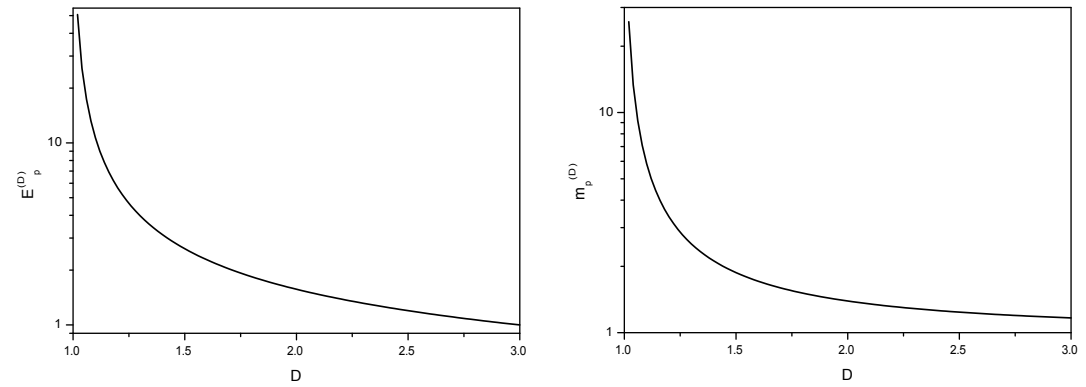

Figure 3.2. Perturbation theory results of the confined polaron in NIDS. (a) The binding energy $E_p^{(D)}$, and (b) effective mass $m_p^{(D)}$ of confined polaron as function of the effective dimensionality ($D = 3 \rightarrow 1$)for the wire-like geometries

ing energy and the effective mass become reasonably deepened for the slab-like geometry. When dimensionality parameter goes from 3 to 2, with continuous transition, polaron cloud starts to be squezzed starting from 0 to 1. For wire-like geometry the behaviour is rather different. Beginning from the bulk case (D=3) and approaching the wire-like geometry, the enhancement in the binding energy and effective mass is particularly apparent. As can be seen from Fig.3.2, as the dimensionality parameter approaches the 1D limit, strength of the electron phonon coupling becomes much stronger and the results for the contributions to the polaron in the ground state diverge at D=1. In view of the results we have obtained, we see that the compact forms of the binding energy, mass shift and effective mass can be reduced to well known results in Eq.(1.32)for bulk polaron (D=3) and Eq.(1.34) for the strictly-2D polaron (D=2) at the limit values. In this way, we can obtain confined polaron results in real 3D space avoiding complex calculations. Another key advantage of NID polaron results is that when we give a non-integer value to the effective dimensionality, we obtain the energy and the mass for the slab-like or wire-like geometries.

3.2. Variational Method in NIDS

In this section, we report on a detailed analysis for not only ground state energy but also effective mass of Fröhlich polarons in NID space. In general, for strong interaction strength, variational method can be used to described polarons. The results of the previous strongly coupled polaron calculations are generalized to non-integer or D-dimensional space by using variational method within adiabatic approximation. Before starting the calculation that is modified according to NIDS algebra, we need to recall the effective Fröhlich Hamiltonian in Eq.(2.13).

$$H = -\nabla_D^2 + \sum_q a_q^\dagger a_q + \sum_q V_q(D)(a_q e^{i\boldsymbol{q}.\boldsymbol{r}} + a_q^\dagger e^{-i\boldsymbol{q}.\boldsymbol{r}}) \tag{3.19}$$

We first construct a wave function which is the adiabatic polaron ground state.

$$\Psi_g \;=\; \Phi_e(r)|0\rangle \tag{3.20}$$

Adiabatic polaron ground state obtained from product ansatz consisting of the electron and phonon parts. And the normalized electronic wave function is given as

$$\Phi_e(r) = \left(\frac{\lambda}{2\pi}\right)^{D/4} \exp\Big(-\frac{1}{4}\lambda r^2\Big) \tag{3.21}$$

Under displaced oscillator transformation effective Hamiltonian conforms to

$$\tilde{H} = \nabla_D^2 + \sum_Q a_Q^\dagger a_Q - \sum_Q f_Q(a_Q^\dagger + a_Q) + \sum_Q {f_Q}^2 \tag{3.22}$$

$$+ \sum_Q V_Q[a_Q e^{i\boldsymbol{Q}.\boldsymbol{r}} + {a_Q}^\dagger e^{-i\boldsymbol{Q}.\boldsymbol{r}}] \tag{3.23}$$

where

$$U = \sum_q u_q(\Phi_e)[a_q - {a_q}^\dagger] \tag{3.24}$$

Here,$u_q(\Phi_e)$ is the lattice variational parameter via which an interrelation is established between the potential well set up by the lattice polarization and the electron which,in turn, becomes trapped in this well. The minimization of the energy functional $\langle\Psi_g|\tilde{H}|\Psi_g\rangle = \langle 0|\langle\Phi_e|\tilde{H}|\Phi_e\rangle|0\rangle$ with respect to u_q yields

$$u_q(\Phi_e) = V_q s_q, \qquad s_q = \langle\Phi_e|\exp(\pm i\boldsymbol{q}.\boldsymbol{r})|\Phi_e\rangle \tag{3.25}$$

With the optimal fit for substituted in, the Hamiltonian becomes

$$\tilde{H} = \langle\Phi_e|H|\Phi_e\rangle \tag{3.26}$$

$$= -\nabla_D^2 + \sum_q {a_q}^\dagger a_q + \sum_q {V_q}^2(D){s_q}^2$$

$$- \sum_q V_q(D)^2 s_q(e^{i\boldsymbol{q}.\boldsymbol{r}} + e^{-i\boldsymbol{q}.\boldsymbol{r}})$$

$$+ \sum_q V_q(D)[(e^{i\boldsymbol{q}.\boldsymbol{r}} - s_q)a_q + (e^{-i\boldsymbol{q}.\boldsymbol{r}} - s_q){a_q}^\dagger] \tag{3.27}$$

$$\begin{aligned}\langle 0|\tilde{H}|0\rangle &= \langle 0| - \nabla_D^2 + \sum_q {V_q}^2(D){s_q}^2 \\ &- \sum_q {V_q}^2(D)s_q\langle 0|(e^{i\boldsymbol{q}.\boldsymbol{r}} + e^{-i\boldsymbol{q}.\boldsymbol{r}})|0\rangle \end{aligned} \tag{3.28}$$

remaining terms gives the ground state energy in a simple form

$$E_g = \epsilon_k - \sum_q {V_q}^2(D){s_q}^2 \tag{3.29}$$

where $\epsilon_k = \langle \Phi_e| - \nabla_D^2|\Phi_e\rangle$
we need to turn q summation into the integration by using weight function

$$\sum_q \rightarrow \upsilon_{\mathrm{D}}(2\pi)^{-\mathrm{D}} \int_0^\infty dq W_D(q) \tag{3.30}$$

where weight function and D-dimensional interaction amplitude

$$W_D(q) = \frac{2\pi^{D/2}}{\Gamma(D/2)} q^{D-1} \tag{3.31}$$

$$|V_q(D)|^2 = \frac{\Gamma(\frac{D-1}{2})(4\pi)^{\frac{D-1}{2}}}{\upsilon_D} \alpha \frac{1}{q^{D-1}} \tag{3.32}$$

The summation in Eq.(3.29) can be calculated exactly. The term

$$s_q^2 = e^{-q^2/\lambda} \tag{3.33}$$

$$\sum_q V_q^2 s_q^2 = \frac{\sqrt{\lambda}}{2} \frac{\Gamma(\frac{D-1}{2})}{\Gamma(\frac{D}{2})} \alpha \tag{3.34}$$

kinetic part of the E_g will be given as follows

$$\begin{aligned}\epsilon_k &= \langle \Phi_e| - \nabla_D^2|\Phi_e\rangle \\ &= \int_0^\infty \Phi_e^*(r)(-\nabla_D^2)\Phi_e(r)W_D(r)dr \\ &= \lambda\frac{D}{4} \end{aligned} \tag{3.35}$$

Then E_g being a function of λ, the optimal value of the variational parameter λ_0, is found by the variation of E_g with respect to λ i.e. $\frac{dE_g}{d\lambda} = 0$;

$$E_g = \lambda\frac{D}{4} - \frac{\sqrt{\lambda}}{2}\frac{\Gamma(\frac{D-1}{2})}{\Gamma(\frac{D}{2})}\alpha \tag{3.36}$$

$$\frac{dE_g}{d\lambda} = 0 \tag{3.37}$$

$$\lambda_0 = \frac{1}{D^2}\left[\frac{\Gamma(\frac{D-1}{2})}{\Gamma(D/2)}\right]^2\alpha^2 \tag{3.38}$$

Substituting λ_0 into the λ in Eq.(3.36), finally we obtain the ground state energy of Fröhlich polaron in NIDS

$$E_g = -\frac{1}{4D}\left[\frac{\Gamma(\frac{D-1}{2})}{\Gamma(D/2)}\right]^2\alpha^2 \tag{3.39}$$

Effective mass of the D-dimensional polaron

$$m_p^{(D)}/m^* = 1 + \frac{4}{D}\sum_Q Q^2 V_Q^2(D)\sigma_Q^2 \tag{3.40}$$

The second term in Eq.(3.40) is the phononic contribution to the mass.

$$\begin{aligned}\mu^{(D)} &= \frac{4}{D}\frac{\omega_D}{(2\pi)^D}\int_0^\infty Q^2 V_Q^2(D)\sigma_Q^2 W_D(Q)dQ \\ &= \frac{\lambda^{3/2}}{D}\frac{\Gamma(\frac{D-1}{2})}{\Gamma(\frac{D}{2})}\alpha\end{aligned} \tag{3.41}$$

substitute λ_0 into the λ above equation which minimizes the ground state energy

$$m_p^D/m^* = 1 + \frac{1}{D^4}\left[\frac{\Gamma(\frac{D-1}{2})}{\Gamma(\frac{D}{2})}\right]^4\alpha^4 \tag{3.42}$$

The curves of the ground state energy and the effective mass corresponding to variational method results shown in Fig.3.3. These curves reveal that, variation of the

$E_g^{(D)}$ and m_p^D of confined polaron as a function of the effective dimensionality parameter during a continuous transition from the bulk geometry to the slab geometry ($D = 3 \rightarrow 2$) in NIDS. It is important to know that the curves are plotted for the value of $\alpha = 1$. In the strongly interacting regime with decreasing the mobility of the polaron namely,reducing the effective dimensionality, the ground state energy and the effective mass are increasing as expected for the slab-like geometry ($D = 3 \rightarrow 2$). Alternatively stating that, the enhancement in the polaron ground state energy and the effective mass are are valid for the wire-like geometry as shown in fig.3.4

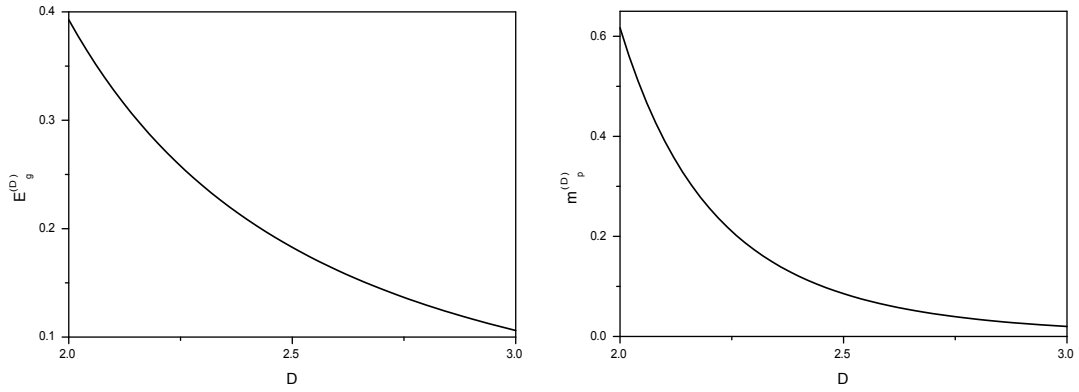

Figure 3.3. (a) The binding energy $E_p^{(D)}$, and (b) effective mass $m_p^{(D)}$of confined polaron as function of the effective dimensionality for the slab-like geometries. The solid lines refer to the results of the strong coupling theory.

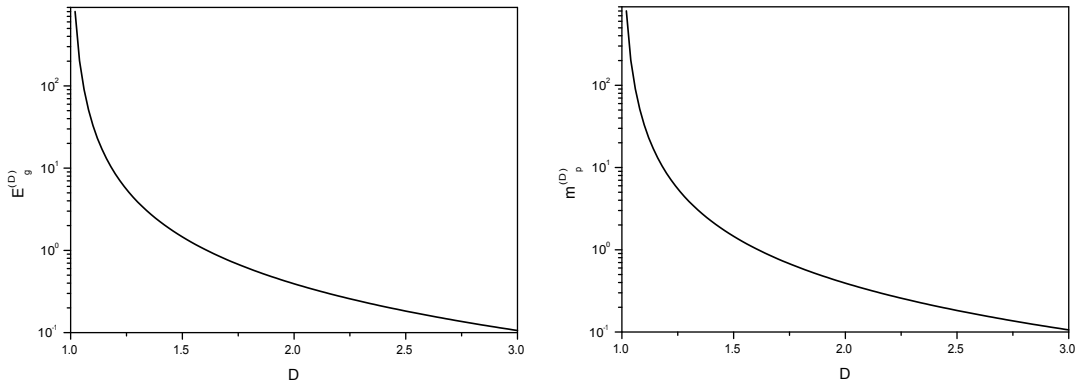

Figure 3.4. (a) The binding energy $E_p^{(D)}$, and (b) effective mass $m_p^{(D)}$of confined polaron as function of the effective dimensionality for the wire-like geometries. The solid lines refer to the results of the strong coupling theory.

Most important of all, we have also determine the relation of the effective dimensionality parameter and degree of confinement corresponds to same ground state energy in large α limit. The dependency of these parameters maps the dynamical space into the conventional Euclidean space where physical interactions occur. As fitting the our results which are found from the strongly interacting system, we have derived simple and handy model which relates the effective dimensionality and degree of confinement. The structure of the relation is given below

$$D = 3 - \exp\left[-\frac{1}{\sqrt{\Omega}}\right] \tag{3.43}$$

Alternatively stating that this relation can be represented by the following form

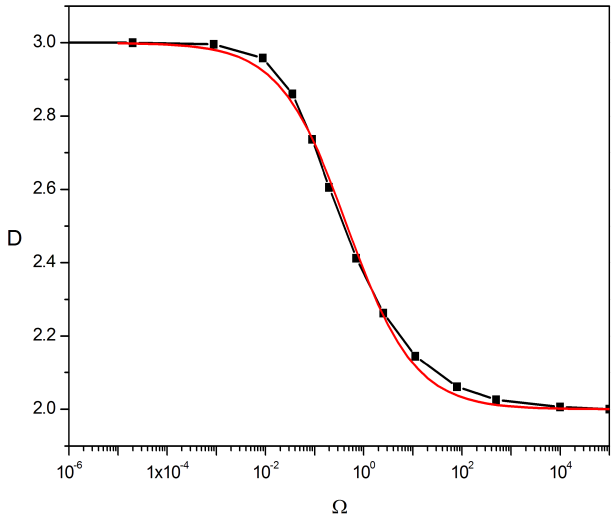

Figure 3.5. Effective dimensionality D as a function of the parabolic confinement Ω for slab-like geometry in strong coupling limit.

$$D = 3 - \exp\left[-\frac{L_z}{R_p}\right] \tag{3.44}$$

where the L_z refers well-width for the slab-like geometry and R_p denotes polaron size. Both of these parameters are unitless in our notation. Examine that in the limiting cases,

as the first case when the well-width goes to infinity ($L_z \to \infty$) we obtain the bulk value (D=3) for the polaron. In the second case when well-width goes to zero ($L_z \to 0$) we reach the slab geometry (D=2). The structure of the effective dimensionality for tunable slab-like confinement is displaced in Fig.3.5. It seems clear that at the rather large or small values of confinement parameter, effective dimensionality does not change nearly. In contrast, for the intermediate values of Ω rather large change is seen in the dimensionality parameter.

Consequently without making complicated calculations, we can obtain results of polaron energy and the mass for any confining potential through dimensionality.

3.3. Variational Perturbative Method in NIDS

The implementation of extended formalism to the polaron problem embedded in low dimensional system with parabolic confinement has been interpreted in the previous section. Now we mostly concentrate the modification is required in order to display a broader insight into the ground state properties of polaron in NID space. We propose a theoretical model re-characterizing the integer space to the case of non-integer space with in the framework of extended formalism. This theoretical model that we mentioned has a crucial advantage based on the fact that all the corrections come from perturbation collected on a single value dimensionality. In other words dimensionality in an NID space can be matched with an effective physical description of confinement in a real low dimensional system. Here we deal with obtaining the $E_g^{(D)}$ and $m_p^{(D)}$ of the polaron by revealing more valid and powerful approach that takes into account intermediate values in NID space. We construct a well-coordinated formalism is inspired by the original study proposed by [28, 29] During the generalization of mathematical structure of the problem, we follow the steps usual in extended formalism which covers all over α values. In this study

Ground state energy and effective mass of the polaron will be calculated by means of a arbitrary coupling approach. We use the Fröhlich Hamiltonian of the entire system in a NID space as stated in Eq.(2.13) and instead of working with the explicit wavefunction which belongs to electron, we set momentum and position in terms of operators. Momentum of the electron moving in non-integer dimensional bulk geometry in terms of operators

$$p_D = \frac{\sqrt{\sigma}}{2}(b_D + b_D^\dagger + p_D^{(0)}) \tag{3.45}$$

where index D denotes D-dimensional coordinates. Our aim is adding to variational quantity $p_D^{(0)}$ in order to set the system in motion.

$$p_D^2 = \frac{\sigma}{4}\sum_D b_D^2 + b_D^{\dagger 2} + b_D b_D^\dagger + b_D^\dagger b_D + 2(\boldsymbol{p}_D^{(0)} b_D + \boldsymbol{p}_D^{(0)} b_D^\dagger) + {p_D^{(0)}}^2 \tag{3.46}$$

fermionic operators satisfy the commutation relation $[b_D, b_{D'}^\dagger] = \delta_{DD'}$. Square of the momentum operator is given

$$p_D^2 = \frac{\sigma}{4}\sum_D b_D^2 + b_D^{\dagger 2} + \delta_{DD} + 2b_D^\dagger b_D + 2(\boldsymbol{p}_D^{(0)} b_D + \boldsymbol{p}_D^{(0)} b_D^\dagger) + p_D^{2^{(0)}} \tag{3.47}$$

by using lagrange multiplier method the functional is given

$$\begin{aligned} F(\sigma, \boldsymbol{v}) &= \langle 0|\tilde{H} - \boldsymbol{v}.\tilde{\Pi}|0\rangle \\ &= \frac{D\sigma}{4} + \frac{D\sigma}{4}p^{(0)} - D\frac{\sqrt{\sigma}}{2}\boldsymbol{v}.\boldsymbol{p}^{(0)} \\ &+ \sum_Q u_Q^2 - 2\sum_Q u_Q V_Q(D) s_Q - \sum_Q \boldsymbol{v}.\boldsymbol{Q} u_Q^2 \end{aligned} \tag{3.48}$$

is the expression of functional depends on dimensionality parameter in NID space. Minimizing the functional gives explicit form of the $p^{(0)}$ which serves our purpose and lattice variational parameter .

$$\boldsymbol{p}^{(0)} = \frac{\boldsymbol{v}}{\sqrt{\sigma}} \qquad u_Q = V_Q(D) s_Q \rho_Q \tag{3.49}$$

where

$$\rho_Q = (1 - \boldsymbol{v}.\boldsymbol{Q})^{-1} \tag{3.50}$$

in which the Lagrange multiplier v is to be identified as the polaron velocity along the D-dimensional bulk geometry. We will follow same procedure as in intermediate coupling theory for real space with one difference. As we mentioned before we use operator formalism instead of explicit variational wavefunction method. Therefore, modified trial

state will be defined in terms of phonon vacuum states as given in the following.

$$\begin{aligned} |0^{'}\rangle &= c|0\rangle + \sum_{Q} V_Q \sum_{i} |i\rangle \frac{\langle i|(\exp(-i\boldsymbol{Q}.\boldsymbol{r}) - s_Q)a_Q^{\dagger}|0\rangle}{\Delta_{\varepsilon_{i-0}}} \\ &= c|0\rangle + \sum_{Q} V_Q g_Q (\exp(-i\boldsymbol{Q}.\boldsymbol{r}) - s_Q)a_Q^{\dagger}|0\rangle \end{aligned} \tag{3.51}$$

From the normalization condition we obtain following expression as a constraint

$$f(c, g_Q) = \langle 0^{'}|0^{'}\rangle = c^2 + \sum_{Q} V_Q^2 g_Q^2 h_Q - 1 = 0 \tag{3.52}$$

One has to minimize the expectation values $\tilde{H} - \boldsymbol{\upsilon}.\tilde{\boldsymbol{\Pi}}$ in the extended trial state in order to find the parameter g_Q as we discussed before

$$\langle 0^{'}|\tilde{H} - \boldsymbol{\upsilon}.\tilde{\boldsymbol{\Pi}}|0^{'}\rangle = \langle 0^{'}|\tilde{H}|0^{'}\rangle - \langle 0^{'}|\boldsymbol{\upsilon}.\tilde{\boldsymbol{\Pi}}|0^{'}\rangle \tag{3.53}$$

and finally, the functional takes the following form without any explicit term

$$\begin{aligned} \Phi(\sigma, \upsilon; c, g_Q) &= c^2(e_0 + \frac{1}{4}\upsilon^2) - \frac{1}{2}\upsilon^2 \\ &+ \sum_{Q} V_Q^2(D) g_Q^2 (e_Q - \delta_{QQ'} + h_Q) \\ &+ \chi(1 - 2c^2) + 2c \sum_{Q} V_Q^2(D) g_Q h_Q \end{aligned} \tag{3.54}$$

Here, c is normalization constant and $\boldsymbol{Q}$ is the *pseudo-wavevector*. Remarkable point in here, all quantities in functional depend on dimensionality parameter.

$$\begin{aligned} \lambda &= \sum_{Q} V_Q^2(D) \left(\frac{g_Q}{c}\right) h_Q \\ &= -\sum_{Q} \frac{V_Q^2(D) h_Q^2}{(1 - \lambda + 2\chi - e_0 - \frac{1}{4}\upsilon^2)h_Q + e_Q - \delta_Q} \\ &= -\sum_{Q} \frac{V_Q^2(D) h_Q^2}{D_Q} \end{aligned} \tag{3.55}$$

- **Effective Mass of Non-Integer Dimensional Polaron ($m_p^{(D)}$)**

  We can get the effective mass of polaron in NID space via virtual velocity. To do this it is necessary isolating the velocity dependent terms from the functional. Hence,we will succeeded to split $\Phi(\sigma, \upsilon)$ into its parts consisting of the binding energy and of the polaron alone and the additional kinetic contribution which shows up having imposed a virtual momentum to the polaron. We are thus tempted to expand quantities in Eq.(3.54) and the summand in Eq.(3.55) in a power series up to second order in υ χ and δ_Q are transformed into the following form after expansion

$$\chi = \chi^{(0)} + \frac{1}{4}\upsilon^2\chi^{(1)} \qquad \text{and} \qquad \delta_Q = \delta_Q^{(0)} + \frac{1}{4}\upsilon^2\delta_Q^{(1)} \tag{3.56}$$

where $\chi^{(n)}$ and $\delta_Q^{(n)}$ (n=0,1) are given by

$$\begin{aligned} \chi^{(n)} &= \sum_Q V_Q^2(D) s_Q^2 [2Q]^{2n}, & (3.57)\\ \delta_Q^{(n)} &= \sum_{Q'} V_{Q'}^2(D) s_{Q'} \Delta_{QQ'} [2Q']^{2n} \\ &= 2\chi^{(n)}(1+s_Q^2) \\ &- 2s_Q \sum_{Q'} V_{Q'}^2 s_{Q'} \times (s_{Q+Q'} + s_{Q-Q'})[2Q']^{2n} & (3.58) \end{aligned}$$

D_Q takes this form with substitution expanded terms

$$\begin{aligned} D_Q &= e_Q^{(0)} - \boldsymbol{\upsilon.Q} h_Q + \frac{1}{4}\upsilon^2 h_Q - \delta_Q^{(0)} - \frac{1}{4}\upsilon^2\delta_Q^{(1)} \\ &+ h_Q - h_Q e_0 - \frac{1}{4}\upsilon^2 h_Q + 2\chi^{(0)} h_Q + \frac{1}{2}\upsilon^2\chi^{(1)} h_Q - \Lambda h_Q \end{aligned} \tag{3.59}$$

We will be calculated contribution to the $E_g^{(D)}$ and $m_p^{(D)}$ comes from D_Q by distinguishing velocity dependent and independent terms.
Hence, setting

$$D_Q^{(0)} = e_Q^{(0)} - \delta_Q^{(0)} + (1 - e_0 + 2\chi^{(0)} - \Lambda) h_Q \tag{3.60}$$

Furthermore, we obtain

$$\Phi(\sigma, \upsilon) = E_g(\sigma) - \frac{1}{4}\upsilon^2 m_p \tag{3.61}$$

where

$$E_g(\sigma) = e_0 - \chi^{(0)} + \Lambda \tag{3.62}$$

shows up the ground state energy and the factor m_p multiplying $\frac{1}{4}\upsilon^2$ is specified as the polaron mass given by

$$m_p = 1 + \chi^{(1)} + \sum_Q \frac{V_Q^2(D) h_Q^2}{D_Q^{(0)}} \left[\frac{4}{D} Q^2 \left(\frac{h_Q}{D_Q^{(0)}} \right)^2 + \frac{\delta_Q^{(1)} - 2\chi^{(1)} h_Q}{D_Q^{(0)}} \right] \tag{3.63}$$

Now, we need to derive explicit analytic forms for the quantities $e_0, s_Q, \chi^{(n)}$, and $\delta_Q^{(n)}$ to obtain explicit expressions of E_g and m_p. These analytical forms is derived using properties of NID space as we mentioned in Chapter 2. We aim to obtain results consistent with both 2D and 3D free polaron are found before in Chapter 1. We have calculated the set of quantities $\chi^{(0)}, \chi^{(1)}, \delta_Q^{(0)}$ and $\delta_Q^{(1)}$ in a explicit form

$$\begin{aligned} \chi^{(0)} &= \sum_Q V_Q^2(D) s_Q^2 = \alpha \frac{\vartheta_D}{(2\pi^D)} \int_0^\infty dQ W_D(Q) V_Q^2(D) s_Q^2 \\ &= \alpha \frac{\sqrt{\sigma}}{2} \frac{\Gamma(\frac{D-1}{2})}{\Gamma(\frac{D}{2})} \end{aligned} \tag{3.64}$$

$$\begin{aligned} \chi^{(1)} &= \frac{4}{D} \sum_Q V_Q^2(D) s_Q^2 Q^2 = \alpha \frac{4}{D} \frac{\vartheta_D}{(2\pi^D)} \int_0^\infty dQ W_D(Q) V_Q^2(D) s_Q^2 Q^2 \\ &= \alpha \sigma^{3/2} \frac{1}{D} \frac{\Gamma(\frac{D-1}{2})}{\Gamma(\frac{D}{2})} \end{aligned} \tag{3.65}$$

$$\delta_Q^0 = 2(1+s_Q^2)\chi^{(0)} - 2s_Q[\sum_{Q'} V_{Q'}^2(D)s_{Q'}s_{Q\pm Q'}] \tag{3.66}$$

We need to first calculate the summation

$$\begin{aligned}
&\sum_{Q'} V_{Q'}^2(D)s_{Q'}s_{Q\pm Q'} \\
&= \alpha\frac{\vartheta_{D-1}}{(2\pi)^{D-1}}\int_0^\infty\int_0^\pi dQ^{'}W_{D-1}(Q^{'})V_{Q'}^2(D)s_{Q'}s_{Q\pm Q'} \\
&= 2s_Q\alpha\sqrt{\sigma}\Gamma\left(\frac{D-1}{2}\right){}_1F_1\left[\frac{1}{2},\frac{D}{2},\frac{Q^2}{4\sigma}\right]
\end{aligned} \tag{3.67}$$

Here, the function in this form ${}_1F_1[a,b,z]$ is the regularized hypergeometric function.
Final form of the $\delta_Q^{(0)}$ is obtained as

$$\delta_Q^{(0)} = 2(1+s_Q^2)\chi^{(0)} - 4s_Q^2\sqrt{\lambda}\Gamma\left(\frac{D-1}{2}\right)\alpha_1F_1\left[\frac{1}{2},\frac{D}{2},\frac{Q^2}{4\sigma}\right] \tag{3.68}$$

$$\begin{aligned}
\delta_Q^{(1)} &= \frac{4}{D}\sum_{Q'} V_{Q'}^2(D)s_{Q'}\Delta_{QQ'}Q^{'^2} \\
&= \frac{4}{D}\sum_{Q'} V_{Q'}^2(D)s_{Q'}Q^{'^2}\left[2s_{Q'}(1+s_Q^2) - 2s_Qs_{Q\pm Q'}\right]
\end{aligned} \tag{3.69}$$

As in the $\delta_Q^{(0)}$ the summation is calculated as

$$\begin{aligned}
&\sum_{Q'} V_{Q'}^2(D)s_{Q'}s_{Q\pm Q'}Q^{'^2} \\
&= \alpha\frac{\vartheta_{D-1}}{(2\pi)^{D-1}}\sigma(D-1)\int_0^\infty\int_0^\pi dQ^{'}d\theta(Q^{'})^{(D-1)}(sin\theta)^{(D-2)}V_{Q'}^2(D)s_{Q'}s_{Q\pm Q'}Q^{'^2} \\
&= \frac{\alpha}{2}\sigma^{3/2}s_Q\Gamma\left(\frac{D-1}{2}\right){}_1F_1\left[\frac{3}{2},\frac{D}{2},\frac{Q^2}{4\sigma}\right]
\end{aligned} \tag{3.70}$$

Final type of the equation is given as

$$\delta_Q^{(1)} = \frac{4}{D}\left[2(1+s_Q^2)\chi^{(1)} - \alpha\sigma^{3/2}s_Q^2\Gamma\left(\frac{D-1}{2}\right){}_1F_1\left[\frac{3}{2},\frac{D}{2},\frac{Q^2}{4\sigma}\right]\right] \tag{3.71}$$

If we return to the Eq.(3.62) we will obtain the following expression clearly for the ground state energy of polaron in NID space via utilization the extended formalism

$$E_g(\sigma) = e_0 - \chi^{(0)} + \lambda \tag{3.72}$$

$$E_g(\sigma) = \frac{\sigma D}{4} - \alpha\frac{\sqrt{\sigma}}{2}\frac{\Gamma(\frac{D-1}{2})}{\Gamma(\frac{D}{2})} - \sum_Q \frac{V_Q^2(D)h_Q^2}{D_Q^{(0)}} \tag{3.73}$$

The polaron ground state energy as a function of the dimensionality parameter is shown in Fig.3.6 with the comparison of the strong, weak and intermediate coupling results for the value $\alpha = 0.1$. It is expected that, the results obtained from extended formalism and the results obtained from perturbation theory should be consistent with each other. In

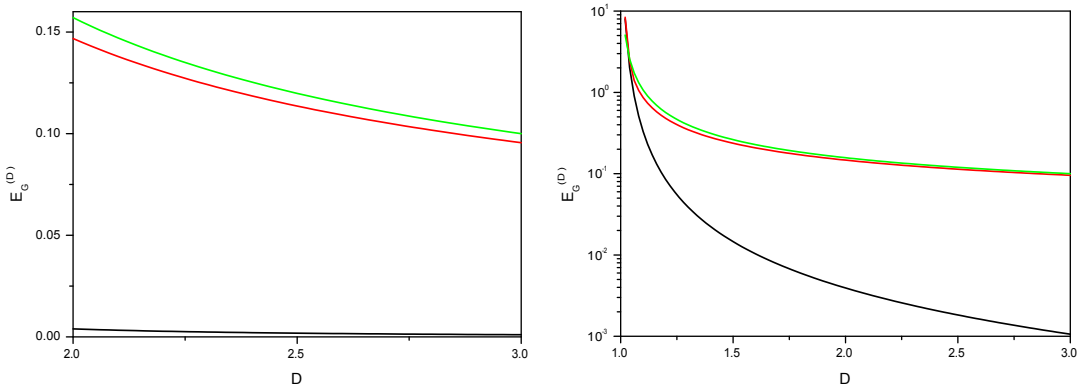

Figure 3.6. The ground state energy $E_g^{(D)}$ versus effective dimensionality D at electron-phonon coupling constant $\alpha = 0.1$ for slab-like and wire-like geometry respectively. Black solid line refers to the results of the strong coupling theory. Green solid line displays the results of the weak coupling theory. Red solid line refers to the results of the generalized extended formalism.

addition to alpha being small, the bulk limit for the polaron leads to rather weak electron phonon interaction. Therefore for the bulk limit (D=3), there is clearly a good agreement between the curves obtained from variational perturbative approach and the perturbation

theory. Moreover the detailed analysis shows that the going from the bulk geometry to the wire-like geometry, by comparing the green,red and black curves we can find that the overlapping to each other because of the strong electron phonon interaction. With the increasing in confinement strong coupling effects begin appear. For not too weak $\alpha = 1$,

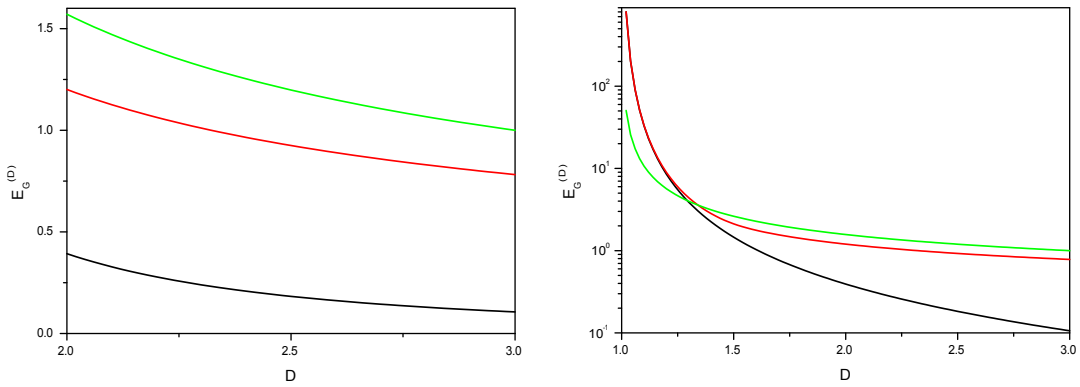

Figure 3.7. The ground state energy $E_g^{(D)}$ versus effective dimensionality D at electron-phonon coupling constant $\alpha = 1$ for slab-like and wire-like geometry, respectively. Black solid line refers to the results of the strong coupling theory. Green solid line displays the results of the weak coupling theory. Red solid line refers to the results of the generalized extended formalism.

weak and intermediate coupling theory results shown in Fig.3.7 may be considered as compatible with each other up to certain value of dimensionality parameter. With reduced dimensionality strong coupling results begin playing an essential role. Around the 1D limit, it is obvious that perturbation theory fails to reflect the features of the polaron.

Fig.3.8 shows that comparison of the strong, weak and intermediate coupling results for the value $\alpha = 10$. For strong α the pure weak coupling treatment is totally inadequate to give accurate results for the ground state energy of the polaron. On the other side, one can easily observe that strong coupling and weak coupling results ing good agreement to each other. We now proceed to discuss the effective mass results derived through the perturbation theory, variational method and variational perturbative method for various α values. In Fig.3.9 we select $\alpha = 0.1$, and compare to the results starting from the bulk limit to the wire-like limit. There is an apparent discrepancy between the black dashed line and the others in the bulk and slab-like geometry regions. This result meets our expectations. On one hand, with reducing dimensionality electron phonon interaction becomes much stronger and it leads to overlap the black dashed line and black solid line corresponds to strong and intermediate coupling results respectively.

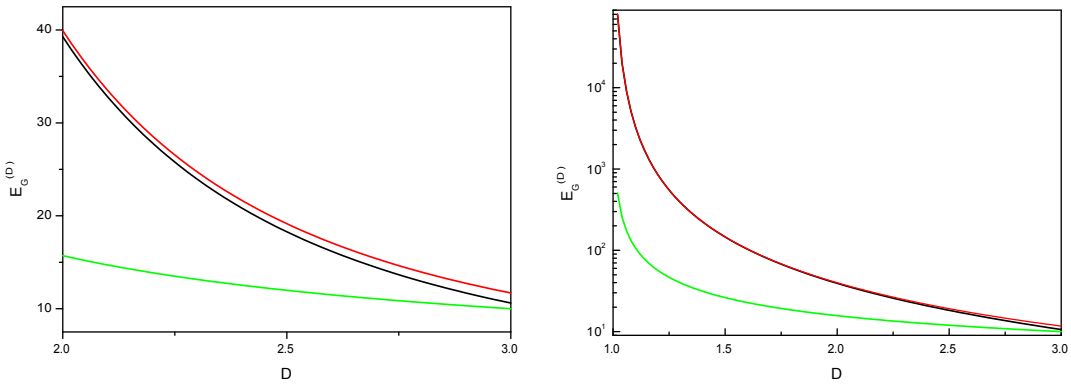

Figure 3.8. The ground state energy $E_g^{(D)}$ versus effective dimensionality D at electron-phonon coupling constant $\alpha = 10$ for slab-like and wire-like geometry, respectively. Black solid line refers to the results of the strong coupling theory. Green solid line displays the results of the weak coupling theory. Red solid line refers to the results of the generalized extended formalism.

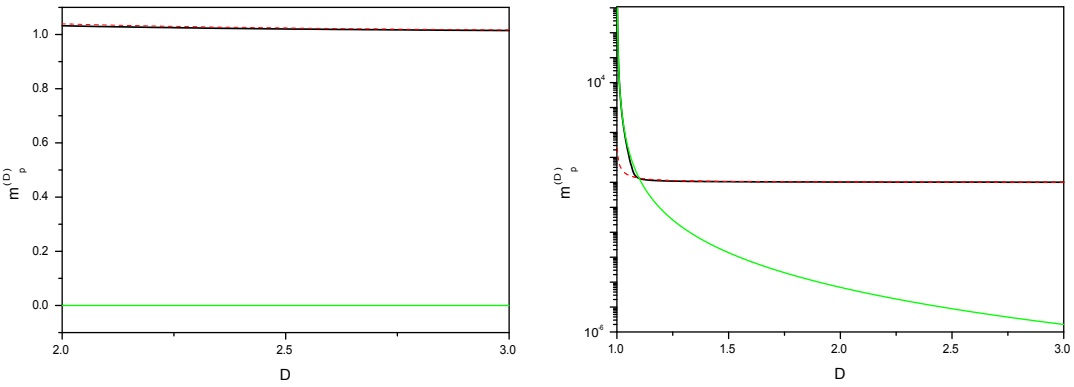

Figure 3.9. The ground state energy $m_p^{(D)}$ versus effective dimensionality D at electron-phonon coupling constant $\alpha = 0.1$ for slab-like and wire-like geometry, respectively. Green solid line refers to the results of the strong coupling theory. Red dashed line displays the results of the weak coupling theory. Black dashed line refers to the results of the generalized extended formalism.

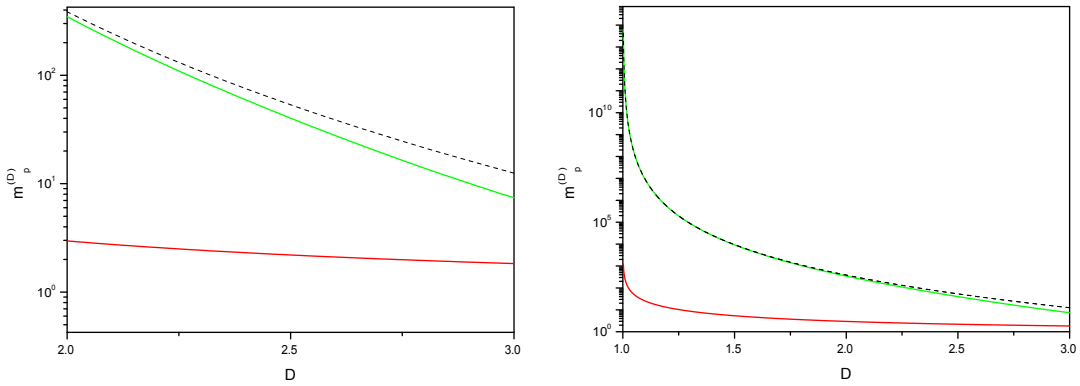

Figure 3.10. The ground state energy $m_p^{(D)}$ versus effective dimensionality D at electron-phonon coupling constant $\alpha = 5$ for slab-like and wire-like geometry, respectively. Green solid line refers to the results of the variational perturbative method. Red solid line displays the results of the weak coupling theory. Black dashed line refers to the results of the strong coupling formalism.

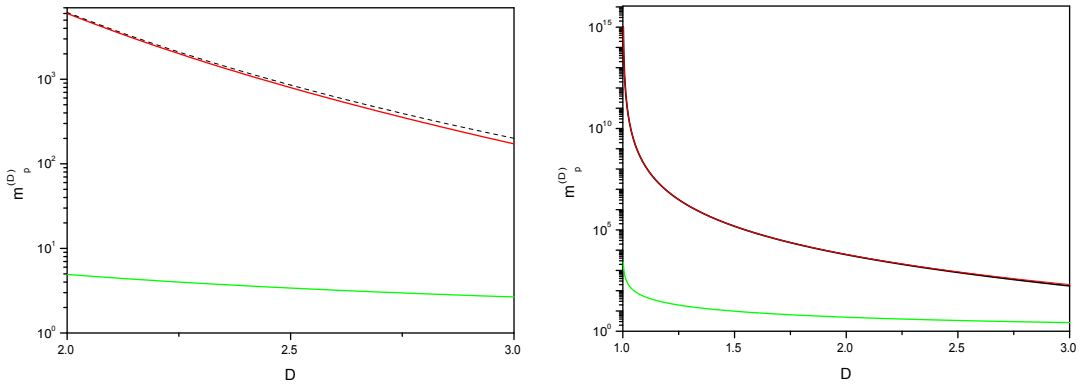

Figure 3.11. The ground state energy $m_p^{(D)}$ versus effective dimensionality D at electron-phonon coupling constant $\alpha = 10$ for slab-like and wire-like geometry, respectively. Black dashed line refers to the results of the strong coupling theory. Green solid line displays the results of the weak coupling theory. Red solid line refers to the results of the variational perturbative method.

Effective mass dependence on the dimensionality parameter for the value of $\alpha = 5$ is addressed in Fig.3.10, showing a drastic increase of the strong and intermediate coupling results. It is seen that, weak coupling theory fails to display the ground state properties of the polaron. However, order of alpha value , in the 3D limit since electron-phonon interaction weaker than the 1D limit, weak coupling theory does not seem to inconsistent with intermediate coupling theory.

Fig.3.11 displays the dependence of effective mass on the dimensionality parameter for the value of $\alpha = 10$. There is an excellent agreement between strong and intermediate coupling theory.

In summary, we have studied the confinement and the corresponding effective dimensionality effect on Fröhlich polaron ground state energy and effective mass in the weak, strong and arbitrary coupling regimes. We see that, for all the coupling constants, with the increasing confinement ground state energy and effective mass of the polaron are enhanced. In contrast, with the reduction of the effective dimensionality, ground state energy is deepened and there is an enhancement in the effective mass of the polaron. It is quite reasonable that more confined geometry leads to more reduced dimensional systems or vice versa.

CHAPTER 4

RESULTS AND DISCUSSIONS

In this work we have examined the problem of Fröhlich polaron in Non-Integer Dimensional Space (NIDS) where the effective dimensionality parameter is continuous in the range from 1 to 3, within the framework of weak, strong and intermediate coupling theory as a model of 3-dimensional polaron with a parabolic confinement. The electron is considered in a NIDS interacting isotropically with the bulk phonons, in order to account for the anisotropic interactions brought about by the spatially confining parabolic potential.

In this regard we have derived expressions for the ground state energy and the effective mass of polaron depend on the effective dimensionality parameter which is the identity of the confinement degree in NIDS. It should be noted that these expressions are obtained straightforwardly in a simple and compact form which recovers the well known results at the limit values . We have also shown that the relation between effective dimensionality and the degree of confinement (anisotropy) in the strong coupling domain. Through this useful relation, we can obtain the energy and the effective mass in the ground state of the strongly coupled polaron, preventing the complex calculations due to the confining potential.

Our results indicate that any confinement effect in our 3-dimensional universe should naturally be modelled in a lower dimensional space, if it can ever be possible. Since essential features of the polaron diverge when $D \rightarrow 1$, we are concerned with in the range 1 to 3.

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APPENDIX A

SUPPLEMENTARY INFORMATION

A.1. Perturbation Theory

$$H = H^{(0)} + H^{(1)} \tag{A.1}$$

It is clear that for the polaron problem we have,

$$H^{(0)} = H_e + H_{ph} \tag{A.2}$$

$$H^{(1)} = H_{e-ph} \tag{A.3}$$

The solution of the time independent Schrödinger equation

$$H|\Psi_n\rangle = E_n|\Psi_n\rangle \tag{A.4}$$

can be expanded in a perturbation series of the form,

$$|\Psi_n\rangle = |\Psi_n^{(0)}\rangle + |\Psi_n^{(1)}\rangle + |\Psi_n^{(2)}\rangle + ... \tag{A.5}$$

$$E_n = E_n^{(0)} + E_n^{(1)} + E_n^{(2)} + ... \tag{A.6}$$

where n stands for all the quantum numbers characterizing the system. Substituting these series in Eq.(...), one can consider the terms with the same order independently. The zeroth-order terms give simply the equation for the unperturbed Hamiltonian,

$$H^{(0)}|\Psi_n^{(0)}\rangle = E_n^{(0)}|\Psi_n^{(0)}\rangle \tag{A.7}$$

which can be assumed to be solved exactly. The first order correction to the energies can be found to be expectation value of $H(1)$ in the unperturbed states,

$$E_n^{(1)} = \langle \Psi_n^{(0)} | H^{(1)} | \Psi_n^{(0)} \rangle \tag{A.8}$$

For some systems, the first order correction $E_n^{(1)}$ vanishes exactly like polaron, so one should consider higher order for the energy,

$$E_n^{(2)} = \sum_m \frac{\left| \langle \Psi_n^{(0)} | H^{(1)} | \Psi_m^{(0)} \rangle \right|^2}{E_n^{(0)} - E_m^{(0)}} \tag{A.9}$$

Finally, for the eigenstates we have

$$|\Psi_n^{(1)}\rangle = \sum_m \frac{\langle \Psi_m^{(0)} | H^{(1)} | \Psi_n^{(0)} \rangle}{E_n^{(0)} - E_m^{(0)}} |\Psi_m^{(0)}\rangle \tag{A.10}$$

as the leading order term in the perturbation series.

A.2. Transformations

Variational and variational perturbative method that we concentrate, in this study, based on using the standard canonical and displaced oscillator transformations in the framework strong coupling and arbitrary coupling formalisms. That is why, we give a brief knowledge concerning transformations. In addition, for the calculation in weak coupling regime, we summarized the usual perturbation theory.

A.2.1. Canonical Transformations

When applying the approximation methods to the polaron problem, instead of writing the wavefunction explicitly, momentum and position operators can be defined in

terms of electron operators as given below

$$p_\nu = \frac{\sqrt{\sigma}}{2}(b_\nu + b_\nu^\dagger) \tag{A.11}$$

$$x_\nu = \frac{i}{\sqrt{\sigma}}(b_\nu - b_\nu^\dagger) \tag{A.12}$$

where $b(b^\dagger)$ annihilation(creation) operators of electron and ν denotes cartesian coordinates.
Canonical transformation of the Hamiltonian is performed by

$$U_1 = exp(-i\sum_Q a_Q^\dagger a_Q \boldsymbol{Q.r}) \tag{A.13}$$

$$H^{'} = U_1^{-1} H U_1 \tag{A.14}$$

Substituting the position operator into the equation (...)

$$U_1 = exp(\frac{1}{\sqrt{\sigma}}\sum_Q Q a_Q^\dagger a_Q (b_\nu - b_\nu^\dagger)) \tag{A.15}$$

It is convenient to use shorthand notation for $U_1 = exp^S$ By using Baker Hausdorff Formula the new Hamiltonian is obtained as given

$$\begin{aligned} H^{'} &= U^{-1}HU = e^{-S}He^S \\ &= (\boldsymbol{P} - \sum_Q \boldsymbol{Q} a_Q^\dagger a_Q)^2 + \sum_Q a_Q^\dagger a_Q + \sum_Q \Gamma_Q (a_Q e^{i\boldsymbol{Q.r}} + a_Q^\dagger e^{-i\boldsymbol{Q.r}}) \end{aligned} \tag{A.16}$$

where $\boldsymbol{P}$ is the total momentum of the system. This result displays that the momentum changes under canonical transformation. In contrast to momentum, phonon term and the interaction term remains invariant.

$$\boldsymbol{P} = \boldsymbol{p} + \sum_Q \boldsymbol{Q} a_Q^\dagger a_Q \tag{A.17}$$

A.2.2. Displaced Oscillator Transformation

Trial wavefunction can be formed as product of the electronic wavefunction and a phonon coherent state consistent with Pekar's product ansatz

$$\Psi_g = U_2|0\rangle \tag{A.18}$$

where $|0\rangle$ represents the states with no phonon.

$$U_2 = \exp \sum_Q f_Q(\Phi_e)[a_Q - a_Q^\dagger] \tag{A.19}$$

is regarded as a unitary operator which acts simply to remove the phonon coordinates a_Q and $a_Q^\dagger$.
Applying the same procedure in Eq.(A.16)

$$\begin{aligned} \tilde{H} &= U_2^{-1} H U_2 \\ &= p^2 + \sum_Q a_Q^\dagger a_Q - \sum_Q f_Q(a_Q^\dagger + a_Q) \\ &+ \sum_Q {f_Q}^2 + \sum_Q V_Q[a_Q e^{i\boldsymbol{Q}.\boldsymbol{r}} + {a_Q}^\dagger e^{-i\boldsymbol{Q}.\boldsymbol{r}}] \end{aligned} \tag{A.20}$$