APPROXIMATION METHODS IN THE POLARON THEORY: APPLICATIONS TO LOW DIMENSIONALLY CONFINED POLARONS

A THESIS
SUBMITTED TO THE DEPARTMENT OF PHYSICS
AND THE INSTITUTE OF ENGINEERING AND SCIENCES
OF BILKENT UNIVERSITY
IN PARTIAL FULFILLMENT OF THE REQUIREMENTS
FOR THE DEGREE OF
MASTER OF SCIENCE

By
Ö. Tuğrul Sevgen
July 1996

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

Prof. Atilla Erçelebi (Supervisor)

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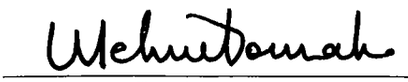

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Abstract

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R. Tuğrul Senger
M. S. in Physics
Supervisor: Prof. Atilla Erçelebi
July 1996

The polaron problem has been of interest in condensed matter physics and field theory for about half a century. Within the framework of vast variety of theoretical approximations, the bulk polaron properties have been extensively explored and fairly well understood in the literature. In the last two decades, with the impressive progress achieved in the microfabrication technology, it became possible to obtain low dimensional microstructures, in which the charge carriers are confined in one or more spatial directions. Consequently, there has appeared quite a large interest in phonon coupling-induced effects and polaronic properties of low dimensionally confined electrons.

In this context, this thesis work is devoted to the study of low dimensional optical polaron properties, with the application of several different formal approaches common in the literature, such as perturbation theory, variational principles and Feynman path integral formalism. The model we adopt in this

work consists of an electron, confined within an external potential (quantum well), and interacting via the Fröhlich Hamiltonian with the bulk LO-phonons of the relevant well material. Therefore, our primary concern is to give a clear view of only the bulk phonon effects on an electron in confined media, and we disregard all other complications that may come about from screening effects, phonon confinement, etc. Under these assumptions, we calculate the ground state energy, the effective mass, and some other quantities of polaron in several confinement geometries. We also provide a broad interpolating overview to the one polaron problem in the overall range of electron-phonon coupling constant and in a general type of confinement, which can be conformed from one geometrical configuration to another.

Another interesting theme of the polaron theory, magneto-polaron, is considered in the context of the confinement effect on the polaron, brought about by the magnetic field. A detailed analysis is given in the case, where the effect of electron-phonon coupling is dominated over by the magnetic field counterpart of the problem.

Keywords:

Optical polaron, electron-phonon interaction, Fröhlich Hamiltonian, low dimensional structures, quantum wire, quantum dot, path integral, magneto-polaron.

Özet

POLARON KURAMINDA YAKLAŞIM YÖNTEMLERİ: DÜŞÜK BOYUTLU POLARONLARA UYGULAMALAR

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Temmuz 1996

Polaron problemi, yaklaşık yarım yüzyıldır, katı hal fiziği ve alanlar kuramının ilgi konusu olagelmiştir. Çeşitli kuramsal yaklaşımlar altında yapılan çalışmalarla, üç boyutlu polaronların özellikleri geniş ölçüde araştırılmış ve oldukça iyi anlaşılmıştır. Son yirmi yıl içinde, çok küçük yapıların üretim teknolojisinde sağlanan etkileyici gelişmeler sayesinde, yüktaşırların bir veya daha çok yönden sınırlandırıldığı düşük boyutlu yapıların üretimi mümkün olmaktadır. Bundan dolayı, düşük boyutlara sıkıştırılmış elektronlarda polaronik özellikler ve fononlarla etkileşim kaynaklı problemler üzerine yoğun bir ilgi uyanmıştır.

Bu bağlamda, bu tez çalışmasının kapsamı içinde, tedirgeme kuramı, değişken ilkesi kuramı ve Feynman yol integralleri yöntemi gibi yaygın olarak kullanılan çeşitli yaklaşımlar çerçevesinde, düşük boyutlu optik polaronların özellikleri ele alındı. Çalışma, bir dış potansitel tarafından sınırlandırılmış ve Fröhlich Hamiltonu yoluyla üç boyutlu boylamsal optik fononlarla etkileşen bir elektron modeli üzerine kuruldu. Başlıca amacımız, sınırlandırılmış ortamlarda bulunan elektronlara üç boyutlu fononlarların etkilerini sergilemek olduğundan, perdeleme etkileri veya fonon sınırlandırılması gibi olası yan etkenler tamamen gözardı

edildi. Bu varsayım altında, temel durum enerjisi, efektif kütle ve diğer bazı polaron nicelikleri değişik geometrilerde hesaplandı. Ayrıca, bir geometrik yapıdan diğerine dönüştürülebilen esnek bir potansiyel kuyusu içinde ve tüm elektron-fonon bağlaşım sabiti değerleri için geçerli olmak üzere tek polaron problemine geniş ve birleştirici bir bakış açısı sunuldu.

Polaron kuramının bir başka ilginç konusu olan manyeto-polaron problemi, manyetik alanın polaron üzerindeki sınırlandırıcı etkisi yönünden ele alındı. Problemin, manyetik alan etkisinin elektron-fonon bağlaşım etkilerine göre daha baskın olduğu durumlar için kapsamlı bir analizi yapıldı.

Anahtar sözcükler:

Optik polaron, elektron-fonon etkileşmesi, Fröhlich Hamiltonu, düşük boyutlu yapılar, kuvantum kuyusu, kuvantum teli, yol integralleri, manyeto-polaron.

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Finally, it is my duty and pleasure to thank my family, and the lovely Süheyla, without whom the life would be boring and less meaningful.

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Chapter 1

INTRODUCTION

The problem of polaron is an old and interesting subject. It has been a long time (more than half a century) since the first appearance of it in the literature of, then newly developing branch, solid state physics, in the early 1930's, but there still occurs a considerable amount of work devoted to the study of polarons. Mainly there are two reasons of the interest on the subject; firstly, it is relevant to the applied physics of semiconductors, which has a wide area of technological applications, secondly, it represents a simple but nontrivial example of a particle coupled to a quantum field, presenting a challenging formal mathematical structure. Besides, with the theoretical prediction and subsequent fabrication of semiconductor based quantum - well confined systems, the subject is enriched with the polarons of lower dimensionality, in the last two decades.

The concept of polaron is based on the motion of an electron in an ionic or polar semiconductor crystal. The long range Coulomb interaction of the electron with the ions of the crystal produces a polarization field around it due to the displacements of ions from their equilibrium positions. Alternatively stating, the electron couples to the phonon modes of the crystal, resulting in a cloud of phonons surrounding and accompanying it, as it moves. The system of electron plus the concomitant phonon cloud (or the lattice deformation) is called the polaron. The interaction with phonons modifies the electron properties, lowering the self energy and increasing the inertia of it by an amount depending on the

strength of the coupling.

The first conceptual approach to polaron problem was by Landau[1] in 1933. He introduced the idea of a self-tapped electron in the polarization potential produced by the Coulomb interaction of the electron with the ions of the ionic crystal. In 1937, introducing the concept of polarization field, Fröhlich[2] gave a quantitative treatment of electron scattering in ionic crystals. After some early semiclassical works[3–5] on the subject, in which the lattice properties were incorporated into a classical macroscopic polarization, the formulation of the problem in the framework of quantum field theory was first given by Fröhlich, Pelzer and Zienau[6] in 1950, by proposing a microscopic model Hamiltonian, which now bears the name of Fröhlich.

Until now, the Fröhlich Hamiltonian remained the basic concept of enormous number of publications on the theory of polarons. Having no exact solution it has been a testing ground for several approximation methods in quantum field theory and quantum statistics. An elaborate summary of the theoretical and experimental developments achieved in the history of polarons can be found in the books edited by Kuper & Whitfield[7] and Devreese.[8] An excellent overview of the approximation methods in the polaron theory is also given in a recent paper by Bogolubov and Plechko.[9] Finally, we should mention about a distinguished review article of Gerlach and Löwen,[10] in which they have considered and formally settled the famous controversy of polaron theory; whether the polaronic phase transitions exist or not, by concluding that the qualitative changes in the polaron quantities take place in a smooth and continuous way, and that any non-analytical behavior encountered is an artifact of the approximating theory rather than the intrinsic property of the Fröhlich Hamiltonian.

The bulk polaron properties have been extensively explored and fairly well understood in the literature, with the development of a variety of theoretical approaches. Recently, the progress in the fabrication techniques, such as molecular beam epitaxy and lithographic methods, made it possible to obtain low dimensional microstructures, where the charge carriers are confined in one or more spatial directions. Consequently, there occurred a renewed interest

in the study of polarons of reduced dimensionality in the context of quantum well structures. Particular emphasis has been given to quasi- and strict-two dimensional systems.[11–15] The quasi-one (quantum wire),[16–18] and zero dimensional (quantum box)[19–21] systems are also extensively studied. Presenting a unified picture for polarons in confined media, covering all these special geometries and smoothly interpolating among them, is one of the motivations of the present work (cf. Chapter 6).

In low dimensional systems, besides the confinement of electron, it is also possible to consider the confinement of phonons with the notion of confined phonon modes,[22–25] and/or the surface and interface phonon modes[26,27] that occur at the boundaries. An alternative or complementary approach in this sense is the so called *bulk phonon approximation*, where the spatially confined electron is visualized as interacting via the Fröhlich Hamiltonian solely with the bulk LO-phonons of the relevant well material. Throughout this thesis, we will apply the bulk phonon approximation for the one polaron problem within the framework of the well known theoretical methodologies common in the literature. We will give most emphasis to the generic low dimensional aspect of the dynamical behavior of the electron confined in an external potential, and leave out all the other effects; thus our concern will primarily be to give a view of the bulk phonon effects stripped from all other perturbing quantities. Apart from omitting the contributions that may come from all other kinds of phonon modes, we will also ignore any screening effects and further complications such as those due to the nonparabolicity corrections to the electron band or the loss of validity of both the effective-mass approximation and the Fröhlich continuum Hamiltonian in very small microstructures.

The rest of this thesis is organized as follows. In the next sections of this chapter, the Fröhlich Hamiltonian will be derived starting from the basic principles, and a brief summary of the approximation methods will be presented. The Chapters 2 through 6, are devoted to the different theoretical approaches, each chapter starting with a short presentation of the essential points of the methodology, is accompanied with an original (except for Chapter 2) application

of it to a low dimensional configuration. In the seventh chapter we will consider the problem of polaron in a magnetic field, where the external field acts as a means of confinement. Finally a short summary together with relevant discussions and conclusions will form the last chapter.

1.1 Fröhlich Hamiltonian

In this section, we shall drive the Hamiltonian describing the system composed of a single electron, confined in an external potential, and interacting with the LO-branch of bulk phonon modes of the crystal. Although the label *Fröhlich Hamiltonian* is used for all class of more complicated systems involving electron-phonon interactions, with such considerations as polaron gas, confined phonon modes, etc., we shall restrict ourselves within the scope of the present work. For a more detailed derivation one may consult to the original paper by Fröhlich *et al.*,[6] and some relevant books.[7,28]

To represent the motion of the electron and of the lattice vibrations in the simplest possible form, we shall consider that, the electron lies close to the lower edge of the band, where the related Bloch functions have small $\vec{k}$-vector values, so that the corresponding wavelengths are large compared with the lattice constant. Then, it is appropriate, to ignore the detailed lattice structure and to treat the lattice as a dielectric continuum, and also, to apply the effective mass approximation for the electron. As a further approximation we shall take the LO-phonon modes to be dispersionless; $\omega(\vec{Q}) = \omega_{\mathrm{LO}}$.

In view of these simplifying considerations, the total polaron Hamiltonian can be stated as composed of three parts,

$$H = H_{\mathrm{e}} + H_{\mathrm{ph}} + H_{\mathrm{e-ph}}, \tag{1.1}$$

where the subscripts '*e*', '*ph*' and '*e-ph*' stand for 'electron', 'phonon', 'electron-phonon interaction' respectively.

The first term in the above, is simply

$$H_{\mathrm{e}} = \frac{p^2}{2m^*} + V_{\mathrm{conf}}(\vec{r}; \{\Omega_i\}) \tag{1.2}$$

where $\vec{r}$ and $\vec{p}$ are electron position and momentum operators, $m^\star$ is the effective band mass of electron and $V_{\rm conf}$ defines the external potential through which the electron is confined. The set of parameters $\{\Omega_i\}$ characterizing the potential, will generally be taken as tunable, by means of which we shall obtain several low dimensional confinement geometries.

For the remaining two terms in Eq.(1.1), we will first consider the energy of the polarization oscillations induced by the electron, and the electron-polarization field interaction energy within the framework of classical electrodynamics. Afterwards, the form of the Hamiltonian in the language of quantum field theory will be obtained through the quantization of the polarization field.

As a model of the polarization $\vec{P}(\vec{r})$ of the medium, consider individual dipoles $\vec{d}_n = e_n^\star \vec{q}_n$, located at the sites of the lattice. The dipoles oscillate with the characteristic frequency $\omega_{\rm LO}$, the frequency of optical lattice vibrations, and they correspond to oscillating masses m_n, with effective charges $e_n^\star$, in the normal coordinates $\vec{q}_n(t)$. With the assumption that the dipoles are not coupled, the total energy is stated as,

$$\frac{1}{2}\sum_n m_n \left(\dot{\vec{q}}^2 + \omega_{\rm LO}^2 \vec{q}^{\,2}\right). \tag{1.3}$$

Switching from the individual dipoles to a dielectric continuum is achieved through the following substitutions;

$$e_n^\star \vec{q}_n \;\rightarrow\; \vec{P}(\vec{r}) \qquad m_n \;\rightarrow\; \varrho(\vec{r}) d^3 r \tag{1.4}$$

where $\varrho(\vec{r})$ is the mass density. If we further let $\varrho(\vec{r})/e^\star(\vec{r}) = \gamma$ to be a constant, the total energy of the polarization field gets the form;

$$\frac{1}{2}\gamma \int d^3 r \left(\dot{\vec{P}}^{\,2}(\vec{r}) + \omega_{\rm LO}^2 \vec{P}^{\,2}(\vec{r})\right). \tag{1.5}$$

Therefore, introducing the momentum variable $\vec{\Pi} = \dot{\vec{P}}/\gamma$, canonically conjugate to $\vec{P}$, one can express the polarization Hamiltonian H_P as,

$$H_P = \int d^3 r \left(\frac{1}{2\gamma}\vec{\Pi}^{\,2} + \frac{\gamma\omega_{\rm LO}^2}{2}\vec{P}^{\,2}\right). \tag{1.6}$$

In the above, the undetermined γ is to be found from the phenomenological theory.

Let us, therefore, consider the interaction energy between the electron and the polarization oscillations. From electrostatics, we know that the interaction energy density between an electric charge e at point $\vec{r}$ and a continuously distributed dipole density $\vec{P}(\vec{r}')$ is given by,

$$-e\vec{\nabla}_r\left(\frac{1}{|\vec{r}-\vec{r}'|}\right)\cdot\vec{P}(\vec{r}')d^3r'. \tag{1.7}$$

Integration with respect to $\vec{r}'$, gives the interaction Hamiltonian H_I,

$$H_I = -e\int d^3r'\vec{\nabla}_r\left(\frac{1}{|\vec{r}-\vec{r}'|}\right)\cdot\vec{P}(\vec{r}')\ . \tag{1.8}$$

To determine the free constant γ, for the time being, let us consider the electron to be stationary and investigate the equations of motion for the polarization vibrations under the influence of the electron. With the Hamiltonian $H = H_P + H_I$, the Hamilton's equations of motion,

$$\dot{P}_i = \frac{\delta H}{\delta \Pi_i} \qquad \dot{\Pi}_i = -\frac{\delta H}{\delta P_i} \qquad i = x, y, z \tag{1.9}$$

lead us to the following equation;

$$\gamma\left(\ddot{\vec{P}}(\vec{r}') + \omega_{\rm LO}^2\vec{P}(\vec{r}')\right) = -e\vec{\nabla}_r\left(\frac{1}{|\vec{r}-\vec{r}'|}\right). \tag{1.10}$$

Notice that the right-hand side of the equation represents simply the dielectric displacement $\vec{D}(\vec{r}')$ due to the electron. In the static case, i.e. $\dot{\vec{P}}(\vec{r}') = 0$, we have,

$$\gamma\omega_{\rm LO}^2\vec{P}(\vec{r}') = \vec{D}(\vec{r}')\ . \tag{1.11}$$

Using the relation between the field strength and the dielectric displacement,

$$\vec{D} = \vec{E} + 4\pi\vec{P}_{\rm tot} = \epsilon_0\vec{E}\ , \tag{1.12}$$

one can write,

$$4\pi\vec{P}_{\rm tot} = \left(1 - \frac{1}{\epsilon_0}\right)\vec{D}. \tag{1.13}$$

Here, $\vec{P}_{\rm tot} = \Delta\vec{P} + \vec{P}$ is the total polarization, which consists of two parts; one from the polarization of the electrons in the ionic shells, $\Delta\vec{P}$, and the other from the ionic displacements, $\vec{P}$. With an applied static field, both contributions develop fully, so that ϵ_0 is the static dielectric constant.

Since the effect of the polarization due to the electrons of ionic shells has already been accounted in the effective mass approximation for the electron, we are only interested in the contribution coming from the polarization of the lattice itself. To isolate this contribution, let us think of the external electron as having been suddenly created, in the lattice. Only the electrons are able to keep up with this sudden switch-on of the field, because the ions are much more inertial than the electrons. Consequently, we obtain a formula relating $\Delta\vec{P}$ to $\vec{D}$, similar to Eq.(1.13), but where now ϵ_0 is replaced by the high frequency dielectric constant ϵ_∞;

$$4\pi\Delta\vec{P} = \left(1 - \frac{1}{\epsilon_\infty}\right)\vec{D}. \tag{1.14}$$

Therefore, for the part of the polarization due to the lattice vibrations, we obtain,

$$4\pi\vec{P} = \left(\frac{1}{\epsilon_\infty} - \frac{1}{\epsilon_0}\right)\vec{D} = \frac{1}{\bar{\epsilon}}\vec{D}. \tag{1.15}$$

Comparing the Eqs.(1.11) and (1,15), the value of γ is obtained as

$$\gamma = \frac{4\pi\bar{\epsilon}}{\omega_{\rm LO}^2} \quad . \tag{1.16}$$

Having found γ, we can proceed with the quantization of the polarization field, as a consequence of which $H_P \rightarrow H_{\rm ph}$ and $H_I \rightarrow H_{\rm e-ph}$. However, before that, let us express the interaction part of the Hamiltonian in Eq.(1.8), in a more convenient form. Using the relation

$$\begin{aligned} \vec{\nabla}_r\left(\frac{1}{|\vec{r}-\vec{r}'|}\right)\cdot\vec{P}(\vec{r}') &= -\vec{\nabla}_{r'}\left(\frac{1}{|\vec{r}-\vec{r}'|}\right)\cdot\vec{P}(\vec{r}') \\ &= -\vec{\nabla}_{r'}\cdot\left(\frac{\vec{P}(\vec{r}')}{|\vec{r}-\vec{r}'|}\right) + \left(\frac{1}{|\vec{r}-\vec{r}'|}\right)\vec{\nabla}_{r'}\cdot\vec{P}(\vec{r}') \end{aligned} \tag{1.17}$$

the contribution coming from the first term after the substitution in Eq.(1.8), becomes zero due to the boundary conditions, and H_I reduces to,

$$H_I = -\int d^3r'\frac{e}{|\vec{r}-\vec{r}'|}\vec{\nabla}_{r'}\cdot\vec{P}(\vec{r}') \ . \tag{1.18}$$

An important remark pertaining to this form of the interaction Hamiltonian is that the plane wave expansion of the term $\vec{\nabla}_{r'} \cdot \vec{P}(\vec{r}')$ contains only longitudinal waves. We are, therefore, confirmed in restricting our considerations only to the longitudinal lattice vibrations, from the beginning.

To quantize the polarization field, the conjugate variables $\vec{P}$ and $\vec{\Pi}$ are to be considered as operators obeying the commutation relation,

$$[\Pi_i, P_j] = -i\hbar\delta_{ij} \qquad i,j = x,y,z \ . \tag{1.19}$$

The phonon annihilation and creation operators are defined as,

$$\begin{aligned} \vec{A}(\vec{r}) &= \sqrt{\frac{\gamma\omega_{\mathrm{LO}}}{2\hbar}}\vec{P}(\vec{r}) + i\frac{1}{\sqrt{2\gamma\hbar\omega_{\mathrm{LO}}}}\vec{\Pi}(\vec{r}) \\ \vec{A}^{\dagger}(\vec{r}) &= \sqrt{\frac{\gamma\omega_{\mathrm{LO}}}{2\hbar}}\vec{P}(\vec{r}) - i\frac{1}{\sqrt{2\gamma\hbar\omega_{\mathrm{LO}}}}\vec{\Pi}(\vec{r}) \end{aligned} \tag{1.20}$$

with

$$\left[A_i(\vec{r}), A_j^{\dagger}(\vec{r}')\right] = \delta_{ij}\ \delta(\vec{r} - \vec{r}') \ . \tag{1.21}$$

Expanding the operators in plane waves;

$$\begin{aligned} \vec{A}(\vec{r}) &= \frac{1}{\sqrt{V}}\sum_Q \frac{\vec{Q}}{Q}\, a_Q\, e^{i\vec{Q}\cdot\vec{r}} \\ \vec{A}^{\dagger}(\vec{r}) &= \frac{1}{\sqrt{V}}\sum_Q \frac{\vec{Q}}{Q}\, a_Q^{\dagger}\, e^{-i\vec{Q}\cdot\vec{r}} \end{aligned} \tag{1.22}$$

where V is the normalization volume and $\vec{Q}$ is the phonon wave vector, the commutation relation (1.21) implies for the new operators,

$$\left[a_i, a_j^{\dagger}\right] = \delta_{ij} \qquad \text{and} \qquad [a_i, a_j] = \left[a_i^{\dagger}, a_j^{\dagger}\right] = 0 \ . \tag{1.23}$$

Inverting the set of equations (1.20) and substituting $\vec{A}(\vec{r})$ and $\vec{A}^{\dagger}(\vec{r})$ as given in Eq.(1.22), we have,

$$\begin{aligned} \vec{P}(\vec{r}) &= \sqrt{\frac{\hbar}{2\gamma\omega_{\mathrm{LO}}V}}\sum_Q \frac{\vec{Q}}{Q}\left(a_Q e^{i\vec{Q}\cdot\vec{r}} + a_Q^{\dagger}e^{-i\vec{Q}\cdot\vec{r}}\right) \\ \vec{\Pi}(\vec{r}) &= i\sqrt{\frac{\gamma\hbar\omega_{\mathrm{LO}}}{2V}}\sum_Q \frac{\vec{Q}}{Q}\left(a_Q^{\dagger}e^{-i\vec{Q}\cdot\vec{r}} - a_Q e^{i\vec{Q}\cdot\vec{r}}\right) \end{aligned} \tag{1.24}$$

Inserting these expressions in equations (1.6) and (1.18), we obtain,

$$\begin{aligned} H_{\rm ph} &= \hbar\omega_{\rm LO}\sum_Q a_Q^\dagger a_Q \\ H_{\rm e-ph} &= \sum_Q \left(V_Q a_Q e^{i\vec{Q}\cdot\vec{r}} + V_Q^* a_Q^\dagger e^{-i\vec{Q}\cdot\vec{r}}\right) \end{aligned} \tag{1.25}$$

where $V_Q = -i4\pi\sqrt{e^2\hbar/2\gamma\omega_{\rm LO}V}(1/Q)$ is the interaction amplitude. With the value of γ as given in Eq.(1.16) substituted in, and choosing $\hbar\omega_{\rm LO}$ as a unit of energy, $u = (\hbar/2m^*\omega_{\rm LO})^{1/2}$ as a unit of length, i.e. making the following scaling transformations,

$$H \rightarrow \hbar\omega_{\rm LO}H \qquad \vec{r} \rightarrow u\,\vec{r} \qquad \vec{Q} \rightarrow \vec{Q}/u \qquad V \rightarrow u^3V \tag{1.26}$$

the dimensionless Fröhlich Hamiltonian, in its well established form, is written as

$$H = p^2 + V_{\rm conf}(\vec{r};\{\Omega_i\}) + \sum_Q a_Q^\dagger a_Q + \sum_Q V_Q\left(a_Q e^{i\vec{Q}\cdot\vec{r}} + a_Q^\dagger e^{-i\vec{Q}\cdot\vec{r}}\right) \tag{1.27}$$

where now,

$$V_Q = \sqrt{\frac{4\pi\alpha}{V}}\frac{1}{Q} \tag{1.28}$$

is taken as real for notational convenience, and in which,

$$\alpha = \frac{e^2}{2}\left(\frac{1}{\epsilon_\infty} - \frac{1}{\epsilon_0}\right)\sqrt{\frac{2m^*\omega_{\rm LO}}{\hbar}}\frac{1}{\hbar\omega_{\rm LO}} \tag{1.29}$$

is the dimensionless electron-phonon coupling constant.

The polaron calculations are performed generally in dimensionless units. It is convenient to choose $\hbar = \omega_{\rm LO} = 1$, to facilitate the notation. If further, $2m^* = 1$ is chosen, the form of the Hamiltonian in Eq.(1.27) remains the same, but if $m^* = 1$ is the choice, the scaling unit length becomes $u = 1/\sqrt{2}$, so that we have a factor of $1/2$ in front of p^2, also the interaction amplitude becomes modified as $V_Q = (2\sqrt{2}\alpha/V)^{1/2}(1/Q)$, where the numerical value of α remains the same for both cases.

The Hamiltonian derived in this section, will be the starting point for all the calculations to be presented in this work. Since the exact solution of the

Material	α	$\hbar\omega_{\mathrm{LO}}$ (meV)
KCl	5.6	26.7
NaCl	5.5	33.6
AgBr	1.56	17.1
CdTe	0.40	20.8
InP	0.11	43.3
GaAs	0.07	36.8
InAs	0.05	30.2

Table 1.1: Coupling constants and LO-phonon frequencies of some common materials
Note that these experimental values correspond to liquid helium temperature and one may expect slightly larger values at 0°K.

Hamiltonian is not available, we will consider several approximation methods, common in the literature, for obtaining the ground state properties of the polaron, giving most emphasis to the bulk phonon effects on the low dimensionally confined electron.

In the next section we will briefly mention those approximation techniques, which will be dealt with in more detail, in the following chapters.

1.2 Approximation Methods

In the Fröhlich Hamiltonian, when expressed in units of $\hbar\omega_{\mathrm{LO}}$, all the material dependent parameters are summed up into the dimensionless constant α. The numerical value of this electron-phonon interaction constant can be quite different for different types of the materials, ranging from ~ 0.01 up to ~ 10. It is large for highly polar materials such as alkali halides, whereas it is small for compound semiconductors. In Table 1.1 we list the values of α and the energy unit $\hbar\omega_{\mathrm{LO}}$ for several common materials, as calculated with the given data in a review article by Kartheuser.[29]

The interpretation of the polaron problem and its mathematical structure are

relatively simple and well understood in the asymptotic limits of the interaction strength. One of the basic points of view is the case where the kinetic energy of the electron is much smaller than the energy of the phonon modes, and $\alpha \ll 1$. In this case the lattice deformation tends to follow the electron, as it moves through the crystal. A reasonable treatment to such a case is to take the electron-phonon interaction, $H_{\mathrm{e-ph}}$, as a perturbation[6,30–35] and to calculate the corrections to the energy eigenvalues brought about by the polaron effect.

Another approach which successfully gives a good description of the behavior of the electron and its concomitant lattice deformation at weak coupling has been developed by Lee, Low and Pines[36] (LLP). This theory is of variational nature and leads to essentially the same results as the perturbation theory in the leading order in α, but this approximation remains valid for a broader domain of the coupling constant, therefore, it is generally referred to as the intermediate coupling theory. They have introduced a canonical transformation which eliminates the electron coordinates from the Hamiltonian. The LLP approximation became particularly influential and it has been applied as an important tool in many subsequent publications.[37–43]

A contrasting point of view originates from the idea that for a strong enough electron-phonon interaction ($\alpha \gg 1$) the electron goes into a bound state with a highly localized wave function in the self-induced potential, which is built up by the field of correlated virtual phonons.[44] If the electron is really deeply bound, one expects the lattice deformation to react back and produce some structure in the electronic wave function, and the presence of the electron in turn determines and maintains the size and shape of the deformation. The point of view presented by these arguments is referred to as the strong coupling (adiabatic) theory. The method, basically consists of proposing a trial wave function for the electron with some parameters, and making use of the variational principle, to calculate the ground state polaron properties. There are several other works on the strong coupling theory,[45,47–53,15,54] in the literature. Since for the bulk, the strong coupling theory gives dependable results only at some unrealistic values of the coupling constant, ($\alpha > 10$), it can be considered as an academic theory,

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

Table 1.2: Results of perturbation and strong coupling theories for the polaron properties
Polaron ground state energy, E_g, is in units of $\hbar\omega_{LO}$ and the polaron mass, m_p, is taken in units of electron band mass m^*.

but however, as we will see, the confinement effects bring about the concept of pseudo-enhancement in the electron-phonon coupling, extending the domain of validity of this approach in low dimensional systems.

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

It is seen that the functional dependences of the ground state energy and phonon contribution to effective mass $(m_p - 1)$, on α, are quite different at the two limiting regimes. Besides, the numerical coefficients get considerably larger with the reduction in the dimensionality (cf. Table 1.3).

Recently, Peeters *et al.*[55] have derived an interesting scaling relation for (2D) polaron properties, taking (3D) case as a reference;

$$E_g^{(2D)}(\alpha) = \frac{2}{3} E_g^{(3D)}\left(\frac{3\pi}{4}\alpha\right) \qquad \text{and} \qquad m_p^{(2D)}(\alpha) = m_p^{(3D)}\left(\frac{3\pi}{4}\alpha\right). \qquad (1.30)$$

Similar relations hold true for other physical quantities of interest, such as mean number of phonons, linear mobility and impedance function. The form of the relations in Eq.(1.30) immediately signals the mentioned pseudo-enhancement of the interaction strength in low dimensional systems.

For a more general view of the problem, not restricted to the limiting regimes, one requires more powerful methods or interpolating approximations. One of

	$E_g(3D \rightarrow 2D)$	$m_p - 1(3D \rightarrow 2D)$
$\alpha \ll 1$	1.57	2.36
$\alpha \gg 1$	3.70	30.82

Table 1.3: Scaling factors for polaron properties from 3D to 2D

such methods, which can be named as a "perturbative variational approach", has been introduced by Devreese *et al.* in an application to bound polaron.[56] The procedure is an extension of the adiabatic approximation, in the sense that a strongly coupled polaron state combined with a first order perturbative extension is used as a variational trial state, by which it is possible to achieve a satisfying extrapolation towards the weak coupling regime. It has been recently applied to 3D and 2D free polarons[57] successfully, and also we will consider the quantum wire[58] and magneto-polaron[59] applications in the following chapters.

The final approach to polaron problem, to be stated here, is the Feynman path integral formalism. It is the most successful theory, in the sense that it provides superior upper bound for the ground state energy of the Fröhlich polaron at arbitrary electron-phonon coupling strength, compared to the other approximations. It has been first applied to bulk polaron by Feynman[60] in 1955, and became an indispensable tool for the study of the Fröhlich polaron. The pioneering work of Feynman, initiated the development of functional-integral methods in the polaron theory, which, with refined variational procedures, proved to be an extremely powerful tool, if not the most powerful. There are very elegant applications of functional-integral methods in the literature,[61–76] and the Feynman path integral formalism applied to the case of general quadratic confinement,[77] will be presented in the sixth chapter.

Chapter 2

PERTURBATION THEORY

When the electron-phonon interaction constant α is small, as it is, in most of the semiconductor compounds, it is appropriate to consider the interaction term of the Fröhlich Hamiltonian as a perturbation. The unperturbed Hamiltonian then, describes a decoupled system of an electron and phonons. The effect of electron-phonon interaction leads to small corrections for the eigenstates and eigenenergies of the unperturbed Hamiltonian, in the form of a power series in α. To demonstrate the approach of the perturbation theory consider the following Hamiltonian, in which $H^{(1)}$ is small compared to the unperturbed part, $H^{(0)}$.

$$H = H^{(0)} + H^{(1)} \tag{2.1}$$

For the polaron problem we have,

$$H^{(0)} = H_{\rm e} + H_{\rm ph}\,, \qquad H^{(1)} = H_{\rm e-ph}\,. \tag{2.2}$$

The solution of the Schrödinger equation

$$H\,|\Psi_n\rangle = E_n\,|\Psi_n\rangle \tag{2.3}$$

can be expanded in a perturbation series of the form,

$$\begin{aligned} |\Psi_n\rangle &= |\Psi_n^{(0)}\rangle + |\Psi_n^{(1)}\rangle + |\Psi_n^{(2)}\rangle + \cdots \\ E_n &= E_n^{(0)} + E_n^{(1)} + E_n^{(2)} + \cdots \end{aligned} \tag{2.4}$$

where n stands for all the quantum numbers characterizing the system. Substituting these series in Eq.(2.3), one can consider the terms with the same order independently. The zeroth-order terms give simply the equation for the unperturbed Hamiltonian,

$$H^{(0)}\,|\Psi_n^{(0)}\rangle = E_n^{(0)}\,|\Psi_n^{(0)}\rangle\,, \tag{2.5}$$

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

$$E_n^{(1)} = \langle\,\Psi_n^{(0)}|\,H^{(1)}\,|\Psi_n^{(0)}\rangle\,. \tag{2.6}$$

For the polaron, as we will see, this first order correction becomes zero, so one should consider the next order correction for the energy,

$$E_n^{(2)} = \sum_m{}' \frac{|\langle\,\Psi_n^{(0)}|\,H^{(1)}\,|\Psi_m^{(0)}\rangle\,|^2}{E_n^{(0)} - E_m^{(0)}}\,. \tag{2.7}$$

Finally, for the eigenstates, the perturbation theory leads to the correction term

$$|\Psi_n^{(1)}\rangle = \sum_m{}' \frac{|\Psi_m^{(0)}\rangle\langle\,\Psi_m^{(0)}|\,H^{(1)}\,|\Psi_n^{(0)}\rangle}{E_n^{(0)} - E_m^{(0)}} \tag{2.8}$$

in the leading order.

2.1 Application: Quasi 2-Dimensional Polaron

Among the polaron papers,[32–34] in which perturbation theory has been applied, we will consider a recent one by Yıldırım and Erçelebi[35] as an example. In that work, they have attempted to give a unifying picture for all confinement geometries of weakly coupled polaron. It is instructive to review the essential steps of the formulation given therein, since in Chapter 6, the same problem will be treated within the framework of path integral formalism and the correspondence between the two methodologies will be discussed.

The simple model adopted in that work, is capable of reflecting the ground state property of the confined polaron, where the degree of confinement can

be chosen flexibly, through the usage of an anisotropic parabolic potential box. However, here we will consider the quasi-2 dimensional slab-like configuration for the confinement of the electron.

With the appropriate units ($2m^* = \hbar = \omega_{\rm LO} = 1$), the Hamiltonian describing the confined electron coupled to LO-phonons is in the form as given in Eq.(1.27). For the confining potential,

$$V_{\rm conf} = \frac{1}{4}\Omega^2 z^2 \tag{2.9}$$

has been chosen, where the dimensionless frequency Ω in units of $\omega_{\rm LO}$ is the measure of the degree of confinement in the z-direction. By varying Ω from zero to values much larger than unity, one can achieve a continuous transition from bulk to the strict 2-dimensional geometry.

The unperturbed states of the system is expressed in a product form of the electron and phonon parts,

$$|\Psi^{(0)}_{\vec{k},\nu,n_Q}\rangle = |\Phi_{\vec{k},\nu}(\vec{\varrho},z)\rangle\ |n_Q\rangle \tag{2.10}$$

where the electronic part satisfies the wave equation

$$H_{\rm e}\,|\Phi_{\vec{k},\nu}(\vec{\varrho},z)\rangle = \epsilon_\nu(\vec{k})\,|\Phi_{\vec{k},\nu}(\vec{\varrho},z)\rangle \qquad \nu = 0,1,2,... \tag{2.11}$$

The electronic wave function is composed of harmonic oscillator states for the z-direction, and since the electron is free in the transverse directions, a plane wave representation is utilized for its motion parallel to the x-y plane,

$$|\Phi_{\vec{k},\nu}(\vec{\varrho},z)\rangle = \frac{1}{\sqrt{2^\nu \nu!}}\left(\frac{\Omega}{2\pi}\right)^{1/4} H_\nu\left(\sqrt{\frac{\Omega}{2}}z\right)\exp(-\frac{1}{4}\Omega z^2)\ \phi_{\vec{k}}(\vec{\varrho}) \tag{2.12}$$

$$\phi_{\vec{k}}(\vec{\varrho}) \sim \exp(i\vec{k}\cdot\vec{\varrho}) \tag{2.13}$$

with H_ν denoting the Hermite polynomial of degree ν. The corresponding energy eigenvalues of Eq.(2.11) are then given by

$$\epsilon_\nu(\vec{k}) = (\nu + \frac{1}{2})\Omega + k^2\,. \tag{2.14}$$

The phonon state $|n_Q\rangle$ is the Fock number state, with the ground state (phonon vacuum), $|0\rangle$, characterized as;

$$a_Q\,|0\rangle = 0\ . \tag{2.15}$$

For the ground state of the polaron, the electron should also be taken in the lowest subband ($\nu = 0$).

The first non-vanishing contribution to the ground state energy comes from the second order term, as given in Eq.(2.7),

$$E_{\rm g}^{(2)} = -\sum_{Q}\sum_{\vec{k}'}\sum_{\nu} \frac{|\langle \Psi^{(0)}_{\vec{k}',\nu,1_Q}| H_{\rm e-ph} |\Psi^{(0)}_{\vec{k},0,0}\rangle|^2}{1+\epsilon_\nu(\vec{k}')-\epsilon_0(\vec{k})} \ . \tag{2.16}$$

With the form (1.27) of the Fröhlich interaction, the above equation can be written alternatively as,

$$E_{\rm g}^{(2)} = -\sum_{Q} V_Q^2 \sum_{\vec{k}'}\sum_{\nu} \frac{|\langle \phi_{\vec{k}'}| \exp(-i\vec{q}\cdot\vec{\varrho})|\phi_{\vec{k}}\rangle|^2}{1+\Omega\nu+k'^2-k^2} |h_\nu(q_z)|^2 \tag{2.17}$$

where

$$\begin{aligned} h_\nu(q_z) &= \frac{1}{\sqrt{2^\nu \nu!}}\left(\frac{\Omega}{2\pi}\right)^{1/2}\int_{-\infty}^{\infty} dz \exp(-iq_z z)\, H_\nu\left(\sqrt{\frac{\Omega}{2}}z\right)\exp(-\frac{1}{2}\Omega z^2) \qquad (2.18)\\ &= \frac{(-i)^\nu}{\sqrt{\nu!}}\left(\frac{q_z^2}{\Omega}\right)^{\nu/2}\exp\left(-\frac{q_z^2}{2\Omega}\right) . \end{aligned}$$

Projecting out the $\vec{k}'$ summation one obtains

$$E_{\rm g}^{(2)} = -\sum_{Q} V_Q^2 \sum_{\nu}\frac{1}{\nu!}\frac{1}{1+\Omega\nu+q^2-2\vec{k}\cdot\vec{q}}\left(\frac{q_z^2}{\Omega}\right)^\nu \exp\left(-\frac{q_z^2}{\Omega}\right) . \tag{2.19}$$

It should be noted that, in the ground state, the electron is stationary ($\vec{k}=0$). However, to keep trace of the effective mass of the polaron, one can consider the electron to have a small momentum ($\vec{k}\simeq 0$), and expand the summand in Eq.(2.19) in a power series up to second order in $\vec{k}\cdot\vec{q}$,

$$E_{\rm g}^{(2)} = -\sum_{Q} V_Q^2 \exp\left(-\frac{q_z^2}{\Omega}\right)\sum_{\nu}\frac{1}{\nu!}\left(\frac{q_z^2}{\Omega}\right)^\nu\left(\frac{1}{1+\Omega\nu+q^2}+\frac{(2\vec{k}\cdot\vec{q})^2}{(1+\Omega\nu+q^2)^3}\right) . \tag{2.20}$$

Using the identity

$$\sum_{\nu=0}^{\infty}\frac{1}{\nu!}\frac{\beta^\nu}{(a+b\nu)^{n+1}} = \frac{1}{n!}\int_0^\infty d\eta\,\eta^n \exp(-a\eta+\beta e^{-b\eta}) \qquad n=0,1,2,\ldots \tag{2.21}$$

and defining

$$\sigma(\eta) = \frac{\Omega\eta}{1 - e^{-\Omega\eta}}\,, \tag{2.22}$$

the ground state energy, $E_{\rm g} = \frac{1}{2}\Omega + k^2 + E_{\rm g}^{(2)}$, can be written as,

$$E_{\rm g} = \frac{1}{2}\Omega - \mathcal{E}_{\rm p} + k^2(1-\mu) \tag{2.23}$$

where

$$\mathcal{E}_{\rm p} = \sum_Q V_Q^2 \int_0^\infty d\eta\, e^{-\eta} \exp\left[-(q^2 + \frac{q_z^2}{\sigma(\eta)})\eta\right] \tag{2.24}$$

and

$$\mu = \sum_Q V_Q^2\, q^2 \int_0^\infty d\eta\, \eta^2\, e^{-\eta} \exp\left[-(q^2 + \frac{q_z^2}{\sigma(\eta)})\eta\right]\ . \tag{2.25}$$

In the above, $\mathcal{E}_{\rm p}$ is the polaron binding energy and μ is the polaronic contribution to the composite inertia of the electron together with the concomitant cloud of virtual phonons, i.e.

$$m_{\rm p} = (1-\mu)^{-1} \simeq 1 + \mu \tag{2.26}$$

is the polaron effective mass in units of $m^\star$.

The evaluation of the integrals in Eq.(2.24) and (2.25) require numerical treatment for arbitrary values of Ω. For the two special cases, however, the analytic results are readily available. In the case of $\Omega = 0$, $\sigma(\eta) = 1$ and one obtains the results relevant to the bulk polaron. For the binding energy one has

$$\mathcal{E}_{\rm p}^{(3D)} = \sum_Q V_Q^2 \int_0^\infty d\eta\, e^{-\eta} \exp\left[-(q^2 + q_z^2)\eta\right] = \sum_Q \frac{V_Q^2}{1+Q^2} = \alpha\ . \tag{2.27}$$

Similarly, Eq.(2.25) reduces to

$$\begin{aligned} \mu^{(3D)} &= \sum_Q V_Q^2 q^2 \int_0^\infty d\eta\, \eta^2 e^{-\eta} \exp\left[-(q^2 + q_z^2)\eta\right] \qquad (2.28)\\ &= \sum_Q V_Q^2 q^2 \frac{2}{(1+Q^2)^3} = \frac{\alpha}{6}\ . \end{aligned}$$

In the strict $2D$ limit ($\Omega \to \infty$), $\sigma(\eta)$ tends to infinity, and the corresponding integrals simplify to

$$\mathcal{E}_{\rm p}^{(2D)} = \sum_Q \frac{V_Q^2}{1+q^2} = \frac{\pi}{2}\alpha \tag{2.29}$$

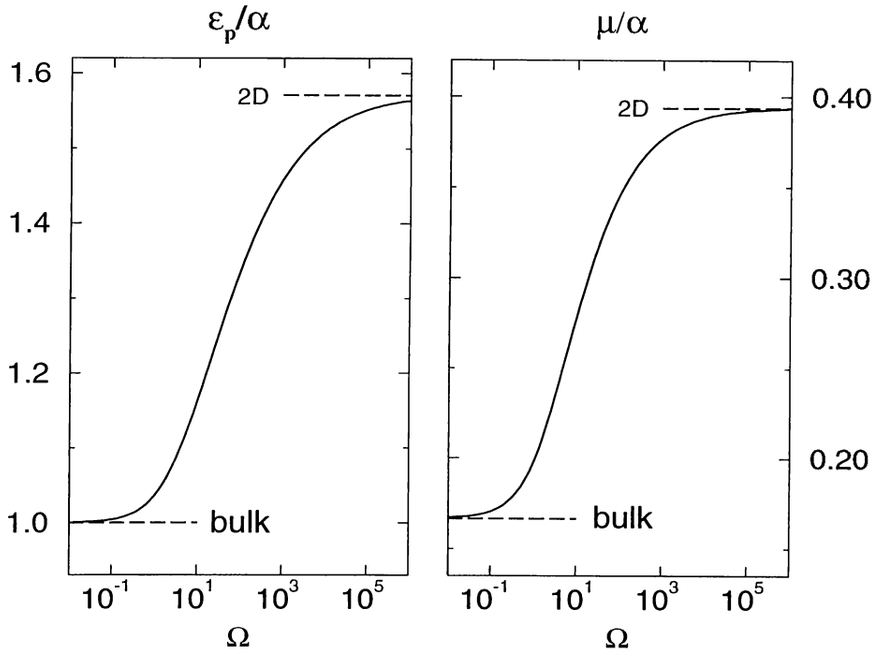

Figure 2.1: Perturbation theory results for quasi-2-dimensional polaron The binding energy $\mathcal{E}_{\rm p}$, and the phonon correction to the effective mass μ as functions of the degree of confinement Ω.

and

$$\mu^{(2D)} = \sum_Q V_Q^2 q^2 \frac{2}{(1+q^2)^3} = \frac{\pi}{8}\alpha \ . \tag{2.30}$$

The binding energy and the phonon contribution to the effective mass as functions of the degree of confinement, are provided in Fig.2.1. With the increasing value of Ω, both $\mathcal{E}_{\rm p}$ and μ approach smoothly to their asymptotic two-dimensional values.

For a total overview interpolating between all possible extremes of the effective dimensionality one should refer back to the Eq.(2.2) and revise the calculations with a more general confining potential,

$$V_{\rm conf} = \frac{1}{4}\Omega_1^2\varrho^2 + \frac{1}{4}\Omega_2^2 z^2 \ . \tag{2.31}$$

The binding energy thus obtained is given in the same form as in Eq.(2.24) where now it reads as

$$\mathcal{E}_{\rm p} = \sum_Q V_Q^2 \int_0^\infty d\eta\, e^{-\eta} \exp\left[-(\frac{q^2}{\sigma_1(\eta)} + \frac{q_z^2}{\sigma_2(\eta)})\eta\right] \tag{2.32}$$

	$\mathcal{E}_p/\alpha$		
Ω_1 and/or Ω_2	slab ($\Omega_1 = 0$)	wire ($\Omega_2 = 0$)	box ($\Omega_1 = \Omega_2$)
10	1.16	1.44	2.02
100	1.33	2.23	5.72

Table 2.1: Comparison of polaron binding energies in different confinement geometries

with

$$\sigma_i(\eta) = \frac{\Omega_i \eta}{1 - e^{-\Omega_i \eta}} \qquad i = 1, 2 \; . \tag{2.33}$$

Projecting out the summations over the wave vector components one obtains,

$$\mathcal{E}_p = \frac{\alpha}{\sqrt{\pi}} \int_0^\infty d\eta e^{-\eta} \sqrt{\frac{\sigma_2(\eta)}{\eta}} \frac{\arctan \gamma(\eta)}{\gamma(\eta)} \tag{2.34}$$

where

$$\gamma(\eta) = \left(\frac{\sigma_2(\eta)}{\sigma_1(\eta)} - 1 \right)^{1/2} \tag{2.35}$$

The solution of Eq.(2.34) requires numerical treatment. By varying the potential parameters Ω_i, one can trace out all possible extremes of the effective dimensionality. For a comparison of the different confinement geometries, consider the data given in Table 2.1. The binding gets deeper as the electron confinement is increased.

The domain of validity of perturbation theory is restricted to small values of α. In certain compound semiconductor structures, such as II-VI compounds, the relevant coupling constants cannot be regarded as sufficiently small ($\alpha \simeq 0.4$ for CdTe, for instance) for the perturbation approach to be totally dependable. Moreover, we have mentioned about the pseudo-enhancement in α, realized in confined systems, bringing about a strong coupling counterpart to the problem. Therefore, one requires alternative methods to deal with intermediate and strong coupling regimes, and yet more powerful interpolating theories to get a unifying picture over the complete range of α. Those theories will be the subject matter of the following chapters.

Chapter 3

STRONG COUPLING THEORY

When the electron-phonon interaction is strong enough, due to the phonon field, there induces a deep deformation potential surrounding the electron, and it appears to be trapped in this potential. With this consideration, the polaron, in strong coupling regime was studied by Pekar[44] (and others[45,46,37]) who hypothesized that in this limit the total ground state wave function could be taken as a product of an electronic function and a phonon part. The Pekar ansatz is based on the physically appealing notion that, at large coupling, the phonons cannot follow the rapidly moving electron (as they do at weak coupling) and so resign themselves to interacting only with the mean electronic density (adiabatic condition).

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

3.1 Displaced Oscillator Transformation

The Fröhlich polaron can be viewed as an assembly of harmonic oscillators interacting with the electron. Thus, considering one of the oscillators that of the assembly, the wave equation describing the coupling of the oscillator to the

electron is given by

$$H_Q \Psi_Q = \left(-\nabla^2_{X_Q} + \frac{1}{4} X_Q^2 - u_Q X_Q \right) \Psi_Q = \epsilon_Q \Psi_Q \tag{3.1}$$

where X_Q and ϵ_Q are the dimensionless coordinate and the energy of the oscillator with the wave vector $\vec{Q}$, and the parameter u_Q is the force term due to the interaction.

After completing to a square, the Eq.(3.1) takes the form

$$\left(-\nabla^2_{X_Q} + \frac{1}{4}(X_Q - 2u_Q)^2 - u_Q^2 \right) \Psi_Q = \epsilon_Q \Psi_Q \tag{3.2}$$

from which $2u_Q$ can be interpreted as the equilibrium coordinate. Assuming that all the phonon modes behave independently in the same way, the total Hamiltonian can be written in terms of the phonon creation and annihilation operators as,

$$H = \sum_Q \left[a_Q^\dagger a_Q - u_Q (a_Q^\dagger + a_Q) \right] . \tag{3.3}$$

The terms linear in $a_Q^\dagger$ and a_Q can easily be made to disappear by defining a set of new operators,

$$\tilde{a}_Q = a_Q - u_Q \qquad \tilde{a}_Q^\dagger = a_Q^\dagger - u_Q \tag{3.4}$$

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

$$\tilde{a}_Q = \mathbf{U}^{-1} a_Q \mathbf{U} \qquad \tilde{a}_Q^\dagger = \mathbf{U}^{-1} a_Q^\dagger \mathbf{U} \tag{3.5}$$

where

$$\mathbf{U} = \exp \sum_Q u_Q (a_Q - a_Q^\dagger) . \tag{3.6}$$

Instead of transforming the phonon operators, one can equivalently consider the phonon ground state to be chosen as $\mathbf{U}|0\rangle$ rather than the bare phonon vacuum $|0\rangle$, where the origin is shifted over to the equilibrium coordinates (cf. Fig.3.1). This kind of representation is widely known as displaced oscillator transformation.

Clearly, the amount by which the origin is to be displaced depends on the interaction strength and further on the electronic charge density in a somewhat

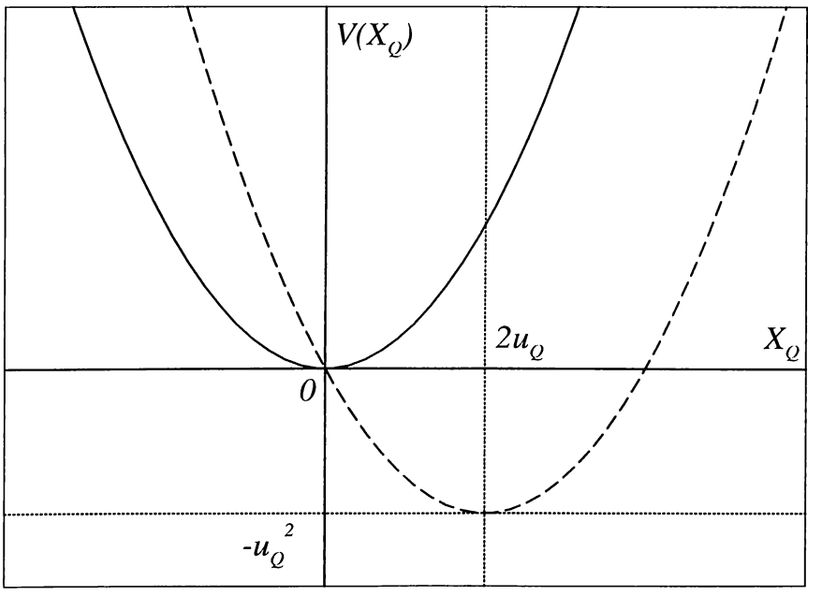

Figure 3.1: Sketch of displaced oscillator potential.
The solid and dashed curves represent undisplaced and displaced oscillators respectively.

implicit manner. Therefore, the procedure of strong coupling theory will consist of proposing a variational wave function for the electron and through the minimization of the ground state energy, determining the variational parameters and the terms u_Q simultaneously. In the rest of this chapter, we will exemplify these arguments in the case of strongly coupled polaron in a cylindrical quantum wire.[54]

3.2 Application: Infinite Boundary Quantum Wire

In this section we retrieve, within the strong-coupling theory, the quasi-one dimensional analog of the standard optical polaron relevant to a cylindrical quantum well wire. Under the assumption of perfect confinement the ground state binding energy, effective polaronic mass and the phonon-coupling - induced

potential well profiles will be given as functions of the wire radius and the electron-phonon interaction strength.

3.2.1 Introduction

Quantum well - heterostructure - type systems with reduced dimensionality have become important as a basis for novel devices, owing to the possibility of tailoring their electronic and optical properties. The impressive progress achieved in microfabrication technology (such as molecular beam epitaxy, lithographic and etching techniques) has created a variety of opportunities for the fabrication of new semiconductor structures. Of particular interest is the quantum well wire (QWW) configuration based on the confinement of electrons in a thin semiconducting wire where the motion is quantized in the transverse directions normal to its length. Since their early prediction[78] and subsequent fabrication,[79–82] there has appeared quite a large interest in phonon-coupling - induced effects and polaronic properties of one dimensionally confined electrons. Some considerable amount of the literature published within this context has been devoted to the interaction of electrons with bulk-like LO-phonons and the study of the relevant polaron properties.[16,17,19,35,53,83,84] The common prediction led by these works is that in quantum wires where the electrons are fundamentally quasi-one dimensional (Q1D) the polaronic binding is far much deeper than in comparable quasi-two dimensional systems. Alternatively stating, high degrees of confinement (as realized in thin wires) lead to a pseudo-enhancement in the effective electron-phonon coupling which in turn brings about the possibility that, in spite of weak polar coupling as in GaAs, for instance, the polaron problem may as well have a strong-coupling counterpart coming from confinement effects. This salient feature can be more prominent in II-VI compound semiconductors or in alkali halides where the relevant coupling strengths are almost an order of magnitude larger or even much stronger than those in III-V materials. We thus feel that for not too weak and pseudo-enhanced electron-phonon coupling, the strong-coupling polaron theory should not be accounted for as a totally academic

formalism but may serve so as to provide some insight into the study of polarons in confined media consisting of materials of somewhat strong polar crystals. Here we refer to the case of an electron perfectly confined within a cylindrical boundary with infinite potential, studying the ground state properties (the binding energy, mass and the phonon-coupling - induced effective potential) of the Q1D strong-coupling polaron as functions of the coupling strength and the QWW radius.

3.2.2 Theory

Hamiltonian and Wave Function

As always, we start with the Fröhlich Hamiltonian in dimensionless units in the form as it is given in Eq.(1.27). For the confining potential we adopt an infinite boundary cylindrical quantum wire of radius R,

$$V_{\rm conf}(\varrho) = \begin{cases} 0 & \text{if } \varrho < R \\ \infty & \text{if } \varrho > R \end{cases} \tag{3.7}$$

In cylindrical coordinates, $\vec{r} = (\vec{\varrho}, z)$, we take the electron trial wave function as consisting of two adjustable parameters λ and μ accounting for the anisotropic nature of the confined system

$$\Phi_e(\varrho, z) = (\lambda^2/\pi)^{1/4} \varphi(\varrho) \exp(-\frac{1}{2}\lambda^2 z^2)\ e^{iwz} \tag{3.8}$$

and

$$\varphi(\varrho) = n_\varrho \, \mathrm{J}_0(\kappa\varrho)\ \exp(-\frac{1}{2}\mu^2\varrho^2)\ . \tag{3.9}$$

In the above, the exponential factor e^{iwz} (with w being a further variational parameter) sets the system in motion, thus enabling one to trace the polaron mass along the wire axis. J_0 is the zeroth order cylindrical Bessel function of the first kind in which $\kappa = j_{0,1}/R$, where $j_{0,1} \approx 2.4048 \cdots$ is its first zero. The normalization constant n_ϱ is given through $2\pi \int_0^R d\varrho\, \varrho\, \varphi^2(\varrho) = 1$. With the form (3) adopted for the lateral part of the electron trial state, the Bessel function takes care of the geometric confinement, and the further confinement induced by phonon coupling is governed by the Gaussian counterpart through parameter μ.

Adiabatic Formulation

In the foregoing approximation we assume a highly rapid charge density fluctuations for the electron to which the lattice responds by acquiring a relaxed static deformation clothing the entire extent of the electron. Due to Pekar,[44] the adiabatic polaron ground state thus formed can be written in a product ansatz consisting of the electron and lattice parts, i.e.,

$$\Psi_{\rm g} = \Phi_e(\varrho, z)\ \mathbf{U}|\,0\,\rangle, \tag{3.10}$$

where $|\,0\,\rangle$ is the phonon vacuum state, and

$$\mathbf{U} = \exp\sum_Q u_Q(\Phi_e)(a_Q - a_Q^\dagger) \tag{3.11}$$

is the unitary displacement operator of the displaced oscillator transformation mentioned in the previous section, changing the reference system of virtual particles by an amount $u_Q(\Phi_e)$. It should be noted that simultaneous optimizations with respect to Φ_e and $u_Q(\Phi_e)$ correspond to the self-trapping picture of the polaron where the electron distribution and the lattice polarization influence each other in such a way that a stable relaxed state is eventually attained. Under the canonical transformation $H \rightarrow \mathbf{U}^{-1}H\mathbf{U}$, the Hamiltonian conforms to

$$\begin{aligned} H' = p^2 \ &+\ V_{\rm conf}(\varrho) + \sum_Q u_Q^2 - \sum_Q V_Q u_Q \left[\exp(i\vec{Q}\cdot\vec{r}) + {\rm cc}\right] \\ &+\ \sum_Q a_Q^\dagger a_Q + \sum_Q \left\{\left[V_Q \exp(i\vec{Q}\cdot\vec{r}) - u_Q\right] a_Q + {\rm hc}\right\} \end{aligned} \tag{3.12}$$

Since the Hamiltonian is invariant to translations of the electron together with its concomitant lattice distortion, the total momentum along the wire axis

$$\mathsf{P}_z = p_z + \sum_Q q_z a_Q^\dagger a_Q \tag{3.13}$$

must be conserved. The variation therefore requires an optimization of the polaron state $\Psi_{\rm g}$ which minimizes $\langle\,\Psi_{\rm g}\,|H|\,\Psi_{\rm g}\,\rangle$ subject to the constraint that $\langle\,\Psi_{\rm g}\,|\mathsf{P}_z|\,\Psi_{\rm g}\,\rangle$ is a constant of motion. Thus, minimizing the functional

$$\mathsf{F}(\lambda, \mu, v_z; w, u_Q) \ \equiv\ \langle\,\Phi_e\,|\,\langle\,0\,|\mathbf{U}^{-1}(H - v_z\mathsf{P}_z)\mathbf{U}|\,0\,\rangle\,|\,\Phi_e\,\rangle \tag{3.14}$$

with respect to w and u_Q yields

$$w = \frac{1}{2}v_z \qquad \text{and} \qquad u_Q(\Phi_e) = V_Q s_Q \eta_Q \tag{3.15}$$

where

$$s_Q = \langle \Phi_e \,|\exp(\pm i\vec{Q}\cdot\vec{r})|\, \Phi_e \rangle \tag{3.16}$$

$$\eta_Q = (1 - v_z q_z)^{-1} \tag{3.17}$$

in which the Lagrange multiplier v_z is to be identified as the polaron velocity[85,86] along the wire axis, as it turns out.

In what follows we adopt the case of a stationary polaron, i.e. take $\langle \Phi_e \,|\mathbf{U}^{-1}\mathsf{P}_z\mathbf{U}|\, \Phi_e \rangle$ as zero, and thus regard v_z as a virtual velocity which we retain in the foregoing steps to keep track of the effective mass of the coupled electron-phonon complex.

In complete form, with the optimal fits for w and u_Q substituted in, Eq.(3.14) takes the form

$$\mathsf{F}(\lambda, \mu, v_z) = \epsilon_k + \sum_Q V_Q^2 s_Q^2(\eta_Q^2 - 2\eta_Q) - \frac{1}{4}v_z^2 - \sum_Q V_Q^2 s_Q^2 \eta_Q^2 v_z q_z \tag{3.18}$$

where $\epsilon_k = \langle \Phi_e \,|p^2|\, \Phi_e \rangle$.

In order to trace out the polaron mass from the above equation we have to split the right hand side into its parts consisting of the binding energy of the polaron alone and the additional kinetic contribution which shows up after having imposed a virtual momentum on the polaron. We are thus tempted to expand the summands in Eq.(3.18) in a power series up to order v_z^2. We obtain

$$\mathsf{F}(\lambda, \mu, v_z) = E_{\mathrm{g}}(\lambda, \mu) - \frac{1}{4}v_z^2 m_{\mathrm{p}} \tag{3.19}$$

where

$$E_{\mathrm{g}}(\lambda, \mu) = \epsilon_k - \sum_Q V_Q^2 s_Q^2 \tag{3.20}$$

refers to the ground state energy and the factor m_{p} multiplying $\frac{1}{4}v_z^2$ is identified as the polaron mass, given by

$$m_{\mathrm{p}} = 1 + \sum_Q V_Q^2 s_Q^2 q_z^2 \tag{3.21}$$

Defining

$$\sigma^{(n)}_{mm'}(x) = \int_0^{j_{0,1}} dt\ t^n \mathrm{J}_m(t)\,\mathrm{J}_{m'}(t)\,\mathrm{J}_0(xt)\exp(-\frac{\mu^2}{\kappa^2}t^2)\ , \tag{3.22}$$

we write the following expressions for ϵ_k and s_Q which take part in Eq.(3.20) and (3.21)

$$\epsilon_k = \frac{1}{2}\lambda^2 + \kappa^2 + \mu^2\{2 - \frac{2\sigma^{(2)}_{10}(0) - (\mu/\kappa)^2\sigma^{(3)}_{00}(0)}{\sigma^{(1)}_{00}(0)}\}\ , \tag{3.23}$$

and

$$s_Q = r_q\ \exp(-\frac{q_z^2}{4\lambda^2})\ , \tag{3.24}$$

with

$$r_q = \frac{\sigma^{(1)}_{00}(q/\kappa)}{\sigma^{(1)}_{00}(0)}\ . \tag{3.25}$$

Projecting out the $\vec{Q}$-summations: $\sum_Q V_Q^2 s_Q^2 q_z^{2n}$, we further write

$$E_{\mathrm{g}}(\lambda,\mu) = \epsilon_k - \alpha\int_0^\infty dq\ r_q^2 f_q\ , \tag{3.26}$$

and

$$m_{\mathrm{p}} = 1 + \alpha\int_0^\infty dq\ r_q^2\ \{\sqrt{\frac{2}{\pi}}\lambda - q f_q\}\ , \tag{3.27}$$

where

$$f_q = \exp(\frac{q^2}{2\lambda^2})\ \mathrm{erfc}(\frac{q}{\sqrt{2}\lambda})\ , \tag{3.28}$$

with erfc denoting the complementary error function.

3.2.3 Results and Conclusions

In order to obtain the binding energy and effective mass correction of the polaron we numerically minimize Eq.(3.26) with respect to the variational parameters μ and λ. The parameters thus determined are displayed against the wire radius for a succession of strong α values in Fig.3.2(a). It is seen that for large wire radii the curves for μ and λ both have the same asymptotic 3D limit ($\mu = \lambda = \sqrt{2/9\pi}\alpha$), and as R is made to approach the bulk - polaron size the curves begin to split depicting the anisotropy due to the confinement imposed by the wire boundary. We note that the place at which the anisotropy starts to show up gets shifted to

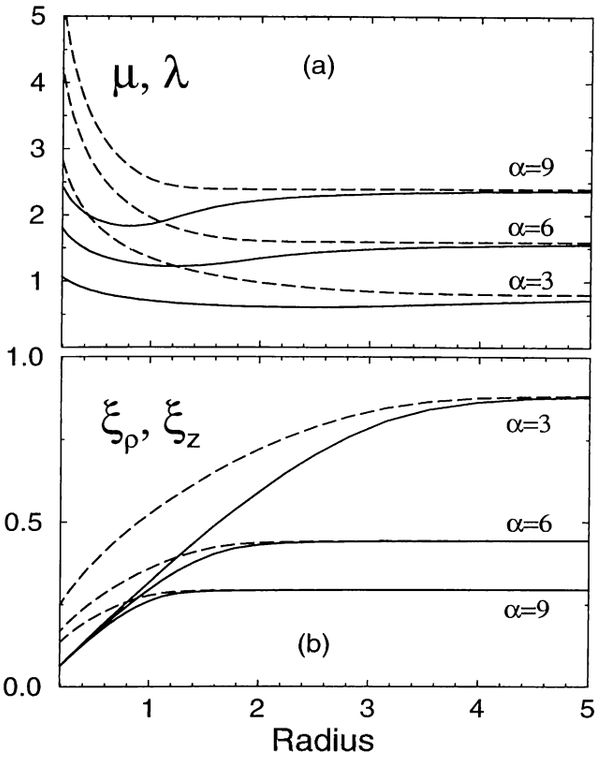

Figure 3.2: The variational parameters and spatial extents as functions of radius (a) The variational parameters μ (solid curve) and λ (dashed curve), and (b) the spatial extents ξ_ϱ (solid) and ξ_z (dashed) of the polaron as a function of the wire radius.

smaller R values for stronger phonon coupling since for large α the starting state of the polaron is already a highly-localized one (as implied by the relatively large values of the parameters μ and λ) and a smaller - sized polaron feels the effect of the confining boundary only for smaller wire radius.

For a complementary understanding of the variation of the spatial extent of the polaron in the lateral and longitudinal directions, we also provide plots (Fig.3.2(b)) of the direct measures of localization of the electron coordinates expressed in terms of the corresponding rms - values given by

$$\xi_\varrho = \left\{ \langle \Phi_e | \frac{1}{2}\varrho^2 | \Phi_e \rangle \right\}^{1/2} = \kappa^{-1}\sqrt{\sigma_{00}^{(3)}/\sigma_{00}^{(1)}} \tag{3.29}$$

and

$$\xi_z = \left\{ \langle \Phi_e | z^2 | \Phi_e \rangle \right\}^{1/2} = (2\lambda^2)^{-1/2} \ . \tag{3.30}$$

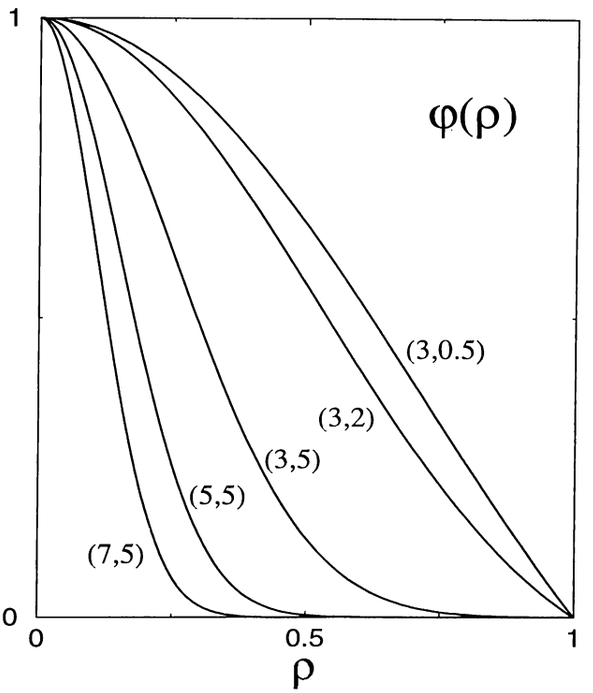

Figure 3.3: Radial part of electronic wave function $\varphi(\varrho)$ versus ϱ for various pairs (α, R) of α $(= 3, 5, 7)$ and R $(= 0.5, 2, 5)$. In the plots the peak value of φ is normalized to unity, and ϱ is expressed in units of R.

It should be remarked that the two parameters (α and R) characterizing the system do not enter the problem in an independent way but together take part in an interrelated manner in the binding, thus inducing an implicit coupling between the transverse and longitudinal coordinates of the electron. Examining the family of curves for μ and λ and for ξ_ϱ and ξ_z we see that, even though there is no geometric confinement along the wire axis, the axial extent of the polaron shrinks monotonically inwards contrary to what one might have expected if the effective electron - LO phonon interaction in the axial direction were insensitive to the variation of R.

Going from the bulk case to the quasi-one dimensional limit (Q1D) there comes about a competitive interrelation between whether the charge distribution (and hence the lattice deformation) will condense onto the origin (the polaron center) or will expand to relax itself in the longitudinal directions along the wire axis.

Starting from $R \gg 1$ and then restricting the transverse spread of the electron the contribution coming from the tendency of the polaron to expand longitudinally is compensated over by the pseudo-enhancement in the effective phonon coupling due to lateral localization towards the wire axis, thus in the overall, leading to a shrinking spatial extent in the $\pm z$ directions. Meanwhile, with contracting wire size there results an alteration in the lateral structure of the electron wave function as depicted by the μ-profile, displaying first a monotonic decrease and then an increase, implying that the radial part, $\varphi(\varrho)$, of the electron wave function conforms to a form structured more by its Bessel-function counterpart, $J_0(\kappa\varrho)$, rather than a narrow Gaussian, $\exp(-\mu^2\varrho^2/2)$, decaying far before the boundary is reached (cf., Fig.3.3). This can alternatively be recognized from that, regardless of α, the curves for ξ_ϱ (cf., Fig.3.2(b)) all tend to the same asymptote meaning that at small wire radii the lateral extent of the polaron is governed mainly by the geometric confinement rather than phonon coupling - induced localization. A complementary feature is that when R is far below unity both μ and λ display rather rapidly growing profiles compatible with a considerably pronounced effective phonon coupling and a highly localized characterization of the polaron in all directions.

For completeness, we also present a pictorial view of the phonon-coupling - induced potential well profiles

$$V(\varrho,z) = \frac{1}{e}\sum_Q V_Q \langle\, \Psi_g \,|(e^{i\vec{Q}\cdot\vec{r}}a_Q + \mathrm{hc})|\, \Psi_g \,\rangle \ , \tag{3.31}$$

along the radial and transverse directions. Using Eq.(3.12) with $u_Q = V_Q s_Q$, Eq.(3.31) conforms to

$$V(\varrho,z) = -\frac{1}{e}\sum_Q V_Q^2 s_Q (e^{i\vec{Q}\cdot\vec{r}} + \mathrm{cc}) \tag{3.32}$$

in which s_Q is given by Eq.(3.24). Setting $z = 0$ and $\varrho = 0$, respectively for the potential profiles along the radial (ϱ)- and longitudinal (z)- directions and projecting out the wave vector summation we obtain

$$V_\varrho \ = \ -\frac{2}{e}\alpha \int_0^\infty dq \ r_q \, e^{t^2}\mathrm{erfc}(t)\, J_0(\varrho q) \tag{3.33}$$

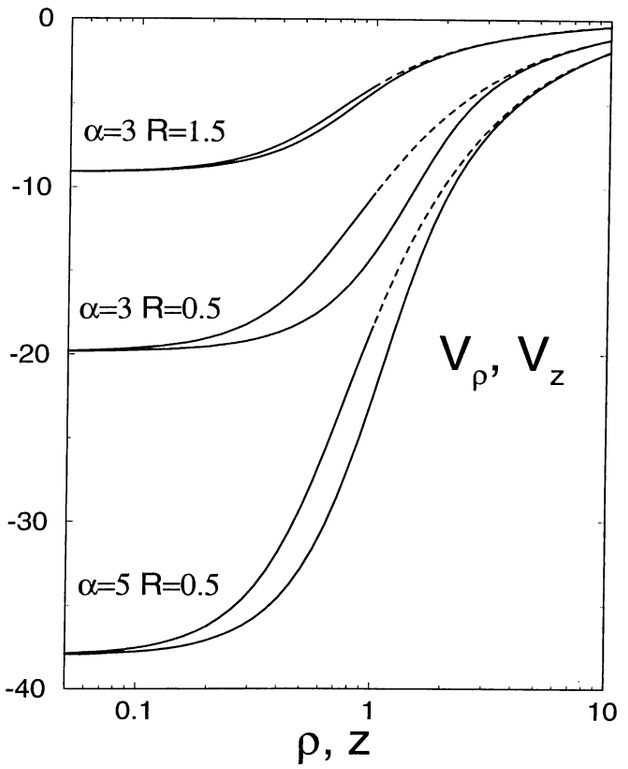

Figure 3.4: Phonon-coupling-induced potential well profiles.
The radial and longitudinal parts are represented respectively by the upper and lower curves. The potentials V_ϱ and V_z are given in arbitrary units on a linear scale, whereas ϱ and z are expressed in terms of R.

$$V_z = -\frac{1}{e}\alpha \int_0^\infty dq\, r_q\, e^{t^2}[h_q(z) + h_q(-z)] \tag{3.34}$$

where

$$t = \frac{q}{2\lambda} \quad \text{and} \quad h_q(z) = e^{zq}\,\mathrm{erfc}(t + \lambda z)\ . \tag{3.35}$$

In Fig.3.4 we plot $V_\varrho \equiv V(\varrho, z = 0)$ and $V_z \equiv V(\varrho = 0, z)$ for different permutations of α $(= 3, 5)$ and R $(= 0.5, 1.5)$. It is readily seen that the interaction potential gets deeper for strong α and/or narrow R where the two parameters together play a combined role in favor of a more effective coupling of the electron to the phonon field. The spatial anisotropy mentioned in the preceding paragraph is also portrayed in the set of curves for the potential profiles in that V_z lies deviated below V_ϱ, the digression being most significant for small R values and at sites more on the boundary side rather than the axial region

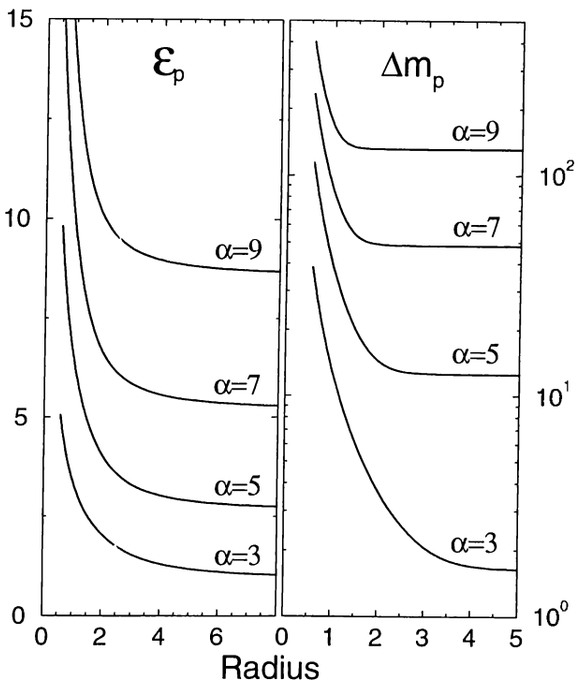

Figure 3.5: Polaronic binding energy and effective mass $\mathcal{E}_p$ and Δm_p as functions of R for several values of α.

$(\varrho/R, z/R \leq 0.1)$ where V_ϱ and V_z join and form spherically symmetric (isotropic) equipotentials.

A more brief content of the arguments given above is provided in Fig.3.5 where we plot the binding energy, $\mathcal{E}_p = (j_{0,1}/R)^2 - E_g$ (relative to the subband), and the polaronic contribution to the band mass, $\Delta m_p = m_p - 1$, against the wire radius for a set of distinctive α-values. We once again note the same qualitative behavior where the growth rates of $\mathcal{E}_p$ and m_p are somewhat moderate for large R, but however on the opposite extreme where R is tuned to smaller values both $\mathcal{E}_p$ and m_p are observed to increase with very pronounced slopes the growth rates of which being significantly greater for stronger α.

The adiabatic theory employed in this work gives $\mathcal{E}_p^{(3D)} = -\alpha^2/3\pi$ in the bulk case, and $\mathcal{E}_p^{(2D)} = (\pi/8)\alpha^2$ for a strictly two dimensional polaron.[12] The general trend that the polaron quantities are inherently pronounced in low dimensional systems is also reflected in our present results. For a wire with $\alpha = 3$ and $R = 1$,

for instance, we obtain $\mathcal{E}_{\rm p} = 3.377$. For thinner wires the binding gets naturally deeper since the electronic wave function becomes even more localized in both directions perpendicular to the wire axis. We obtain $\mathcal{E}_{\rm p} = 5.485$ when $R = 0.5$ and $\mathcal{E}_{\rm p} = 9.920$ when $R = 0.2$. A comparison of these values with the corresponding three- ($\mathcal{E}_{\rm p}^{(3D)} = 0.955$) and two- ($\mathcal{E}_{\rm p}^{(2D)} = 3.534$) dimensional values reveals that the polaron binding energy is much greater when the effective dimensionality is reduced from three to Q1D than when reduced from three to two. The same is true for the polaron mass where $\Delta m_{\rm p}$ in quantum wires of small dimensions are much larger than those in comparable two dimensional wells.

Chapter 4

INTERMEDIATE COUPLING THEORY

In the last two chapters, we have considered the two methods appropriate to the small and large values of the electron phonon interaction strength. However, in some cases of interest, the interaction constant has intermediate values, being so large that the perturbation theory breaks down, but on the other hand it is still small for the adiabatic approximation to be totally valid. The earliest attempt to deal with this intermediate coupling regime has been made by Lee, Low and Pines (LLP).[36] The method is based on a variational technique, which is equivalent to a simple canonical transformation. At weak coupling, LLP approximation reproduces the results of perturbation theory, and moreover, it has a considerable validity for intermediate values of the coupling constant up to $\alpha \sim 4$.

4.1 LLP Transformation

In quantum mechanics, the symmetry properties of the physical system lead to important conservation laws. In this regard, the conservation of linear momentum is a consequence of translational symmetry. For the polaron problem, the total

momentum operator,

$$\vec{\mathsf{P}} = \vec{p} + \sum_Q \vec{Q} a_Q^\dagger a_Q \ , \tag{4.1}$$

of the system is a constant of motion and commutes with the Fröhlich Hamiltonian, which we restate here for the bulk polaron and in the usual dimensionless units (and $2m^\star = 1$),

$$H = p^2 + \sum_Q a_Q^\dagger a_Q + \sum_Q V_Q \left(a_Q e^{i\vec{Q}\cdot\vec{r}} + \mathrm{hc} \right) \ . \tag{4.2}$$

Therefore, it is possible to transform to a representation in which the electron coordinates are totally eliminated and in which the total momentum $\vec{\mathsf{P}}$ becomes a c-number. The required unitary transformation, introduced by Lee, Low and Pines,[36] is generated by,

$$\mathbf{U}_1 = \exp\left\{ i(\vec{\mathsf{P}} - \sum_Q \vec{Q} a_Q^\dagger a_Q) \cdot \vec{r} \right\} \ . \tag{4.3}$$

Since a unitary transformation preserves the eigenvalues of the Schrödinger equation, the basic polaron Hamiltonian can equivalently be taken as

$$\mathcal{H} = \mathbf{U}_1^{-1} H \mathbf{U}_1 \tag{4.4}$$

in this approximation.

The form of $\mathcal{H}$ is easily obtained by considering the transformation of the operators $\vec{p}$, a_Q, $a_Q^\dagger$ and $e^{i\vec{Q}\cdot\vec{r}}$. In the new representation one finds,

$$\mathbf{U}_1^{-1} \vec{p} \mathbf{U}_1 = \vec{\mathsf{P}} - \sum_Q \vec{Q} a_Q^\dagger a_Q + \vec{p} \tag{4.5}$$

and

$$\mathbf{U}_1^{-1} a_Q \mathbf{U}_1 = a_Q e^{-i\vec{Q}\cdot\vec{r}} \ ; \quad \mathbf{U}_1^{-1} a_Q^\dagger \mathbf{U}_1 = a_Q^\dagger e^{i\vec{Q}\cdot\vec{r}} \ , \tag{4.6}$$

while $e^{i\vec{Q}\cdot\vec{r}}$ is left invariant under this transformation. Setting $\vec{p} = 0$, the new Hamiltonian now gets the form,

$$\mathcal{H} = \left(\vec{\mathsf{P}} - \sum_Q \vec{Q} a_Q^\dagger a_Q \right)^2 + \sum_Q V_Q \left(a_Q + a_Q^\dagger \right) \ . \tag{4.7}$$

The problem is then reduced to the calculation of the ground state energy $E_g(\mathsf{P})$ of this Hamiltonian, for a given momentum P. For the low-lying energy levels of the electron, $E_g(\mathsf{P})$ can be represented by a power series expansion in P^2. Thus, up to first order in P^2, one can write $E_g(\mathsf{P}) \simeq -\mathcal{E}_p + \mathsf{P}^2/m_p$, where $\mathcal{E}_p$ is the polaronic binding energy and m_p is identified as the polaron mass (in units of m^*).

The calculation of $E_g(\mathsf{P})$ requires a variational procedure. It is the expectation value of the Hamiltonian $\mathcal{H}$ in the ground state Ψ_g, chosen in the form,

$$\Psi_g = \mathbf{U}_2|0\rangle, \tag{4.8}$$

where $|0\rangle$ is the phonon vacuum, and

$$\mathbf{U}_2 = \exp \sum_Q u_Q(a_Q - a_Q^\dagger) \tag{4.9}$$

is the generator of displaced oscillator transformation that we have introduced previously in the strong coupling theory. The parameters u_Q here are to be determined variationally to minimize the ground state energy.

In their original work, using the outlined procedure, LLP have found the ground state polaronic binding energy in the leading order of α,

$$\mathcal{E}_p = \alpha \ , \tag{4.10}$$

same as in second order perturbation theory, but the effective mass is obtained in the form

$$m_p = 1 + \alpha/6 \tag{4.11}$$

regardless of the value of coupling constant. In contrast to that obtained by perturbation theory, $m_p = 1/(1 - \alpha/6)$, this form of effective mass does not suffer from the unacceptable divergence at $\alpha \sim 6$. Therefore, it seems that LLP approximation expands the domain of validity of perturbation theory results up to intermediate values of α.

In the next section, we will apply the arguments of LLP approximation, in a somewhat modified manner, to the same problem of previous chapter; the polaron in an infinite boundary quantum well wire.

4.2 Application: Quantum Wire

4.2.1 Introduction

Under the assumption of perfect confinement, i.e. with

$$V_{\text{conf}}(\varrho) = \begin{cases} 0 & \text{if } \varrho < R \\ \infty & \text{if } \varrho > R \end{cases} \tag{4.12}$$

we have calculated the polaron quantities, within the framework of strong coupling theory, in the previous chapter. In thin wires, due to the high degree of confinement brought about in the lateral directions, even when the electron phonon interaction is not dominantly strong enough, the adiabatic theory gives a reasonable description of the polaron. To demonstrate this feature, we choose to compare the polaronic binding energy results of strong coupling[53] and path integral[77] theories applied to the polaron in a parabolic quantum wire problem. Both works have been performed with a form $V_{\text{conf}} \sim \Omega^2\varrho^2$ taken as the wire boundary. Although the two types of boundary potentials (rigid and parabolic) are qualitatively different in nature, we mention the results of those works here, just to seek the domain of validity of strong coupling theory.

An immediate glance at Fig.4.1 reveals that the strong coupling theory is totally inadequate for small values of α, giving binding energies far below the path integral results, but when the strength of the coupling is increased to larger values, the results of the two theories tend to approach each other, and eventually match, becoming almost identical in the large α limit. It is also seen that the point where the two theories start to be equivalent, shifts down to smaller values of α, with the increased degree of localization. For $\Omega = 10^3$ (the topmost curves), which corresponds to a rather thin wire, strong coupling theory remains successful down to the intermediate values of $\alpha \sim 2$. The qualitative understanding of the situation is possible. In the Q1D-configuration, the polaron becomes highly localized towards the axis of the wire due to the boundary potential squeezing the charge density of the electron inward in all transverse directions, leading to a pseudo-enhancement in the value of the effective α, through the increased

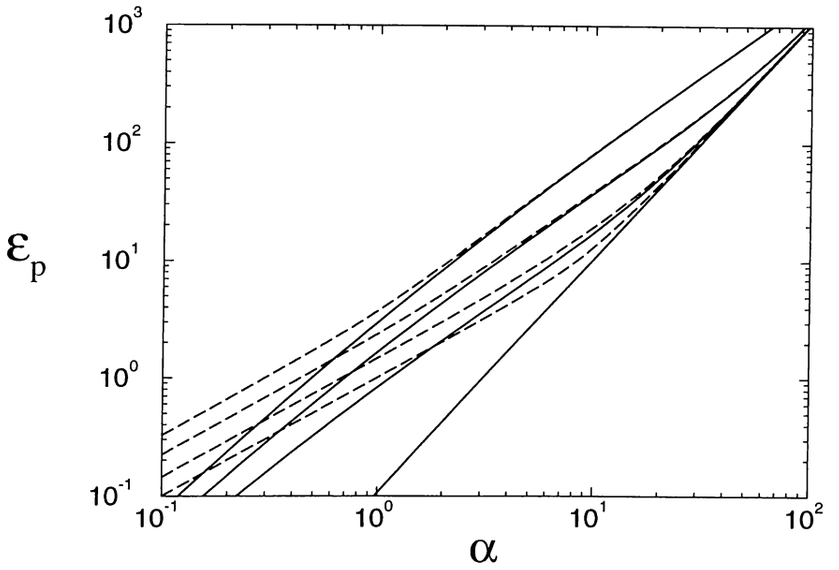

Figure 4.1: The extended domain of validity of strong coupling theory in highly confined systems.
The polaron binding energy as a function of coupling constant, in the parabolic boundary wire configuration. The solid and dashed curves are respectively the results of strong coupling [53] and path integral [77] theories. For each set of curves, from bottom to top, $\Omega = 0$, 10, 10^2, 10^3.

efficiency of the electron coupling to the phonons. Hence, even in weak polar materials (e.g., GaAs), the polaron problem may show up a strong-coupling aspect brought about by confinement effects and this feature becomes even more prominent in II–VI compound semiconductors where the relevant coupling strengths are almost an order of magnitude larger than those in III–V materials.

We thus feel that, even for weak or intermediate coupling strengths, the lattice may acquire a relaxed static deformation, clothing the entire extent of the rapidly fluctuating electron in the directions transverse to the axis of a thin wire. Still, however, in the case of a weak coupling, the ions may respond to the instantaneous position of the electron along the length of the wire. Consequently, one has an adiabatic (strong-coupling) condition obtained along the two transverse axes, and weak-coupling along the third (z) direction. We refer to this picture as mixed coupling.

In this particular situation, the strong coupling theory can be refined to give

better results, by treating the almost free (z) direction with a more suitable approximation such as LLP transformation. In the following we apply an admixture of strong coupling and LLP intermediate coupling approximations, for the characterization of the ground state polaron properties in the highly anisotropic Q1D systems.

4.2.2 Theory

Hamiltonian and Wave Function

We start with the Hamiltonian (1.27), where the confining potential is again taken in the form as given in Eq.(4.12). To account for the cylindrical confinement, we shall impose the lateral wave function of the electron to be given in the product form

$$\Phi_e(\varrho) = N\, \mathrm{J}_0(\kappa\varrho)\, \exp(-\frac{1}{2}\mu^2\varrho^2) \tag{4.13}$$

where the constant N serves for normalization. Clearly, J_0, the zeroth order cylindrical Bessel function of the first kind, takes care of the geometric confinement, and the further confinement induced by phonon coupling is governed by the Gaussian counterpart through parameter μ. In the above, $\kappa = j_{0,1}/R$, where $j_{0,1}$ is the first zero of J_0.

Canonical Transformations

The polaron Hamiltonian is invariant to translations of the electron together with its concomitant lattice distortion, and the total momentum along the wire axis is conserved, i.e., H commutes with

$$\mathsf{P}_z = -i\frac{\partial}{\partial z} + \Pi_z \tag{4.14}$$

in which

$$\Pi_z = \sum_Q q_z a_Q^\dagger a_Q \tag{4.15}$$

refers to the phonon momentum. Therefore, it is possible to transform to a representation in which the relevant coordinate of the electron is totally

eliminated and the total momentum P_z becomes a c-number. On this purpose, applying the one dimensional analogue of LLP unitary transformation (4.4), with

$$\mathbf{U}_1 = \exp\left\{i(\mathsf{P}_z - \Pi_z)\, z\right\}\,, \tag{4.16}$$

the Hamiltonian conforms to

$$\begin{aligned} H' &= \mathbf{U}_1^{-1} H \mathbf{U}_1 \\ &= -\frac{1}{\varrho}\frac{\partial}{\partial\varrho}\left(\varrho\frac{\partial}{\partial\varrho}\right) + (\mathsf{P}_z - \Pi_z)^2 + \sum_Q a_Q^\dagger a_Q + \sum_Q V_Q(a_Q e^{i\vec{q}\cdot\vec{\varrho}} + \mathrm{hc})\,. \end{aligned} \tag{4.17}$$

With the above form achieved for the polaron Hamiltonian, the problem reduces to the evaluation of the ground state energy for a given momentum P_z. The functional form, $E_{\mathrm{g}}(\mathsf{P}_z)$, thus obtained can then be expanded in a power series to second order in the momentum, i.e.,

$$E_{\mathrm{g}}(\mathsf{P}_z) \simeq E_{\mathrm{g}}(0) + c\,\mathsf{P}_z^2\,,$$

where the reciprocal of the factor multiplying P_z^2 is identified as the polaron mass along the length of the wire.

For the calculation of E_{g} a variational approach is adopted, and the polaron ground state is postulated in a product ansatz consisting of the electron and lattice parts, i.e.,

$$\Psi_{\mathrm{g}} = \Phi_{\mathrm{e}}\, \mathbf{U}_2 |0\rangle, \tag{4.18}$$

where $|0\rangle$ is the phonon vacuum state, and

$$\mathbf{U}_2 = \exp \sum_Q u_Q(\Phi_{\mathrm{e}})\,[a_Q - a_Q^\dagger], \tag{4.19}$$

is the displaced oscillator transformation.

Thus, subjecting the Hamiltonian further to the transformation

$$H' \rightarrow \mathbf{U}_2^{-1} H' \mathbf{U}_2\,,$$

we finally obtain

$$H'' = -\frac{1}{\varrho}\frac{\partial}{\partial\varrho}\left(\varrho\frac{\partial}{\partial\varrho}\right) + \sum_Q a_Q^\dagger a_Q + \sum_Q u_Q^2$$

$$
\begin{aligned}
&- \sum_Q V_Q u_Q \left(e^{i\vec{q}\cdot\vec{\varrho}} + \text{cc}\right) + \sum_Q \left\{[V_Q e^{i\vec{q}\cdot\vec{\varrho}} - u_Q]a_Q + \text{hc}\right\} \\
&+ (\mathsf{P}_z - \Pi_z)^2 + \mathsf{P}_z^2 - 2\mathsf{P}_z\Pi_z^{(0)} \\
&+ 2\left\{\mathsf{P}_z - \Pi_z^{(0)}\right\}\Pi_z^{(1)} + \left\{\Pi_z^{(1)} - 2\Pi_z\right\}\Pi_z^{(1)} \qquad (4.20)
\end{aligned}
$$

where

$$\Pi_z^{(0)} = \sum_Q u_Q^2 q_z\,, \qquad (4.21)$$

$$\Pi_z^{(1)} = \sum_Q u_Q q_z (a_Q + a_Q^\dagger)\,. \qquad (4.22)$$

Before we proceed with our main theme we should remark that, if the first transformation were by-passed (i.e. $\mathbf{U}_1$ were selected as the identity operator), the theory would then diverse to the strong coupling approximation for which simultaneous optimizations with respect to Φ_e and $u_Q(\Phi_e)$ correspond to the self-trapping picture of the polaron where the electron distribution and the lattice polarization influence each other in such a way that a stable relaxed state is eventually attained. The calculations and results pertaining to such a case (with $\alpha \gg 1$) have already been discussed in Chapter 3.

Variational Calculation

Calculating the expectation value of H'' (4.20) in the state $\Phi_e|0\rangle$, we obtain the ground state energy, given by

$$
\begin{aligned}
E_g &= \epsilon_k + \mathsf{P}_z^2 - 2\mathsf{P}_z\Pi_z + [\Pi_z^{(0)}]^2 \\
&+ \sum_Q u_Q^2(1 + q_z^2) - 2\sum_Q V_Q u_Q s_q \qquad (4.23)
\end{aligned}
$$

where

$$\epsilon_k = \langle\Phi_e\,| - \frac{1}{\varrho}\frac{\partial}{\partial\varrho}\left(\varrho\frac{\partial}{\partial\varrho}\right)|\,\Phi_e\rangle\,, \qquad (4.24)$$

$$s_q = \langle\Phi_e\,|e^{\pm i\vec{q}\cdot\vec{\varrho}}|\,\Phi_e\rangle\,. \qquad (4.25)$$

Defining, for notational convenience,

$$\sigma_{mm'}^{(n)}(x) = \int_0^{j_{0,1}} dt\; t^n \mathrm{J}_m(t)\,\mathrm{J}_{m'}(t)\,\mathrm{J}_0(xt)\exp(-\frac{\mu^2}{\kappa^2}t^2)\,, \qquad (4.26)$$

and adopting the form (4.13) for the electron wave function, we obtain ϵ_k and s_q, Eqs.(4.24) and (4.25), to be expressible in the following concise forms

$$\epsilon_k = \kappa^2 + \mu^2 \left\{ 2 - \frac{2\sigma_{10}^{(2)}(0) - (\mu/\kappa)^2 \sigma_{00}^{(3)}(0)}{\sigma_{00}^{(1)}(0)} \right\} , \tag{4.27}$$

and

$$s_q = \frac{\sigma_{00}^{(1)}(q/\kappa)}{\sigma_{00}^{(1)}(0)} . \tag{4.28}$$

The variational function $u_Q(\Phi_e)$ minimizing Eq.(4.23) is found to be given by the following nonlinear equation

$$\{1 - 2(\mathsf{P}_z - \Pi_z^{(0)})q_z + q_z^2\}u_Q - V_Q s_q = 0 , \tag{4.29}$$

which can easily be handled with the consideration that, from symmetry arguments, the term $\Pi_z^{(0)}$ (4.21) can only differ from the total momentum by a scalar factor. Hence, setting

$$\Pi_z^{(0)} = \eta \mathsf{P}_z , \tag{4.30}$$

the condition (4.29) for $u_Q(\Phi_e)$ conforms to a convenient expression. We obtain

$$u_Q = \frac{V_Q s_q}{1 - 2(1-\eta)\mathsf{P}_z q_z + q_z^2} \tag{4.31}$$

in which the unknown scalar, η, is determined by the transcendental equation

$$\eta \mathsf{P}_z = \sum_Q \frac{V_Q^2 s_q^2 q_z}{[1 - 2(1-\eta)\mathsf{P}_z q_z + q_z^2]^2} . \tag{4.32}$$

In what follows we adopt the case of a stationary polaron, i.e. take

$$\langle \Phi_e | \mathbf{U}_2^{-1} \mathbf{U}_1^{-1} \mathsf{P}_z \mathbf{U}_1 \mathbf{U}_2 | \Phi_e \rangle = 0 ,$$

and thus regard P_z as a virtual momentum which we retain to keep track of the effective mass of the coupled electron-phonon complex.

In complete form, with the optimal fit for $u_Q(\Phi_e)$ substituted in, and the wave vector sums involving powers of first and second order in P_z projected out, Eq.(4.23) takes the form

$$E_g = \epsilon_k - \sum_Q V_Q^2 s_q^2 \frac{1}{1+q_z^2} + (1-\eta)\mathsf{P}_z^2 , \tag{4.33}$$

from which we identify the effective polaron mass as

$$m_{\rm p} = \frac{1}{1-\eta} \ . \tag{4.34}$$

For a virtual translation ($\mathsf{P}_z \simeq 0$), Eq.(4.32) can be expanded in powers of P_z to yield

$$\eta = 4(1-\eta) \sum_Q V_Q^2 \, s_q^2 \, \frac{q_z^2}{(1+q_z^2)^3} + \mathcal{O}(\mathsf{P}_z^2) \ , \tag{4.35}$$

which, upon solving for η and substituting in the mass expression (4.34), we obtain

$$m_{\rm p} = 1 + 4 \sum_Q V_Q^2 \, s_q^2 \, \frac{q_z^2}{(1+q_z^2)^3} \ . \tag{4.36}$$

Projecting out the $\vec{Q}$-summations in Eqs.(4.33) and (4.36), we finally arrive at the following integral - expressions for the ground state energy and the longitudinal mass

$$E_{\rm g} = \epsilon_k - \alpha \int_0^\infty dq \, \frac{1}{1+q} \, s_q^2 \, , \tag{4.37}$$

$$m_{\rm p} = 1 + \frac{\alpha}{2} \int_0^\infty dq \, q \, \frac{q+3}{(1+q)^3} \, s_q^2 \ . \tag{4.38}$$

4.2.3 Results and Conclusions

The energy expression (4.37) depends on the variational parameter μ in a complicated manner through the set of equations (4.26-4.28). The optimal fit to μ which minimizes $E_{\rm g}$ can therefore be performed by numerical techniques. In the following we give our results in terms of the binding energy of the polaron, $\mathcal{E}_{\rm p} = (j_{0,1}/R)^2 - E_{\rm g}$ (relative to the subband).

It should be re-emphasized that the theory we have used in this work constrains the validity of our results to narrow wires and to electron phonon coupling strengths that are not too strong. Clearly, for a small α one requires correspondingly a high degree of lateral confinement to compensate for weak phonon coupling and make the polaron go over to a "pseudo-strong" coupling characterization in the lateral plane achieved by the radially inward localization towards the wire axis. In the meantime, however, the effective phonon coupling

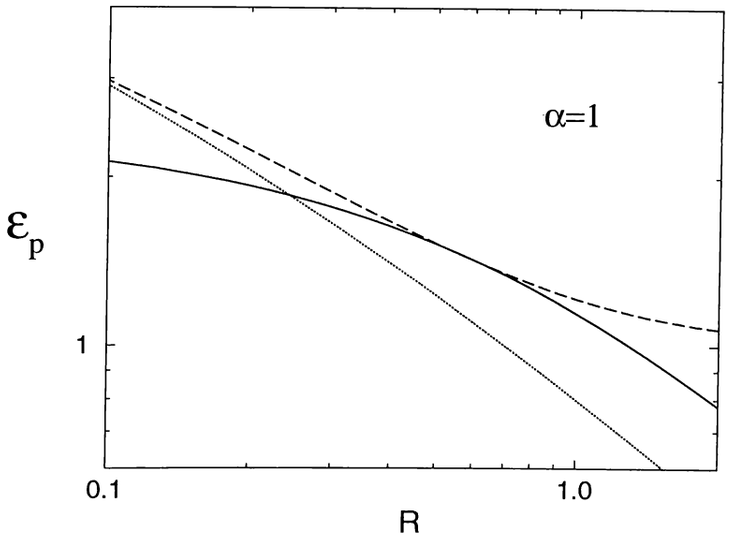

Figure 4.2: Comparison of alternative approaches.
The binding energy $\mathcal{E}_{\rm p}$ as a function of the wire radius for $\alpha = 1$. The solid and dashed curves display the results of the mixed coupling and path integral[77] theories, respectively. The dotted curve refers to the results derived within the pure strong coupling approach.[54]

in the longitudinal direction will be assumed to remain weak or at least, to grow not too powerful to violate the LLP - weak-coupling condition that we have undertaken for the polaron behavior along the z axis. Within the framework of the "mixed coupling" description thus constructed, one obtains a means of studying the ground state polaron properties in thin wires of weak polar materials.

Selecting $\alpha = 1$, an intermediate coupling strength for which the LLP-theory proves to work rather well, we display the results of the present theory as a function of the wire radius for $R \leq 2$. In Fig.4.2 we also supply the energy values of the pure strong coupling treatment of the same problem where the canonical transformation (4.17) is by-passed and the electron wave function (4.13) is extended to include a Gaussian spread along the wire axis, i.e., $\Phi_{\rm e}(\varrho) \rightarrow \Phi_{\rm e}(\varrho)\exp(-\frac{1}{2}\lambda^2 z^2)$ as was done in Chapter 3. A comparison of the two theories reveals that the strong coupling binding energy values lie deviated below the present results except for very small values of R simply because, for an intermediate coupling strength like $\alpha = 1$, the pure adiabatic

approach can be convenient at only very high degrees of confinement where the pseudo-enhancement in α is dominantly realized. In this extreme, with α scaled to effective values considerably larger than 1, the pure strong coupling treatment becomes even superior to the LLP-framework and yields better results since now the effective interaction along the length of the wire should be characterized with a projection more on the strong coupling side as the wire is made thinner. On the contrary, as the geometric confinement is released allowing the polaron the expand and relax itself laterally, the strong coupling theory starts to become inadequate and rapidly loses its validity due to that in a comparatively delocalized configuration the effective phonon coupling strength falls far below to sustain the adiabatic condition. With the LLP - canonical transformation U_1 turned on, however, the deficiency encountered for comparatively large R ($R \geq 0.3$) gets removed and the strong coupling approach becomes refined by a great extent yielding considerably improved energy upper bounds. To see this we also make reference to the available data from a similar problem treated under the Feynman path integral formulation applied to the case of a wire with parabolic boundary potential, $V(\varrho) = \frac{1}{2}\Omega^2\varrho^2$ (cf. [77]). Even though the nature of the problem treated therein[77] is qualitatively different from that for the rigid-boundary potential, we find it useful to generate a plot of the path integral results (cf. dashed curve in Fig.4.2) to shed some insight into the applicability of the present formalism. We correlate the two theories by comparing the relevant subband energies, and simply use $R = j_{0,1}/\sqrt{2\Omega}$ as the corresponding effective radius. We clearly see that within the range $0.4 < R < 1$, the present and the path integral theories are in fairly close agreement. Beyond this range, with increasing wire radius, the present theory is seen to display an increasingly large deviation from the Feynman results due to that a delocalized nature of the electron in the lateral directions violates the pseudo-adiabatic condition which we have imposed a priori in this problem.

The basic qualitative features practiced for $\alpha = 1$ are seen to be retained for smaller values of α also. It is observed that, in spite of a coupling constant smaller by an order of magnitude or even more, a sufficiently high degree of localization

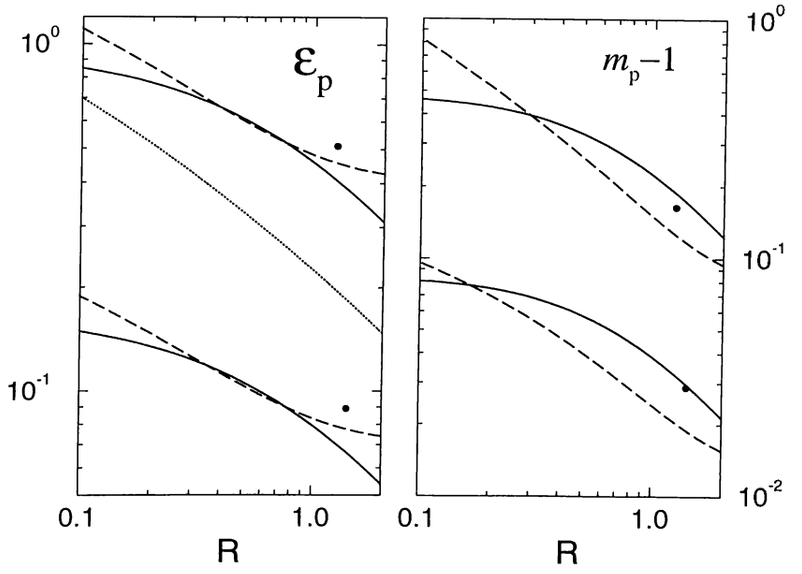

Figure 4.3: The results at weak coupling.
The binding energy $\mathcal{E}_p$ and the effective polaron mass m_p as functions of the wire radius. The upper (lower) set of curves are for CdTe (GaAs) based wires where α = 0.40 (0.07). The solid and dashed curves display the results of the mixed coupling and path integral[77] theories, respectively. The heavy dots included for further comparison, represent the available data obtained for a square cross section wire under perturbation theory[87] where we have correlated the side length L to R through $R = (j_{0,1}/\sqrt{2}\pi)L$. In the plots, the energy and length units correspond, respectively, to 35 (18) meV and 40 (44) $\mathring{A}$, for GaAs (CdTe).

can still compensate for weak phonon coupling and lead the theory to show up a strong coupling aspect in the transverse directions perpendicular to the wire axis. As reference to weak electron phonon coupling, we select CdTe ($\alpha \approx 0.40$) and GaAs ($\alpha \approx 0.07$) based wires, which are of particular interest as typical examples of II-VI and III-V compound semiconductors. In Fig.4.3 we provide plots of the binding energy $\mathcal{E}_p$ and the longitudinal mass m_p in these materials as a function of the wire radius. In the energy plot for $\alpha = 0.40$ we inspect rather prominently that the LLP transformation employed along the z-axis enhances the results considerably in good quality over to the values achieved within the pure strong coupling treatment of the problem. For $\alpha = 0.07$, the digression in the adiabatic approximation is even much greater, and the corresponding strong coupling binding energy values (not shown in the figure) lie drastically deviated, by almost

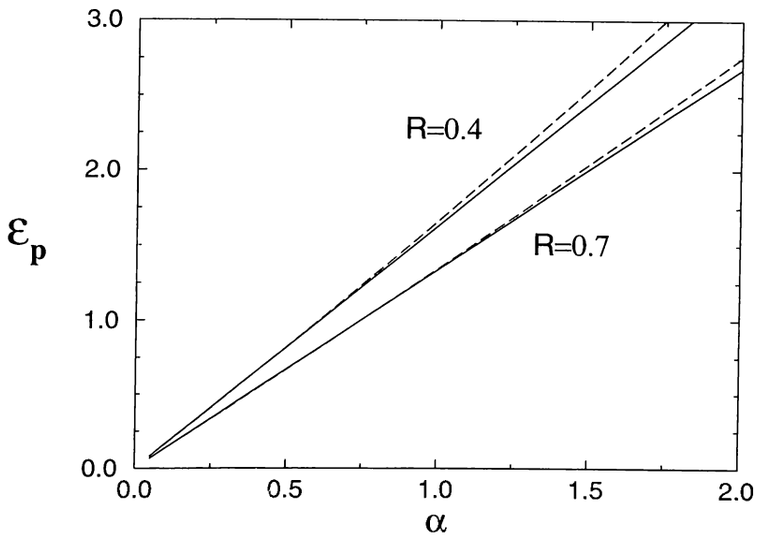

Figure 4.4: The coupling constant dependence of the binding energy. The binding energy $\mathcal{E}_p$ as a function of α in the weak/intermediate coupling regime. The upper (lower) set of curves are for $R = 0.4\,(0.7)$. The solid and dashed curves display the results of the mixed coupling and path integral[77] theories, respectively.

an order of magnitude, below the present results. The overall feature displayed by the succession of curves calculated within the mixed coupling approximation used in this work and the Feynman path integral theory is that the range of validity of the present results is limited, from above and below, to not too broad and not too thin wires, yet however, the relevant values within this range are found to be commendable and are in somewhat close agreement with the corresponding path integral results (cf. Fig.4.4). For large and small values of R lying beyond this range, the mixed-coupling approach fails to yield a satisfying description due to that, for not thin enough wires, the strong coupling requirement which we have imposed in the lateral directions is not adequately satisfied, or else, in very thin wires, the LLP - weak-coupling approximation employed along the length of the wire becomes violated as a consequence of the pseudo-enhancement in the overall effective phonon coupling strength. Nevertheless, we feel that the mixed coupling theory employed in this work can be regarded as capable of reflecting a sensible characterization of the Q1D-polaron within a reasonable range of the wire diameter lying within $30 - 80\,\mathring{A}$ units in GaAs- and CdTe-based wires.

Chapter 5

PERTURBATIVE VARIATIONAL APPROACH

5.1 Introduction

We have seen that for not too weak and pseudo-enhanced electron-phonon interaction the strong coupling polaron theory, though not capable of reflecting a totally dependable quantitative description, may serve so as to provide some qualitative insight into the study of polarons in confined media consisting of materials of somewhat strong polar crystals. On the other hand, a pure perturbation treatment may also be not perfectly appropriate except for too weak phonon coupling. We are therefore tempted to formulate the Q1D - polaron problem within the framework of a more convenient approach accounting for its weak and strong coupling counterparts simultaneously. The formalism we follow in this chapter consists of the usage of a perturbative variational approach used previously by Devreese *et al.*[56] in their application to the bulk optical polaron bound to a Coulomb center. The procedure is structured on basing the starting ansatz on the standard displaced oscillator transformation of the Pekar strong coupling theory[44] and then modify the adiabatic polaron state by a variationally determined perturbative extension serving for the theory to interpolate in the overall range of the coupling constant.

As the model, we consider the interaction of a confined electron with bulk polar-optical phonons in a cylindrical quantum well wire with infinite boundary potential. Expressions for the polaron self energy and mass will be derived within the mentioned variational scheme over reasonably broad ranges of the wire radius and the phonon coupling strength. We aim to provide a broad interpolating overview to the one - polaron problem consisting of an electron perfectly confined within a cylindrical boundary with infinite potential. In the next section we give the basic essentials of the variational theory that we adopt in this calculation and derive analytic expressions for the ground state binding energy and mass of the Q1D polaron. In section 5.3 we present our numerical results over reasonably wide ranges of the wire radius and the electron-phonon interaction strength. Interestingly, contrary to the general trend that the electron-phonon interaction is inherently stronger in systems of lower dimensionality, our results indicate that at weak coupling the binding energy of the polaron can be smaller and its mass less inertial compared with the bulk case when the wire is made narrow.

5.2 Application: Quantum Wire

Scaling energies by the phonon quantum $\hbar\omega_{\rm LO}$ and lengths by $(\hbar/2m^*\omega_{\rm LO})^{1/2}$, the Hamiltonian of an electron confined in a wire and interacting with the bulk LO–phonons is given by

$$H = -\nabla^2 + V_{\rm conf}(\varrho) + \sum_Q a_Q^\dagger a_Q + \sum_Q V_Q(a_Q e^{i\vec{Q}\cdot\vec{r}} + a_Q^\dagger e^{-i\vec{Q}\cdot\vec{r}}) \qquad (5.1)$$

in which $\vec{r} = (\vec{\varrho}, z)$ denotes the electron position in cylindrical coordinates. We assume that the electron is perfectly confined to a cylindrical wire with infinite potential boundary at $\varrho = R$, and take $V_{\rm conf}(\varrho) = 0$ inside the wire.

We set the electron wave function as separable in the transverse and longitudinal coordinates in the form

$$\Phi_{\rm e}(\vec{\varrho}, z) = \varphi(\vec{\varrho})\, Z(z)\, e^{i\kappa z} \qquad (5.2)$$

wherein the exponential factor $e^{i\kappa z}$ (with κ to be determined variationally) sets the system in motion, thus enabling one to trace the polaron mass along the length of the wire.

5.2.1 Displaced Oscillator Transformation

The variational approach that we adopt in this paper is based on utilizing the usual canonical transformation of the strong–coupling formalism and then extend the adiabatic polaron state by including an approximate first order perturbative correction by which it is possible to interrelate the strong and weak coupling counterparts of the coupled electron-phonon system. Regardless of the strength of the coupling constant the starting step in the foregoing theory is to assume a highly rapid charge density fluctuations for the electron to which the lattice responds by acquiring a relaxed deformation clothing the entire extent of the electron. The adiabatic polaron ground state thus formed is given through a product ansatz consisting of the electron and phonon parts, i.e.,

$$\Psi_{\rm g} = \Phi_{\rm e}(\vec{\varrho}, z) \mid 0 \rangle \ , \tag{5.3}$$

together with the Hamiltonian subjected to the displaced oscillator transformation

$$H \rightarrow \tilde{H} = e^{-\mathbf{U}} H e^{\mathbf{U}} \tag{5.4}$$

where

$$\mathbf{U} = \sum_{Q} u_Q(\Phi_{\rm e})[a_Q - a_Q^{\dagger}] \ . \tag{5.5}$$

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

Under the transformation (5.4), the Hamiltonian conforms to

$$\tilde{H} = -\nabla^2 + V_{\rm conf}(\varrho) \quad + \quad \sum_{Q} u_Q^2 - \sum_{Q} V_Q u_Q [\exp(i\vec{Q} \cdot \vec{r}) + {\rm cc}]$$

$$+ \sum_Q a_Q^\dagger a_Q + \sum_Q \{[V_Q \exp(i\vec{Q}\cdot\vec{r}) - u_Q]a_Q + \text{hc}\} \quad (5.6)$$

Since the Hamiltonian is invariant to translations of the electron together with its concomitant lattice distortion, the total momentum along the wire axis

$$\mathsf{P}_z = -i\frac{\partial}{\partial z} + \sum_Q q_z a_Q^\dagger a_Q \quad (5.7)$$

must be conserved. The variation therefore requires an optimization of the polaron state $e^{\mathbf{U}}\Psi_{\mathrm{g}}$ which minimizes H subject to the constraint that P_z is a constant of motion. Thus, minimizing the functional

$$\mathsf{F}(\beta, v \mid u_Q, \kappa) \equiv \langle \Psi_{\mathrm{g}} \mid e^{-\mathbf{U}}(H - v\mathsf{P}_z)e^{\mathbf{U}} \mid \Psi_{\mathrm{g}} \rangle \quad (5.8)$$

with respect to κ and u_Q yields

$$\kappa = \frac{1}{2}v \qquad \text{and} \qquad u_Q(\Phi_{\mathrm{e}}) = V_Q s_Q \rho_Q \quad (5.9)$$

where

$$s_Q = \langle \Phi_{\mathrm{e}} \mid \exp\{\pm i(\vec{q}\cdot\vec{\varrho} + q_z z\} \mid \Phi_{\mathrm{e}} \rangle \quad (5.10)$$

$$\rho_Q = (1 - vq_z)^{-1} \quad (5.11)$$

in which the Lagrange multiplier v is to be identified as the polaron velocity along the wire axis.[85] In equation (5.8) the symbol β stands for the variational parameter(s) contained in $\Phi_{\mathrm{e}}(\vec{\varrho}, z)$.

In complete form, with the optimal fits for κ and u_Q substituted in, the Hamiltonian which we shall be referring hereafter is

$$\begin{aligned}\tilde{H} = -\nabla^2 + V_{\mathrm{conf}}(\varrho) \; &+ \sum_Q a_Q^\dagger a_Q + \sum_Q V_Q^2 s_Q^2 \rho_Q^2 \\ &- \sum_Q V_Q^2 s_Q \rho_Q (e^{i\vec{Q}\cdot\vec{r}} + e^{-i\vec{Q}\cdot\vec{r}}) \\ &+ \sum_Q V_Q(\eta_Q a_Q + \eta_Q^* a_Q^\dagger) \end{aligned} \quad (5.12)$$

where

$$\eta_Q = e^{i\vec{Q}\cdot\vec{r}} - s_Q\rho_Q \; . \quad (5.13)$$

Similarly, for the total momentum transformed accordingly, $\mathsf{P}_z \rightarrow e^{-\mathbf{U}}\mathsf{P}_z e^{\mathbf{U}}$, we have

$$\hat{\mathsf{P}}_z = -i\frac{\partial}{\partial z} + \sum_Q q_z a_Q^\dagger a_Q + \sum_Q V_Q^2 q_z s_Q^2 \rho_Q^2 - \sum_Q V_Q q_z s_Q \rho_Q (a_Q + a_Q^\dagger) \qquad (5.14)$$

In what follows we shall consider the case of a stationary polaron, i.e. take $\langle\, \Psi_{\rm g} \mid \tilde{\mathsf{P}}_z \mid \Psi_{\rm g} \,\rangle$ as zero, and thus regard v as a virtual velocity which we retain in our calculations to keep track of the effective mass of the coupled electron-phonon complex.

In the case where the coupling constant is thought to be really strong the visualization of the problem is relatively simple and a reasonable description of the system can readily be achieved by requiring an optimization of the transformed Hamiltonian $\tilde{H}$ with respect to the ground state, $\Phi_{\rm e}(\vec{\varrho}, z) \mid 0\,\rangle$, of the polaron. We shall retain the results and discussions pertaining to the large α limit until later and point them out as a special case of the more general results which we derive in the last section. Here, our concern is to make correspondence with the variational scheme of Devreese *et al.*[56] where the adiabatic polaron trial state is modified accordingly so as to cover the overall range of the coupling strength. For the sake of completeness, in the foregoing two subsections we choose to include a brief revision of the basic essentials in the variational ansatz advanced in [56]. The major distinction which sets the present concern apart from that in [56] is that we confine ourselves to a one dimensionally confined polaron model with a virtual momentum imposed to the coupled electron–phonon complex through the factor ρ_Q multiplying the term s_Q in the Hamiltonian (5.12).

5.2.2 Variational State for Arbitrary Coupling

Regardless of the value of α, no matter how small it is, the procedure is still to continue with our considerations from Eq.(5.12), since with decreasing α the degree of localization of the electron becomes reduced in a significant manner; eventually s_Q tends to zero on the average and thus $\tilde{H}$ converts back to its original form H stripped from the displaced oscillator transformation. In view

of this reasoning one is led to include a first order correction to the trial state (5.3) with the last term in Eq.(5.12) treated as a perturbation. Since at present we limit ourselves to the case of a stationary polaron, we first would like to bring about an insight into the problem with ρ_Q in Eq.(5.12) set to unity, thereby obtain a means of characterizing the polaron (i.e., calculating the optimal Φ_e and hence the binding energy, for instance) for the case when $v = 0$. Thereafter we shall turn on the velocity to keep trace of the polaron mass under a virtual translation of the electron and the lattice distortion together.

In the perturbation treatment of the Fröhlich interaction, the first non-vanishing contribution to the ground-state energy comes from the term which is of second order in the interaction amplitude. Correspondingly, the leading correction to the trial state defined through Eqs.(5.3) and (5.4) is of first order. The ground state trial wave function for $\tilde{H}$ and for the constraint that the total momentum $\tilde{\mathsf{P}}_z$ be conserved, then becomes extended to

$$\Psi_g \rightarrow \tilde{\Psi}_g \;=\; c\Psi_g \;+\; \sum_Q V_Q \sum_i \mid \Psi_i \rangle \frac{\langle \Psi_i \mid (e^{-i\vec{Q}\cdot\vec{r}} - s_Q) a_Q^\dagger \mid \Psi_g \rangle}{\Delta\varepsilon_{i-g}} \tag{5.15}$$

In the above, c is a constant which serves for normalization, and the index i refers to the intermediate states consisting those of the electron and one-phonon with wave vector $\vec{Q}$. The summation over the intermediate states is a rather difficult task since now the states themselves and the corresponding energies depend on α and the lattice coordinates in involved manners. Nevertheless, this shortcoming can be eliminated by replacing the energy denominator $\Delta\varepsilon_{i-g}$ by an average quantity

$$g_Q = \left\langle \frac{1}{\Delta\varepsilon_{i-g}} \right\rangle_i \tag{5.16}$$

which in the calculation will be determined variationally. Using completeness the i-summation in Eq.(5.15) can be projected out to yield[56]

$$\tilde{\Psi}_g \;=\; \{c \;+\; \sum_Q V_Q g_Q (e^{-i\vec{Q}\cdot\vec{r}} - s_Q) a_Q^\dagger\} \Psi_g \tag{5.17}$$

The variational parameter g_Q sets up a fractional admixture of the strong and weak coupling counterparts of the coupled electron–phonon system and thus is

expected to serve for the theory to interpolate between the extreme limits of the coupling constant.

5.2.3 Formulation

The requirement that the extended trial state $\tilde{\Psi}_g$ be normalized yet poses a further constraint interrelating the parameters c and g_Q through

$$f(c, g_Q) = c^2 + \sum_Q V_Q^2 g_Q^2 h_Q - 1 = 0 \tag{5.18}$$

in which

$$h_Q = \langle 0 \mid (e^{i\vec{Q}\cdot\vec{r}} - s_Q)(e^{-i\vec{Q}\cdot\vec{r}} - s_Q) \mid 0 \rangle = 1 - s_Q^2 \ . \tag{5.19}$$

In order to find the optimal fit to g_Q one has to minimize the expectation value of $\check{H} - v\tilde{\mathsf{P}}_z$ in the trial state (5.17) subject to the constraint (5.18). Within the framework of the modified trial state $\tilde{\Psi}_g$ the functional (5.8) now takes the form

$$\begin{aligned} \mathsf{F}(\beta, v \mid c, g_Q) &= c^2(e_0 + \frac{1}{4}v^2) - \frac{1}{2}v^2 + (1 - 2c^2)\chi \\ &+ 2c\sum_Q V_Q^2 g_Q h_Q + \sum_Q V_Q^2 g_Q^2 (e_Q - \delta_Q + h_Q) \end{aligned} \tag{5.20}$$

where

$$e_0 = \langle \Phi_e \mid -\nabla^2 \mid \Phi_e \rangle \tag{5.21}$$

$$\begin{aligned} e_Q &= \langle \Phi_e \mid (e^{i\vec{Q}\cdot\vec{r}} - s_Q)(-\nabla^2)(e^{-i\vec{Q}\cdot\vec{r}} - s_Q) \mid \Phi_e \rangle \\ &= e_Q^{(0)} - v(q_z - \frac{1}{4}v)h_Q \end{aligned} \tag{5.22}$$

with

$$e_Q^{(0)} = q^2 + \frac{1}{2}q_z^2 + (e_0 + \frac{1}{2}q_z^2)h_Q \ , \tag{5.23}$$

and furthermore,

$$\chi = \sum_Q V_Q^2 s_Q^2 \rho_Q, \tag{5.24}$$

$$\delta_Q = \sum_{Q'} V_{Q'}^2 s_{Q'} \Delta_{QQ'} \rho_{Q'} \tag{5.25}$$

wherein

$$\Delta_{QQ'} = \langle\, 0 \mid (e^{i\vec{Q}\cdot\vec{r}} - s_Q)(e^{i\vec{Q}'\cdot\vec{r}} + e^{-i\vec{Q}'\cdot\vec{r}})(e^{-i\vec{Q}\cdot\vec{r}} - s_Q) \mid 0\,\rangle\ . \tag{5.26}$$

The variational fit to g_Q (and to the normalization constant c) is achieved by requiring

$$\frac{\partial}{\partial g_Q}\{\mathsf{F}(\beta, v \mid c, g_Q) - \Lambda f(c, g_Q)\} = 0 \tag{5.27}$$

with Λ being a Lagrange multiplier. It then follows that the functional F is given by

$$\mathsf{F}(\beta, v) = e_0 - \chi - \frac{1}{4}v^2 + \Lambda \tag{5.28}$$

where Λ is derived through the transcendental equation

$$\Lambda = \sum_Q V_Q^2[g_Q/c]h_Q \tag{5.29}$$

in which

$$\frac{g_Q}{c} = -\frac{h_Q}{D_Q} \tag{5.30}$$

and

$$D_Q = e_Q - \delta_Q + (1 - e_0 - \frac{1}{4}v^2 + 2\chi - \Lambda)h_Q\ . \tag{5.31}$$

In order to trace out the polaron mass from Eq.(5.28) we have to split $\mathsf{F}(\beta, v)$ into its parts consisting of the binding energy of the polaron alone and the additional kinetic contribution which shows up under having imposed a virtual momentum to the polaron. We are thus tempted to expand Eqs.(5.24), (5.25) and the summand in Eq.(5.29) in a power series up to second order in v. We therefore conform χ and δ_Q into the forms

$$\chi = \chi^{(0)} + \frac{1}{4}v^2\chi^{(1)} \qquad \text{and} \qquad \delta_Q = \delta_Q^{(0)} + \frac{1}{4}v^2\delta_Q^{(1)} \tag{5.32}$$

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

$$\chi^{(n)} = \sum_Q V_Q^2 s_Q^2 [2q_z]^{2n} \tag{5.33}$$

$$\begin{aligned}\delta_Q^{(n)} &= \sum_{Q'} V_{Q'}^2 s_{Q'} \Delta_{QQ'} [2q'_z]^{2n} \\ &= 2\chi^{(n)}(1 + s_Q^2) - 2s_Q \sum_{Q'} V_{Q'}^2 s_{Q'}(s_{Q+Q'} + s_{Q-Q'})[2q'_z]^{2n}\end{aligned} \tag{5.34}$$

in which $s_{Q\pm Q'}$ refers to the same expression as for s_Q, cf. Eq.(5.10), in which $\vec{q}$ is to be replaced by $\vec{q} \pm \vec{q}\,'$, and q_z by $q_z \pm q'_z$.

Furthermore, setting

$$D_Q^{(0)} = e_Q^{(0)} - \delta_Q^{(0)} + (1 - e_0 + 2\chi^{(0)} - \Lambda)h_Q \tag{5.35}$$

we obtain

$$\mathsf{F}(\beta, v) = E_{\rm g}(\beta) - \frac{1}{4}v^2 m_{\rm p} \tag{5.36}$$

where

$$E_{\rm g}(\beta) = e_0 - \chi^{(0)} + \Lambda \tag{5.37}$$

refers to the ground state energy and the factor $m_{\rm p}$ multiplying $\frac{1}{4}v^2$ is identified as the polaron mass given by

$$m_{\rm p} = 1 + \chi^{(1)} + \sum_Q V_Q^2 \frac{h_Q^2}{D_Q^{(0)}}\{[2q_z h_Q/D_Q^{(0)}]^2 + [\delta_Q^{(1)} - 2\chi^{(1)}h_Q]/D_Q^{(0)}\}\ . \tag{5.38}$$

The explicit analytic forms for the quantities e_0, s_Q, $\chi^{(n)}$ and $\delta_Q^{(n)}$ involved in Eqs.(5.37),(5.38) can be derived using the functional form for $\Phi_{\rm e}(\vec{\varrho}, z)$ which we introduce in the next section. They are however lengthy to write here and therefore, we list them in the Appendix 5.2.5.

It should be clear that in deriving Eq.(5.36) we have regarded parameter Λ as to be obtained from Eq.(5.29) for when $g_Q/c = -h_Q/D_Q^{(0)}$, i.e., for the case where the polaron is taken as stationary.

5.2.4 Results and Conclusions

Due to the analytic complexity the optimal fits to Λ and $\Phi_{\rm e}$ are to be performed by numerical methods within an iterative scheme. In our calculations we select the electron wave function $\Phi_{\rm e}(\vec{\varrho}, z)$ given by Eq.(5.2) in a reasonably simplest form where its transverse and longitudinal parts are given by

$$\varphi(\vec{\varrho}) = \frac{\mathrm{J}_0(j_{0,1}\varrho/R)}{\sqrt{\pi}R\mathrm{J}_1(j_{0,1})} \tag{5.39}$$

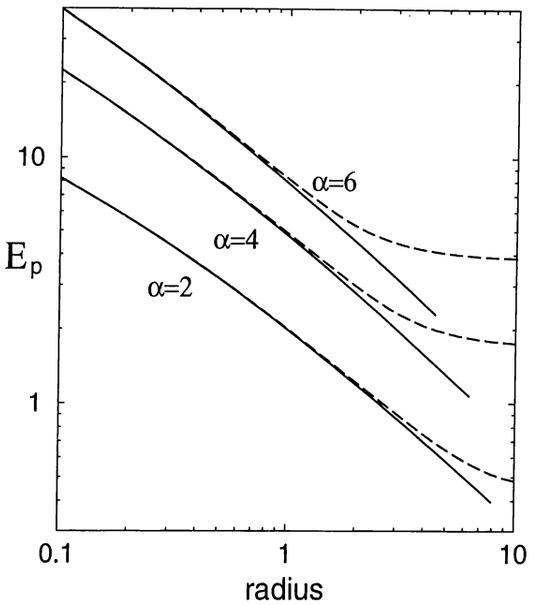

Figure 5.1: Comparison of two forms for the wave function
The binding energy as a function of the wire radius calculated within the strong coupling theory. The solid and dashed curves are for $\varphi(\vec{\varrho})$ taken as given by Eqs.(5.39) and (5.42), respectively.

and

$$Z(z) = (\frac{\beta^2}{\pi})^{1/4} \exp(-\frac{1}{2}\beta^2 z^2) \ . \tag{5.40}$$

Here, J_n denotes the nth order cylindrical Bessel function of the first kind and $j_{0,1} \approx 2.4048$ is the first zero of J_0. Parameter β is to be adjusted variationally and provides a measure of the spatial extent of the electron along the wire axis, i.e., the root mean square of the coordinate z is related to β through

$$\begin{aligned} \xi_z &= \{\langle \tilde{\Psi}_g \mid z^2 \mid \tilde{\Psi}_g \rangle\}^{1/2} \\ &= \frac{1}{\sqrt{2}\beta} \sqrt{\frac{1 + \sum_Q V_Q^2 (g_Q/c)^2 [1 - (1 - q_z^2/\beta^2) s_Q^2]}{1 + \sum_Q V_Q^2 (g_Q/c)^2 h_Q}} \ . \end{aligned} \tag{5.41}$$

We think that for not too large α the choice (5.39) for $\varphi(\vec{\varrho})$ is well suited for thin wire structures as the transverse localization is provided most dominantly by the wire–boundary potential rather than the phonon–coupling – induced localization.

We could as well have chosen $\varphi(\vec{\varrho})$ as more general like

$$\varphi(\vec{\varrho}) \rightarrow \varphi(\vec{\varrho}) \exp(-\beta'^2 \varrho^2), \tag{5.42}$$

consisting of a Gaussian extension, for instance. This latter waveform duplicates the same features at small wire radii and is expected to give better results in the range of large R, and moreover, to depict asymptotically the bulk limit when $R \rightarrow \infty$. However we still adopt the former expression (5.39) for Φ_e mainly to facilitate the analytic and numeric computations. In the following we therefore restrict our considerations solely to thin wires rather than bulk–like media where the relevant polaron properties have already been well understood in the literature. In this regard we shall be content with a comparison of the two waveforms (5.39) and (5.42) within only the framework of the strong–coupling approximation with α selected as larger than 1 where the discrepancy is expected to be somewhat more prominent than that in the intermediate and weak coupling regimes (cf, Fig.5.1). From the succession of curves for $\alpha = 2, 4$ and 6 we observe that the energy values derived from (5.39) exhibit a considerable amount of digression from what one expects for large R, and in particular, the digression grows larger for stronger α. We also note that the place at which the curves for (5.39) and (5.42) start to get deviated shifts down to smaller R values for stronger phonon coupling since for large α the polaron is already in a highly localized state and a small sized polaron becomes influenced by the confining boundary only for small wire radius. On the contrary however, we see that for not too large α both wave functions, (5.39) and (5.42), give almost identical binding energies for $R \leq 2$, and that the waveform (5.39) which we use in our calculations becomes capable to reflect a reasonable description of the system over a broader range of R when α is made weaker.

In displaying the results of the present formulation we first refer to the regime of strong phonon coupling and provide plots of the binding energy $E_{\rm p} = (j_{0,1}/R)^2 - E_{\rm g}$ and the polaron mass $m_{\rm p}$ against the wire size for a succession of large α values. An immediate glance at the set of curves in Fig.5.2 reveals that with increasing degree of confinement (i.e., with increasing R^{-1} as well as with increasing α) the binding becomes substantially deepened

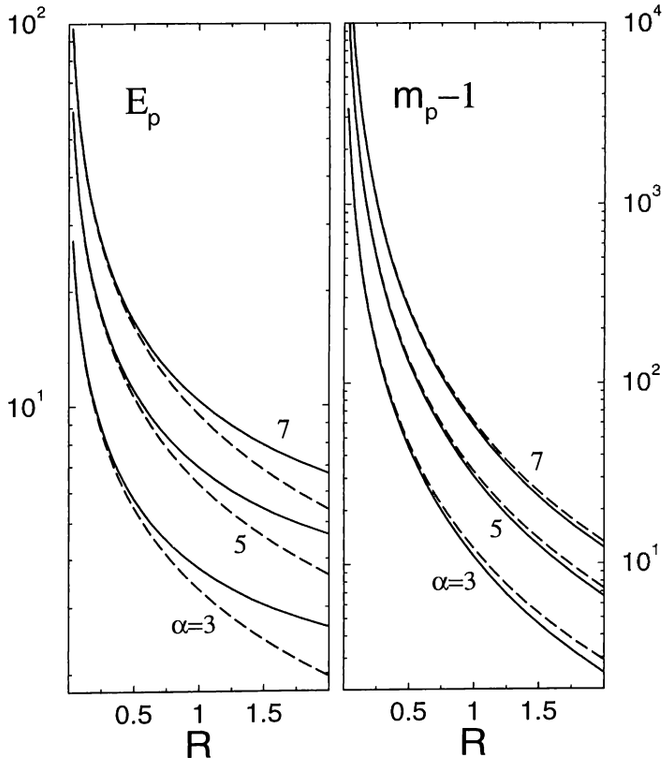

Figure 5.2: The binding energy and the effective mass of polaron at strong coupling.
(a) $E_{\rm p}$, (b) $m_{\rm p}$ as a function of the wire radius. The solid and dashed curves reflect the results of the present and strong coupling approximations, respectively.

where correspondingly the effective polaronic mass scales to large values with very pronounced slopes. Comparing our results with those derived from the strong-coupling theory (cf. dashed curves) we note that the present approach yields significantly improved energy upper bounds and that the strong coupling approximation deviates considerably from the present formalism as α is made weaker and/or R is increased. Indeed, it is only for large α and small R that the two approaches become identical since in this limit the electron gets highly localized, s_Q (5.10) becomes unity on the average, and thus h_Q (5.19), and hence Λ (5.29), tend to zero and the present theory readily reproduces the strong coupling limit, i.e.,

$$E_{\rm g} = e_0 - \chi^{(0)} \qquad \text{and} \qquad m_{\rm p} = 1 + \chi^{(1)} \tag{5.43}$$

as depicted by that the curves (solid and dashed) become closer and eventually match as the phonon coupling is made stronger and R is tuned to small values.

Alternatively stating, for not too strong α the pure strong coupling treatment of the problem is totally inadequate to reflect any weak coupling aspect and this shortcoming is eliminated in the present approach by solving the transcendental equation (5.29) for the term Λ in the energy expression, since it is only through this term that a detailed interbalance is set up between the strong and weak coupling counterparts of the coupled electron-phonon system. As α is shifted down to small values the role Λ plays becomes very prominent and in case the electron is loosely bound the polaron binding is mostly determined by this term. In particular, for a reduced degree of confinement ($R \gg 1$) and at weak coupling ($\alpha \ll 1$), it is easy to see that the terms e_0, δ_Q, χ and Λ in Eq.(5.31) become far too small to yield any significant contribution to the summand in the transcendental equation (5.29). Therefore, in Eqs.(5.37) and (5.38) retaining only $h_Q \approx 1$ and $e_Q \approx Q^2$ we readily obtain

$$E_{\rm g} \approx \Lambda \approx -\sum_Q V_Q^2 (1+Q^2)^{-1} = -(2/\pi)\alpha \int_0^\infty dq (1+Q^2)^{-1} = -\alpha$$

and

$$m_{\rm p} \approx 1 + 4\sum_Q V_Q^2 q_z^2 (1+Q^2)^{-3} = 1 + \frac{1}{6}\alpha$$

which are the well established energy and mass values for the bulk polaron in the weak α limit; thus exemplifying the essential role which Λ plays in conforming the adiabatic approximation over to the results derived from the perturbation theory.

An important remark pertaining to a weakly coupled polaron in a narrow wire is that the electron now has to choose in between two contrasting aspects of whether to conform to a delocalized state with correspondingly large spread when $\alpha \ll 1$, or to acquire a localized configuration as the wire is made thinner. It should be mentioned that, the parameters α and R characterizing the system do not enter the problem in an independent way but together take part in a related manner in the binding, dominating the effect of one another, and yet acting

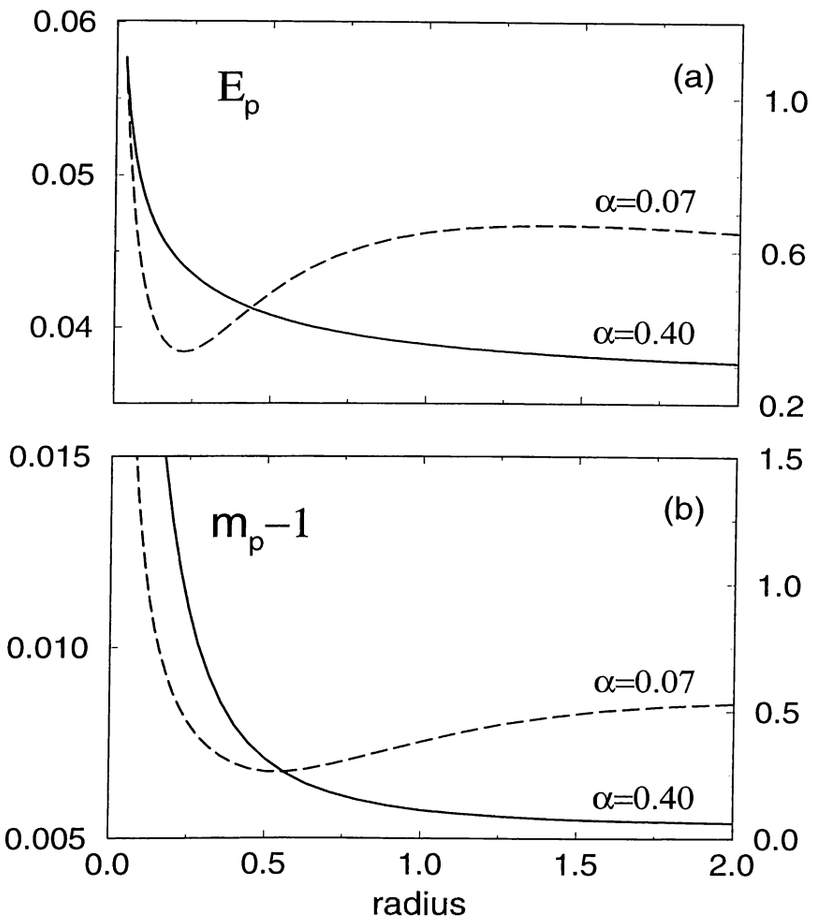

Figure 5.3: Results for CdTe and GaAs based quantum wires (a) The binding energy E_p, and (b) the effective polaron mass m_p, as a function of wire radius. The solid and dashed curves are for CdTe (right scale) and GaAs (left scale) based quantum wires respectively. In the plots, the energy and length units correspond, respectively, to 18 (35) meV and 44 (40) $\mathring{A}$, for CdTe(GaAs).

collaboratively in favor of stronger binding. Thus, a high degree of localization in reduced dimensionality is expected to lead to a pseudo-enhancement in the effective electron–phonon coupling which in turn brings about the possibility that, in spite of weak polar coupling as in compound semiconductors, the polaron binding may as well have a strong-coupling counterpart coming from confinement effects in narrow wires.

As reference to weak electron–phonon coupling we select CdTe ($\alpha \simeq 0.40$)

and GaAs ($\alpha \simeq 0.07$) based quantum wires which are of particular interest as typical examples of II–VI and III–V compound semiconductors. An examination of the curves for CdTe and GaAs in Fig.5.3 reveals that both $E_{\rm p}$ and $m_{\rm p}$ undergo rather distinctive types of variations when we vary R. We observe that for $\alpha = 0.40$ the binding (and hence the mass) become monotonically stronger and more inertial as the dimensionality is tuned from three to quasi-one. This is totally consistent with what one usually expects for systems of reduced dimensionality, and originates essentially from that, with decreasing R, the wave function is squeezed onto the wire axis in all transverse directions, resulting in a reduction in the overall spatial extent of the polaron on the average and hence in the effective dimensionality, thus leading to deeper polaronic binding.

For even weaker coupling (as in GaAs, for instance – cf., the dashed curves in Fig.5.3) the behavior is rather different. Beginning from the bulk case and approaching the one–dimensional limit there comes about a competitive interrelation between whether the charge density fluctuations of the electron will condense onto the polaron center or will expand to relax itself in the longitudinal ($\pm z$) directions along the wire axis. Starting from $R \gg 1$ and then restricting the transverse spread of the electron the contribution coming from the tendency of the electron to expand longitudinally dominates first, causing a decrease in the binding energy, and correspondingly leads to a smaller effective mass of the polaron. Meanwhile, with contracting wire radius the electronic spread experiences an increasingly large restriction towards the wire axis and therefore, below a certain wire size, the effective degree of localization of the electron–phonon system starts to increase, leading to a considerably pronounced effective phonon coupling and hence to deeper polaronic binding. For comparatively stronger α this salient feature becomes less prominent and does not even show up, since the starting state of the system is already a localized one.

In Fig.5.4, we provide a global comprehensive summary of the variation of the binding energy as a function of α and R. We observe that, regardless of the wire width, $E_{\rm p}$ (and $m_{\rm p}$ – not pictured in the figure) always increase monotonically with increasing α. So is true with decreasing R as well, only however, for α

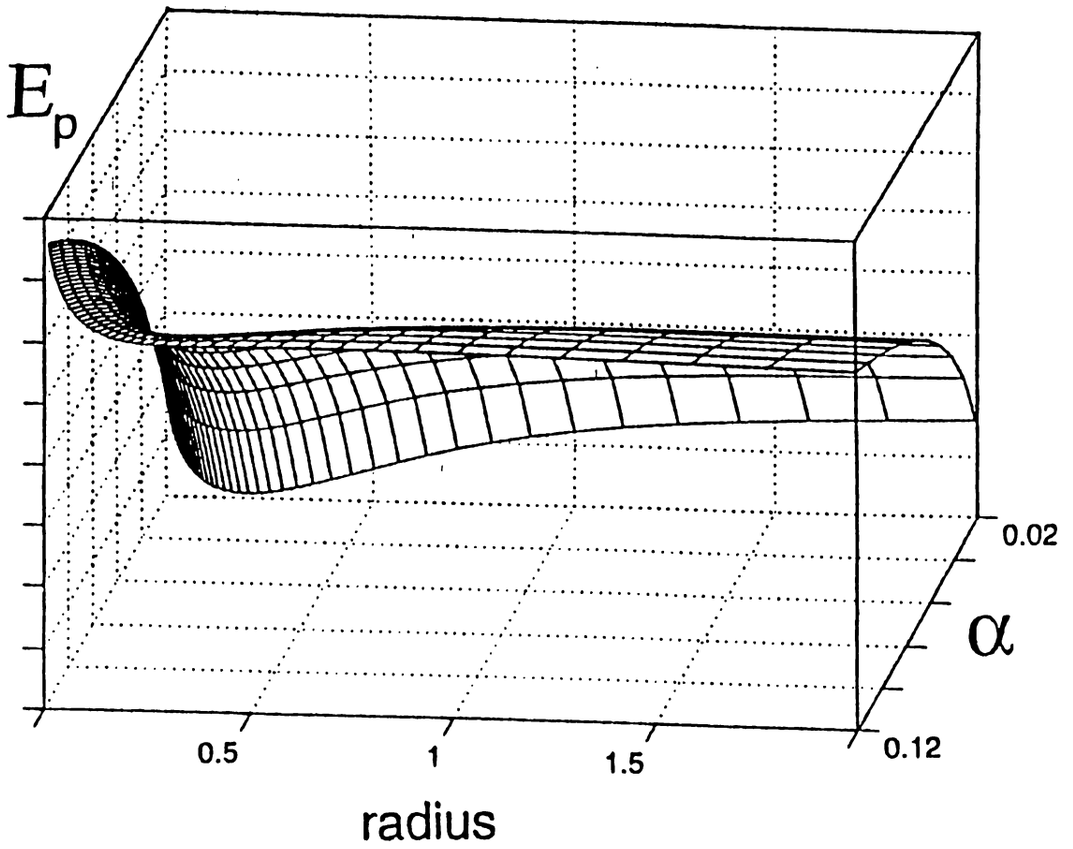

Figure 5.4: A global view of polaronic binding energy
The binding energy (in arbitrary units on a logarithmic scale), as a function of the coupling constant α and the wire radius.

lying above some value around 0.10. Below this value of α, the energy and mass profiles (viewed as a function of decreasing R) are seen to decrease first, and then increase after having gone through a minimum as in the aforementioned description given for the GaAs–wire. To give somewhat more impact to this interesting type of variation of the polaronic binding, we portray the longitudinal extent of the polaron, ξ_z (5.41), over the relevant range of weak–α and the wire radius (cf., Fig.5.5). We note that when α is small, ξ_z has first a tendency to expand and, after having displayed a peaked profile, shrinks as the wire radius is reduced to smaller values. For large values of α, however, ξ_z is seen to shrink

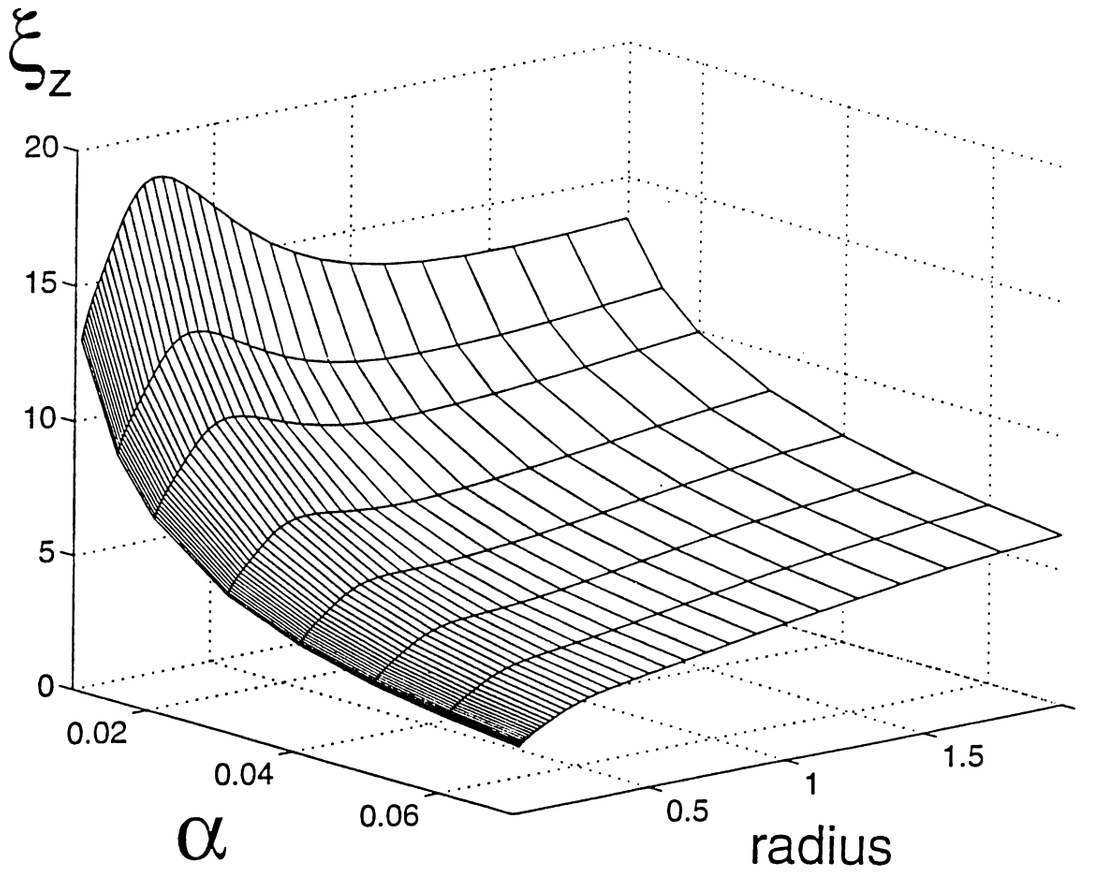

Figure 5.5: A global view of polaron longitudinal spatial extent ξ_z is given as a function of the coupling constant and the wire radius.

monotonically without showing up any prominent increase, since in this case the polaron has already a comparatively deeper self-induced potential, and an increase in the degree of confinement makes the polaron even more deeply bound and more localized.

An interesting remark pertaining to the regime of weak coupling is that even for coupling constants as small as $\alpha \sim 0.01$, a "pseudo - strong coupling" condition can be reached at high degrees of confinement. For completeness, we exemplify this feature in Fig.5.6 where we plot ξ_z (calculated from both the strong coupling and present theories) against the wire size. From the succession of the pairs of curves for $\alpha = 0.01$, 0.02 and 0.03, we readily note that at highly confined configurations of the polaron, the ξ_z - profiles calculated from Eq.(5.42) are fairly

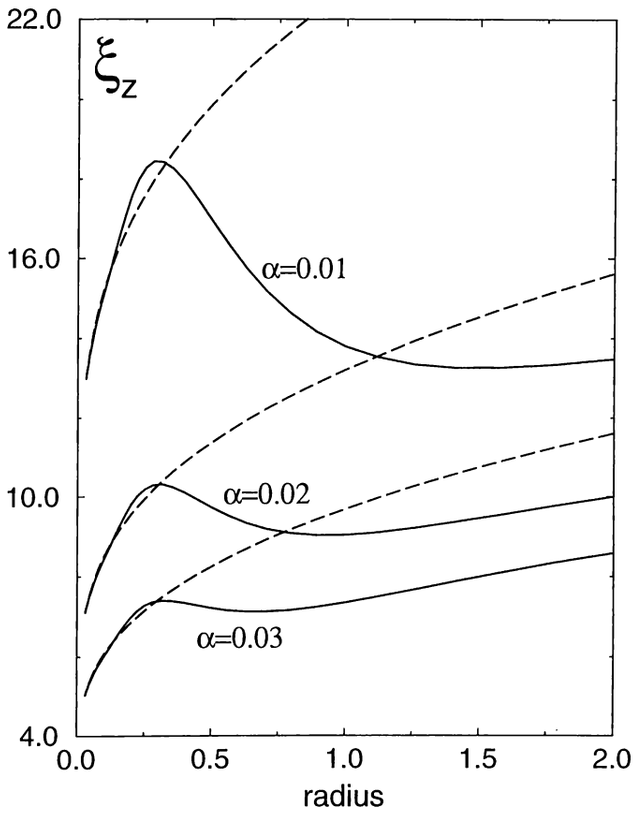

Figure 5.6: The longitudinal spatial extent at weak coupling. The solid and dashed curves reflect the results of the present and strong coupling approximations, respectively.

close to those derived from the strong coupling theory: $\xi_z = 1/\sqrt{2}\beta$, where now the optimal β is to be obtained by minimizing the energy expression given by Eq.(5.43). As the confining boundary is made to expand, however, the strong coupling theory rapidly loses its validity and deviates rather drastically from the present formalism both in terms of magnitude and qualitative nature; and the digression grows at much faster rates for smaller values of the coupling constant.

In summary, we have revised the ground state property of the optical polaron confined in a cylindrical quantum wire of infinite boundary potential. The formalism adopted here allows one to trace out the polaron quantities of general interest within an interpolating scheme accounting for the fractional admixture of the weak and strong coupling counterparts of the coupled electron phonon

complex. Contrary to the general trend that the effective electron phonon coupling is inherently stronger in systems of lower dimensionality, we find that at weak α and for thin wires the polaronic binding may get loose and even become weaker than for the bulk case.

5.2.5 Appendix

The functional forms for the quantities e_0, s_Q, $\chi^{(n)}$ and $\delta_Q^{(n)}$, (n=0,1), calculated using Eqs.(5.39) and (5.40) are given by

$$
\begin{aligned}
e_0 &= (j_{0,1}/R)^2 + \frac{1}{2}\beta^2 \\
s_Q &= A(qR)\ \exp(-\frac{q_z^2}{4\beta^2}) \\
\chi^{(0)} &= \alpha \int_0^\infty dq\, A^2(qR)\, e^{\gamma^2}\mathrm{erfc}(\gamma) \\
\chi^{(1)} &= \sqrt{32/\pi}\,\alpha\beta \int_0^\infty dq\, q\, A^2(qR)\, \{1 - \sqrt{\pi}\,\gamma\, e^{\gamma^2}\mathrm{erfc}(\gamma)\} \\
\delta_Q^{(n)} &= 2\chi^{(n)}(1+s_Q^2) - \frac{8}{\pi^2}\alpha\, s_Q \int d^3q' \frac{q_z'^{2n}}{q'^2+q_z'^2}\, s_{Q'}\, A(\mid \vec{q}+\vec{q}' \mid R) \\
&\qquad \times \exp(-\frac{q_z^2+q_z'^2}{4\beta^2})\cosh(\frac{q_z q_z'}{2\beta^2})
\end{aligned}
$$

where in the above, we have defined $\gamma = q/\sqrt{2}\beta$, and

$$
A(qR) = \frac{2}{[j_{0,1}\mathrm{J}_1(j_{0,1})]^2} \int_0^{j_{0,1}} dt\ t\, \mathrm{J}_0^2(t)\, \mathrm{J}_0(\frac{qR}{j_{0,1}}t)
$$

Chapter 6

PATH INTEGRAL FORMALISM

6.1 Introduction

Feynman's path integral approach has become a unifying formalism in several branches of physics, with such applications in Brownian motion, quantum mechanics, quantum field theory, solid state physics, quantum electro-dynamics, etc. A diverse treatment of the formalism and its applications can be found in the excellent textbook by Feynman and Hibbs,[88] also in some recent publications.[89-91]

In this introductory section we intend to summarize only some basic features of the formalism, required for the treatment of the polaron with path integrals.

6.1.1 Basic Concepts

In quantum mechanics, we deal with the occurrence probabilities of the physical events. The probability of a particle to reach a space-time point $(\vec{r}_b, t_b)$ starting from a space-time point $(\vec{r}_a, t_a)$ is denoted by

$$P(b,a) = |K(\vec{r}_b, t_b; \vec{r}_a, t_a)|^2 \ . \tag{6.1}$$

Here, $K(\vec{r}_b, t_b; \vec{r}_a, t_a)$ is the probability amplitude (or quantum mechanical propagator) for that event, and it is the sum over the the amplitudes of all possible

paths $\vec{r}(t)$ with $\vec{r}(t_a) = \vec{r}_a$ and $\vec{r}(t_b) = \vec{r}_b$. The amplitude associated with each path $\vec{r}(t)$ is proportional to $\exp\{i\mathcal{S}[\vec{r}(t)]/\hbar\}$ where $\mathcal{S}[\vec{r}(t)]$ is the classical action for the trajectory $\vec{r}(t)$:

$$K(\vec{r}_b, t_b; \vec{r}_a, t_a) = \int \mathcal{D}\vec{r}\ e^{i\mathcal{S}[\vec{r}]/\hbar} \tag{6.2}$$

with $\mathcal{D}\vec{r}$ denoting the functional integral over the paths.

If $\Psi(\vec{r}, t) \equiv \langle\vec{r}|\Psi(t)\rangle$ is the wave function of the system in the position representation at time t, the propagator $K(\vec{r}_b, t_b; \vec{r}_a, t_a)$, by definition relates $\Psi(\vec{r}_b, t_b)$ to $\Psi(\vec{r}_a, t_a)$:

$$\Psi(\vec{r}_b, t_b) = \int d\vec{r}_a\, K(\vec{r}_b, t_b; \vec{r}_a, t_a)\Psi(\vec{r}_a, t_a) \tag{6.3}$$

which establishes the relation between path integrals and the operator formulation of quantum mechanics. The path integral in Eq.(6.2) corresponds to a matrix element in position representation of the time-evolution operator in the operator formulation of quantum mechanics. For a time-independent Hamiltonian,

$$K(\vec{r}_b, t; \vec{r}_a, 0) = \langle\vec{r}_b|e^{-itH/\hbar}|\vec{r}_a\rangle\ . \tag{6.4}$$

With the use of time-independent Schrödinger equation, $H|\Psi_n\rangle = E_n|\Psi_n\rangle$ it is possible to write,

$$\begin{aligned} K(\vec{r}_b, t; \vec{r}_a, 0) &= \sum_n \langle\vec{r}_b|e^{-itH/\hbar}|\Psi_n\rangle\langle\Psi_n|\vec{r}_a\rangle \\ &= \sum_n \langle\vec{r}_b|\Psi_n\rangle\langle\Psi_n|\vec{r}_a\rangle e^{-itE_n/\hbar} \end{aligned} \tag{6.5}$$

i.e. the Fourier expansion of the path integral allows to determine the eigen energies of a stationary system:

$$K(\vec{r}_b, t; \vec{r}_a, 0) = \sum_n \Psi_n^*(\vec{r}_b)\Psi_n(\vec{r}_a)e^{-itE_n/\hbar}\ . \tag{6.6}$$

Replacing the time variable t by an *imaginary time* variable $t \to -i\hbar\beta$, (with β to be interpreted as $1/k_BT$, where T is the temperature and k_B the Boltzmann constant), it is clear that the behavior of the resulting *propagator for imaginary times* is governed by the ground state energy in the asymptotic limit $\beta \to \infty$;

$$K(\vec{r}_b, -i\hbar\beta; \vec{r}_a, 0) \overset{\beta\to\infty}{\longrightarrow} \Psi_0^*(\vec{r}_b)\Psi_0(\vec{r}_a)e^{-\beta E_0} \tag{6.7}$$

whereas for arbitrary β one readily obtains the relation between the propagator and the partition function;

$$\mathcal{Z} \equiv \mathrm{Tr}\, e^{-\beta H} = \int d\vec{r}_0\, K(\vec{r}_0, -i\hbar\beta; \vec{r}_0, 0)\ . \tag{6.8}$$

6.1.2 Elimination of the Phonon Field

The Fröhlich Hamiltonian describes the coupling of the electron to the harmonic phonon modes. Therefore, here, we will state the form of partition function for the system of an electron linearly coupled to a harmonic oscillator. Consider the Hamiltonian

$$H = H_e + \hbar\omega(a^\dagger a + 1/2) + fa + f^\dagger a^\dagger \tag{6.9}$$

where H_e is the part related to the electron and $f, f^\dagger$ sets up the interaction with the oscillator. The partition function can be evaluated by using the ordered operator technique to yield a form independent of the oscillator operators $a, a^\dagger$. In the language of path integrals, the final form of $\mathcal{Z}$ after the elimination of the oscillator, is written as,

$$\mathcal{Z} = \frac{e^{-\beta\hbar\omega/2}}{1 - e^{-\beta\hbar\omega}} \int d\vec{r}_0 \int_{\vec{r}_0}^{\vec{r}_0} \mathcal{D}\vec{r} e^{\mathcal{S}_e + \mathcal{S}'} \tag{6.10}$$

where $\mathcal{S}_e$ is the part of the action corresponding to H_e and

$$\mathcal{S}' = \frac{1}{2}\int_0^\beta d\lambda \int_0^\beta d\lambda'\, G_\omega(|\lambda - \lambda'|) f(\lambda) f(\lambda') \tag{6.11}$$

belongs to the interaction. Here, λ, λ' are the imaginary time variables, and

$$G_\omega(u) = \frac{\cosh((\beta - 2u)\hbar\omega/2)}{\sinh(\beta\hbar\omega/2)} \xrightarrow{\beta\to\infty} e^{-\omega u} \tag{6.12}$$

is the Green's function of the harmonic oscillator. Note that the price paid for the elimination of the oscillator is the retarded interaction occurring in $\mathcal{S}'$.

6.1.3 A Variational Principle

When the exact evaluation of the path integrals is not possible or hard to manage, one can use a variational principle, namely Jensen-Feynman inequality for the approximate evaluation of certain type of them.

Suppose we wish to evaluate the free energy F of a system. The partition function can be expressed in the form ($\hbar = 1$)

$$\mathcal{Z} = \int d\vec{r}_0 \int_{\vec{r}_0}^{\vec{r}_0} \mathcal{D}\vec{r} e^{\mathcal{S}} = e^{-\beta F} \ . \tag{6.13}$$

The action $\mathcal{S}$ in the above, is real in ordinary cases without a magnetic field, and the following principle is applicable for real $\mathcal{S}$. (However, recently, the conditions for its validity with imaginary actions have been explored and discussed in detail[89,92]).

To obtain an approximate value of F, one should find another trial action $\mathcal{S}_0$ (with variational parameters) satisfying two conditions. First, $\mathcal{S}_0$ should be simple enough that expressions such as $\int \mathcal{D}\vec{r} e^{\mathcal{S}_0}$ or the weighted averages like $\langle \mathcal{A} \rangle_{\mathcal{S}_0} = (\int \mathcal{D}\vec{r}\, \mathcal{A}\, e^{\mathcal{S}_0})/(\int \mathcal{D}\vec{r} e^{\mathcal{S}_0})$, for simple functionals $\mathcal{A}$ can be evaluated. Second, $\mathcal{S}_0$ should resemble $\mathcal{S}$ as much as possible to be a representative of the general character of it.

Assume that F_0, the free energy associated with $\mathcal{S}_0$, is calculated. That is

$$e^{-\beta F_0} = \int d\vec{r}_0 \int_{\vec{r}_0}^{\vec{r}_0} \mathcal{D}\vec{r} e^{\mathcal{S}_0} \tag{6.14}$$

so that

$$\frac{\int d\vec{r}_0 \int_{\vec{r}_0}^{\vec{r}_0} \mathcal{D}\vec{r} e^{\mathcal{S}}}{\int d\vec{r}_0 \int_{\vec{r}_0}^{\vec{r}_0} \mathcal{D}\vec{r} e^{\mathcal{S}_0}} = e^{-\beta(F-F_0)} \ . \tag{6.15}$$

Then since $e^{\mathcal{S}} = e^{\mathcal{S}-\mathcal{S}_0} e^{\mathcal{S}_0}$, we can write Eq.(6.15) as

$$\langle e^{\mathcal{S}-\mathcal{S}_0} \rangle_{\mathcal{S}_0} = e^{-\beta(F-F_0)} \ . \tag{6.16}$$

At this point we can make a rigorous approximation. The average value of e^x when x is a random variable, always exceeds or equals the exponential of the average value of x, as long as x is real and the weights used in the averaging process are positive (Jensen's inequality). That is

$$e^{\langle x \rangle} \leq \langle e^x \rangle \tag{6.17}$$

where $\langle x \rangle$ is the weighted average of x. This relation is true for any concave upward function like the exponential function. A pictorial presentation of the

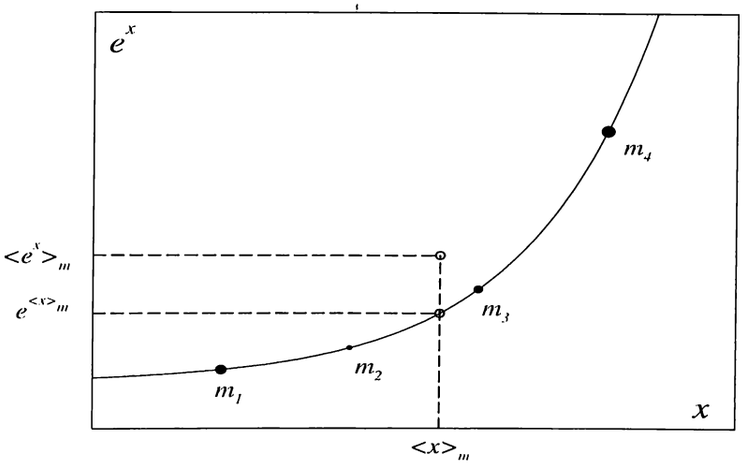

Figure 6.1: Illustration of Jensen's inequality.
The masses m_i have different weights and $\langle\ \rangle_m$ denotes the weighted average.

relation (6.17) can be clearly seen in Fig.6.1 where a number of masses are placed on the curve e^x.

Changing the left-hand side of Eq.(6.16), we have

$$e^{\langle \mathcal{S}-\mathcal{S}_0\rangle_{\mathcal{S}_0}} \leq e^{-\beta(F-F_0)} \ . \tag{6.18}$$

This implies that

$$F \leq F_0 - \frac{1}{\beta}\langle \mathcal{S}-\mathcal{S}_0\rangle_{\mathcal{S}_0} \ . \tag{6.19}$$

The right-hand side of the above equation constitutes an upper bound for the exact free energy F. The nearest approximation to F can be determined through the minimization of $F_0 - \frac{1}{\beta}\langle \mathcal{S}-\mathcal{S}_0\rangle_{\mathcal{S}_0}$ with respect to the variational parameters involved in $\mathcal{S}_0$.

The same variational principle can be used for the ground state energy of the system by simply taking the low temperature limit ($\beta \to \infty$) of Eq.(6.19), since we have $E_g = \lim_{\beta\to\infty} F$.

The important relation given in Eq.(6.19) is referred to as Jensen-Feynman inequality, which we will make use of in the next section on the path integral treatment of confined polaron.

6.2 Application: General Parabolic Confinement

6.2.1 Introduction

In this application, we are tempted to formulate the confined polaron problem within the framework of the Feynman path integral theory[60] which proves to be a convenient and powerful technique in the treatment of the Fröhlich interaction over the entire range of the electron-phonon coupling strength and the degree of confinement. A description of the lowest polaron bound state has already been reviewed previously by Yıldırım and Erçelebi[35,53] within a generalized confining potential which can be tuned to all geometric configurations and interesting regimes of the effective dimensionality. However, the relevant discussions therein have been restricted separately to either the strong- or the weak-coupling limit. In what follows we refer to the same model used in these papers and present a means of formulating the problem somewhat differently by utilizing the Feynman path integral technique, thus enabling us to provide a wider comprehensive insight into polaron properties in confined media with arbitrary electron-phonon coupling strength.

In the foregoing theory we consider a low dimensionally confined electron assuming a simple situation, namely an anisotropic potential box with adjustable parabolic barriers. The composite assembly will then be visualized as immersed in a bosonic reservoir where the electron couples to the LO-branch of the bulk phonon spectrum. Under the bulk-phonon approximation, we provide a broad interpolating overview to the one-polaron problem consisting of an electron confined within a deformable box which can be conformed from one geometric configuration to another.

6.2.2 Theory

Using units appropriate to a polaron calculation ($m^\star = \hbar = \omega_{LO} = 1$), the Hamiltonian describing the confined electron coupled to LO-phonons is given by

$$H = H_{\rm e} + \sum_Q a_Q^\dagger a_Q + H_{\rm e-ph} \tag{6.20}$$

where

$$H_{\rm e} = \frac{1}{2}p^2 + V_{\rm conf}(\varrho, z) \tag{6.21}$$

is the electron part with $V_{\rm conf}(\varrho, z)$ denoting the confining potential, and

$$H_{\rm e-ph} = \sum_Q V_Q(a_Q e^{i\vec{Q}\cdot\vec{r}} + {\rm hc}) \tag{6.22}$$

is the Fröhlich Hamiltonian. In the above, $\vec{r} = (\vec{\varrho}, z)$ denotes the electron position in cylindrical coordinates. The interaction amplitude is related to the electron-phonon coupling constant α and the phonon wave vector $\vec{Q} = (\vec{q}, q_z)$ through $V_Q = (2\sqrt{2}\pi\alpha)^{1/2}/Q$ (notice that we take $m^\star = 1$ this time).

For the confining potential we adopt a three dimensional box with adjustable barrier slopes, i.e., we set

$$V_{\rm conf}(\varrho, z) = \frac{1}{2}(\Omega_1^2\varrho^2 + \Omega_2^2 z^2) \tag{6.23}$$

in which the dimensionless frequencies $\Omega_i\,(i = 1, 2)$ serve for the measures of the potential barrier strengths and the degree of confinement of the electron in the respective lateral (ϱ) and $\pm z$ directions. By tuning Ω_1 and/or Ω_2 from zero to values much larger than unity one can display a unifying picture tracing the transition from the bulk to all possible extremes of the effective dimensionality, such for instance, to the two dimensional slab-like confinement ($\Omega_1 = 0$, $\Omega_2 \gg 1$) or else, to the quasi-one dimensional quantum well wire (QWW) - like tubular geometry ($\Omega_1 \gg 1$, $\Omega_2 = 0$). The rationale behind imposing quadratic potential profiles is that such a form for the confining barriers, besides facilitating the calculations, is further compatible with the harmonic charge density fluctuations of the electron due to random scattering in the phonon field.

Ground State Energy

In the Feynman path integral representation of the polaron the phonon variables can be projected out exactly to yield the partition function of the polaron in the form

$$\mathcal{Z}_{\rm pol} = {\rm Tr}\, e^{-\beta H} = \mathcal{Z}_{\rm ph}\, \mathcal{Z} \tag{6.24}$$

where

$$\mathcal{Z}_{\rm ph} = \prod_{Q} \left[1 - e^{-\beta}\right]^{-1} \tag{6.25}$$

is the phonon part, and

$$\mathcal{Z} = \int d\vec{r}_0 \int_{\vec{r}_0}^{\vec{r}_0} \mathcal{D}\vec{r}\; e^{\mathcal{S}} \tag{6.26}$$

is the path integral in which the action $\mathcal{S}$ consists of two parts, one pertaining to the electron part of the Hamiltonian and the other to the electron-phonon interaction. In imaginary time variables ($t \rightarrow -i\lambda$), we express

$$\mathcal{S} = \mathcal{S}_{\rm e} \; + \; \frac{1}{2} \sum_{Q} V_Q^2 \int_0^\beta d\lambda \int_0^\beta d\lambda' \; e^{i\vec{Q}\cdot[\vec{r}(\lambda) - \vec{r}(\lambda')]}\, G_{(\omega_{\rm LO}=1)}(|\lambda - \lambda'|) \tag{6.27}$$

and

$$\mathcal{S}_{\rm e} = -\frac{1}{2} \int_0^\beta d\lambda \left\{ \dot{\vec{r}}^2(\lambda) + \Omega_1^2 \varrho^2(\lambda) + \Omega_2^2 z^2(\lambda) \right\} \tag{6.28}$$

in which the dimensionless parameter β stands for the inverse temperature, and the memory function G_ω is the Green's function of a harmonic oscillator with frequency ω, as given in Eq.(6.12). In principle, in the low temperature limit, we have $\mathcal{Z}_{\rm pol} = \mathcal{Z}$, and the polaron ground state energy, $E_{\rm g} = -\lim_{\beta\rightarrow\infty} \beta^{-1} \log \mathcal{Z}$, can be calculated exactly provided the path integral (6.26) can be evaluated. Since this is not possible due to the analytic complexity of the integral expressions in the action $\mathcal{S}$, Eqs.(6.27) and (6.28), we choose to proceed with the solvable trial action

$$\mathcal{S}_0 = \mathcal{S}_{\rm e} \; - \; \frac{{\rm w}(\nu^2 - {\rm w}^2)}{8} \int_0^\beta d\lambda \int_0^\beta d\lambda' \, [\vec{r}(\lambda) - \vec{r}(\lambda')]^2 \, G_{\rm w}(|\lambda - \lambda'|) \tag{6.29}$$

which provides us with a convenient variational upper bound led by the Jensen-Feynman inequality

$$E_{\rm g} \leq E_0 - \lim_{\beta\rightarrow\infty} \frac{1}{\beta} \langle \mathcal{S} - \mathcal{S}_0 \rangle_{\mathcal{S}_0} \tag{6.30}$$

where the notation $\langle\ \rangle_{\mathcal{S}_0}$ denotes a path-integral average with density function $e^{\mathcal{S}_0}$, and E_0 is the trial ground state energy corresponding to $\mathcal{S}_0$. In Eq.(6.29) w and ν are the variational parameters introduced within the same context as in the original paper by Feynman.[60] The problem then reduces to the evaluation of three quantities, E_0, A and B such that

$$E_{\rm g} = E_0 - B - A \tag{6.31}$$

is an upper bound, where the last two terms are given by

$$A = \lim_{\beta\to\infty} \frac{1}{2\beta} \sum_Q V_Q^2 \int_0^\beta d\lambda \int_0^\beta d\lambda' \left\langle e^{i\vec{Q}\cdot[\vec{r}(\lambda)-\vec{r}(\lambda')]} \right\rangle_{\mathcal{S}_0} G_{(\omega_{\rm LO}=1)}(|\lambda-\lambda'|), \tag{6.32}$$

$$B = \lim_{\beta\to\infty} \frac{1}{\beta} \frac{{\rm w}(\nu^2-{\rm w}^2)}{8} \int_0^\beta d\lambda \int_0^\beta d\lambda' \left\langle [\vec{r}(\lambda)-\vec{r}(\lambda')]^2 \right\rangle_{\mathcal{S}_0} G_{\rm w}(|\lambda-\lambda'|). \tag{6.33}$$

Since the trial action and the path-integral averages involved in A and B are all separable in the Cartesian coordinates, the calculations can be performed all in identical manners for each spatial direction. Denoting the Cartesian components of the electron position and momentum in any chosen direction by x and p_x, the corresponding Hamiltonian

$$H_0 = \frac{p_x^2}{2} + \frac{p_\phi^2}{2m_\phi} + \frac{1}{2}\Omega^2 x^2 + \frac{1}{2} m_\phi {\rm w}^2 (x-\phi)^2 \tag{6.34}$$

(in which Ω stands for either Ω_1 or Ω_2) can be related to the one dimensional analogue, $\mathcal{S}_0^{(1{\rm D})}$, of the trial action. Eliminating the harmonic oscillator variables ϕ and p_ϕ, one readily obtains

$$\mathcal{Z}_0 = \int dx_0 \int_{x_0}^{x_0} \mathcal{D}x\ \exp\left[\mathcal{S}_0^{(1{\rm D})}\right] = 2\sinh(\frac{1}{2}\beta{\rm w})\ {\rm Tr}\, e^{-\beta H_0} \tag{6.35}$$

so that

$$E_0^{(1{\rm D})} = \lim_{\beta\to\infty} -\frac{1}{\beta} \log\, \mathcal{Z}_0. \tag{6.36}$$

The Hamiltonian H_0, in which the term $\frac{1}{2}\Omega^2 x^2$ is the relevant part of the confining potential (6.23) along the chosen coordinate, describes the coupling of the harmonically confined electron to a fictitious particle of mass $m_\phi = (\nu^2 - {\rm w}^2)/{\rm w}^2$ which, in turn, gives the overall effect of the interaction of the

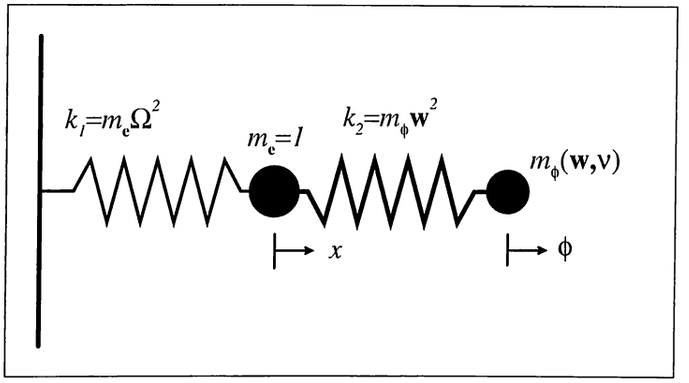

Figure 6.2: The model of confined polaron.
The coordinates and configuration of the coupled particles corresponding to $\mathcal{S}_0^{(1D)}$.

electron with the phonon field (cf. Fig.6.2). Under a suitable coordinate transformation

$$\begin{pmatrix} x \\ \phi \end{pmatrix} \rightarrow \begin{pmatrix} X \\ \Phi \end{pmatrix},$$

H_0 can be diagonalized in the normal coordinates X and Φ yielding the eigen frequencies

$$\left\{ \begin{array}{c} \xi_1(\Omega) \\ \xi_2(\Omega) \end{array} \right\} = \left\{ \frac{\Omega^2+\nu^2}{2} \mp \sqrt{(\frac{\Omega^2+\nu^2}{2})^2 - \Omega^2 w^2} \right\}^{\frac{1}{2}} \tag{6.37}$$

in terms of which H_0 conforms to the canonical form

$$H_0 = \frac{p_X^2}{2M} + \frac{p_\Phi^2}{2\mu} + \frac{1}{2}M\xi_1^2 X^2 + \frac{1}{2}\mu\xi_2^2\Phi^2 \tag{6.38}$$

where $M = \nu^2/w^2$ is sum of the mass of the electron and that of the fictitious particle. Using Eqs.(6.35) and (6.36), the part of the ground state energy contributing from the particular coordinate relevant to $\mathcal{S}_0^{(1D)}$ is obtained simply as

$$E_0^{(1D)} = \frac{1}{2}[\xi_1(\Omega) + \xi_2(\Omega) - w]. \tag{6.39}$$

Noting that the confinement potential $V_{conf}(\varrho, z)$ is characterized by only two parameters, Ω_1 and Ω_2, the former governing the degree of localization of the

electron in the lateral directions isotropically and the latter relevant to the z axis, the expression for $E_0^{(1D)}$ can be extended to account for each of the Cartesian coordinates all at once to yield

$$E_0 = \sum_{n=1}^{2} \frac{1}{n} [\, \xi_1(\Omega_n) + \xi_2(\Omega_n) - \mathrm{w} \,]\,. \tag{6.40}$$

Expanding the path-integral average in the integrand in Eq.(6.32) up to order Q^2, i.e.,

$$\left\langle e^{i\vec{Q}\cdot[\vec{r}(\lambda)-\vec{r}(\lambda')]} \right\rangle_{\mathcal{S}_0} \approx 1 + i\vec{Q}\cdot\langle[\vec{r}(\lambda)-\vec{r}(\lambda')]\rangle_{\mathcal{S}_0} - \frac{1}{2}Q^2 \left\langle [\vec{r}(\lambda)-\vec{r}(\lambda')]^2 \right\rangle_{\mathcal{S}_0}, \tag{6.41}$$

and using the integral transform

$$\int_0^\beta d\lambda \int_0^\beta d\lambda' F(|\lambda-\lambda'|) = \beta \int_0^\beta d\eta F(\eta/2), \qquad [F(\beta-\eta) = F(\eta)] \tag{6.42}$$

the quantities A and B can be cast into more convenient forms. We obtain

$$\begin{aligned} A &= \int_0^\infty d\eta\, e^{-\eta} \sum_Q V_Q^2 \, \exp\left[-\frac{1}{2}\left(\frac{q^2}{\sigma_1(\eta)} + \frac{q_z^2}{\sigma_2(\eta)}\right)\eta\right] \\ &= \frac{\alpha}{\sqrt{\pi}} \int_0^\infty d\eta\, e^{-\eta} \sqrt{\frac{\sigma_2(\eta)}{\eta}}\, \frac{\arctan\gamma}{\gamma} \end{aligned} \tag{6.43}$$

where

$$\gamma = \left\{ \frac{\sigma_2(\eta)}{\sigma_1(\eta)} - 1 \right\}^{1/2}, \tag{6.44}$$

and

$$\begin{aligned} B &= \frac{\mathrm{w}(\nu^2 - \mathrm{w}^2)}{4} \int_0^\infty d\eta\, \eta\, e^{-\mathrm{w}\eta} \left(\frac{2}{\sigma_1(\eta)} + \frac{1}{\sigma_2(\eta)} \right) \\ &= \sum_{n=1}^{2} \frac{1}{2n} [\, b_1(\Omega_n) + b_2(\Omega_n) \,]\,. \end{aligned} \tag{6.45}$$

In the above, the parameters $\sigma_n(\eta)$ and $b_i(\Omega_n)$, $(n = 1, 2$ and $i = 1, 2)$, are given by the following expressions

$$\sigma_n(\eta) = \eta \left\{ \sum_{i=1}^{2} \frac{d_i(\Omega_n)}{\xi_i(\Omega_n)} [1 - e^{-\xi_i(\Omega_n)\eta}] \right\}^{-1} \tag{6.46}$$

with

$$d_i(\Omega_n) = \left\{ 1 + \frac{\mathrm{w}^2(\nu^2 - \mathrm{w}^2)}{[\,\mathrm{w}^2 - \xi_i^2(\Omega_n)\,]^2} \right\}^{-1} \tag{6.47}$$

and

$$b_i(\Omega_n) = \frac{1}{\mathrm{w} + \xi_i(\Omega_n)} \left\{ \frac{1}{\nu^2 - \mathrm{w}^2} + \frac{\mathrm{w}^2}{[\,\mathrm{w}^2 - \xi_i^2(\Omega_n)\,]^2} \right\}^{-1} \tag{6.48}$$

Effective Mass

The variational model used in this work can be extended to yield the effective polaronic mass in various limits of the confinement geometry. When the system is set in virtual motion with a small velocity $\vec{u} = (\vec{u}_\varrho, u_z)$, the total energy attains an additional kinetic contribution of the form

$$\delta K = \frac{1}{2} \left(m_{\mathrm{p}}^{(\varrho)} u_\varrho^2 + m_{\mathrm{p}}^{(z)} u_z^2 \right),$$

in which, $m_{\mathrm{p}}^{(\varrho)}$ and $m_{\mathrm{p}}^{(z)}$ are to be identified as the respective masses in the $\hat{\varrho}$ and $\hat{z}$ directions. Imposing a virtual velocity in the theory is straightforward.[60] In Eq.(6.26), the partition function $\mathcal{Z}$ has been written for all the paths with initial coordinate $\vec{r} = \vec{r}_0$ at zero time and final coordinate $\vec{r} = \vec{r}_0$ at the imaginary time β. With the virtual velocity $\vec{u}$ turned on, the final coordinate should now be $\vec{r}(\beta) = \vec{r}_0 + \beta\vec{u}$; and it is through this coordinate that one keeps trace of the composite translational inertia of the coupled electron+phonon complex. We are thus tempted to reformulate all the terms in Eq.(6.31), where each of E_0, A and B now becomes extended to consist of a part of the binding energy of the polaron alone and a part of the kinetic contribution which shows up having imposed a virtual displacement to the polaron.

The additional kinetic extension involved in E_0 can be written readily as $\frac{1}{2}Mu^2$, where M is the total mass (that of the electron and the fictitious particle), i.e., E_0 scales as

$$E_0 \to E_0 + \frac{1}{2}\frac{\nu^2}{\mathrm{w}^2}(u_\varrho^2 + u_z^2). \tag{6.49}$$

For the remaining two quantities, A and B, we have the following modifications:

$$A \to \int_0^\infty d\eta\, e^{-\eta} \sum_Q V_Q^2 \exp\left\{ -\frac{1}{2}\left(\frac{q^2}{\sigma_1(\eta)} + \frac{q_z^2}{\sigma_2(\eta)}\right)\eta + i(\vec{q}\cdot\vec{u}_\varrho + q_z u_z)\eta \right\} \tag{6.50}$$

and

$$B \rightarrow \frac{\mathrm{w}(\nu^2-\mathrm{w}^2)}{4}\int_0^\infty d\eta\, e^{-\mathrm{w}\eta}\left[(\frac{2}{\sigma_1(\eta)}+\frac{1}{\sigma_2(\eta)})+(u_\varrho^2+u_z^2)\eta^2\right]$$
$$= B+\frac{1}{2}\frac{\nu^2-\mathrm{w}^2}{\mathrm{w}^2}(u_\varrho^2+u_z^2)\ . \qquad (6.51)$$

Expanding Eq.(6.50) up to second order in u_ϱ and u_z (the first order terms in $\vec{u}$ vanish after having projected out the $\vec{Q}$-summation), and arranging the relevant terms in Eq.(6.31) to yield the form $E_{\mathrm{g}} \rightarrow E_{\mathrm{g}}+\delta K$, we obtain the following expressions for the effective mass

$$\left\{\begin{array}{c} m_{\mathrm{p}}^{(\varrho)} \\ m_{\mathrm{p}}^{(z)} \end{array}\right\} = 1+\frac{\alpha}{2\sqrt{\pi}}\int_0^\infty d\eta\,\frac{\sqrt{\eta\sigma_2^3(\eta)}}{\gamma^2}\,e^{-\eta}\left\{\begin{array}{l} \gamma^{-1}\arctan\gamma-(1+\gamma^2)^{-1} \\ 2[1-\gamma^{-1}\arctan\gamma] \end{array}\right\} \qquad (6.52)$$

in which the variational parameters w and ν have to be assigned their optimal-fit values which minimize the ground state energy with $\vec{u}$ set equal to zero.

6.2.3 Results and Conclusions

When $\Omega_i^{-1/2}$, (i=1 and/or 2), is reduced to values comparable with the polaron size, the boundary effects start to become significant and the system enters the regime of reduced dimensionality. Setting $\Omega_1 = 0$ and varying Ω_2 from zero to infinity, one can trace the bulk polaron properties go over to those of a strictly 2D-polaron. On the other hand, deleting the confining potential along the z-axis ($\Omega_2 = 0$) and fixing Ω_1 at non-zero finite values, the theory reflects the Q1D-description in a QWW-like tubular structure. Hereafter, we will consider the polaron binding energy relative to the subband level as $\mathcal{E}_{\mathrm{p}} = \Omega_1+\frac{1}{2}\Omega_2-E_{\mathrm{g}}$, and use Ω to mean $\Omega_1(\Omega_2)$ when $\Omega_2(\Omega_1) = 0$. In the spherically symmetric box-type configuration we simply set $\Omega_1 = \Omega_2 = \Omega$. Similarly, we shall use $\sigma(\eta)$ to mean $\sigma_1(\eta)$ and/or $\sigma_2(\eta)$.

Since analytical minimization of E_{g} (6.31) is not possible, the determination of the optimal fits to w and ν and the polaron quantities of interest, requires treatment on a computer. Before we present our numerical results over a broad

range of the confining parameters and the coupling constant, we find it useful to make correspondence with a few extreme cases which have already been treated and well understood in the literature.

Integer Space Limits

Setting $\Omega_1 = 0$ and $\Omega_2 = 0$ or ∞, we attain the bulk (3D) and strict two dimensional (2D) limits where the general expressions (6.40, 6.43, 6.45 and 6.52) for the ground state energy and mass conform to more tractable and simple forms. For $\Omega_1 = \Omega_2 = 0$ the theory duplicates the results of the original paper by Feynman.[60] In this limit the eigen frequencies (6.37) reduce to $\xi_1(0) = 0$ and $\xi_2(0) = \nu$, and we obtain

$$\sigma(\eta) = \left\{ \frac{\mathrm{w}^2}{\nu^2} + \left(1 - \frac{\mathrm{w}^2}{\nu^2}\right) \frac{1 - e^{-\nu\eta}}{\nu\eta} \right\}^{-1}, \tag{6.53}$$

$$E_0 = \frac{3}{2}(\nu - \mathrm{w}), \tag{6.54}$$

$$B = \frac{3}{4}(\nu^2 - \mathrm{w}^2)/\nu \tag{6.55}$$

yielding the binding energy

$$\mathcal{E}_\mathrm{p} = -E_\mathrm{g} = A - \frac{3(\nu - \mathrm{w})^2}{4\nu}, \tag{6.56}$$

where

$$A = \frac{\alpha}{\sqrt{\pi}} \int_0^\infty d\eta\, e^{-\eta} \sqrt{\frac{\sigma(\eta)}{\eta}}. \tag{6.57}$$

Furthermore, from Eq.(6.52) we obtain the 3D-(isotropic) mass to be given by

$$m_\mathrm{p} = 1 + \frac{\alpha}{3\sqrt{\pi}} \int_0^\infty d\eta\, e^{-\eta} \sqrt{\eta \sigma^3(\eta)}\ . \tag{6.58}$$

Going over to the strict 2D characterization of the polaron we have

$$\lim_{\Omega_2 \to \infty} \left\{ \begin{array}{c} \xi_1(\Omega_2) \\ \xi_2(\Omega_2) \end{array} \right\} = \left\{ \begin{array}{c} \mathrm{w} \\ \infty \end{array} \right\}, \tag{6.59}$$

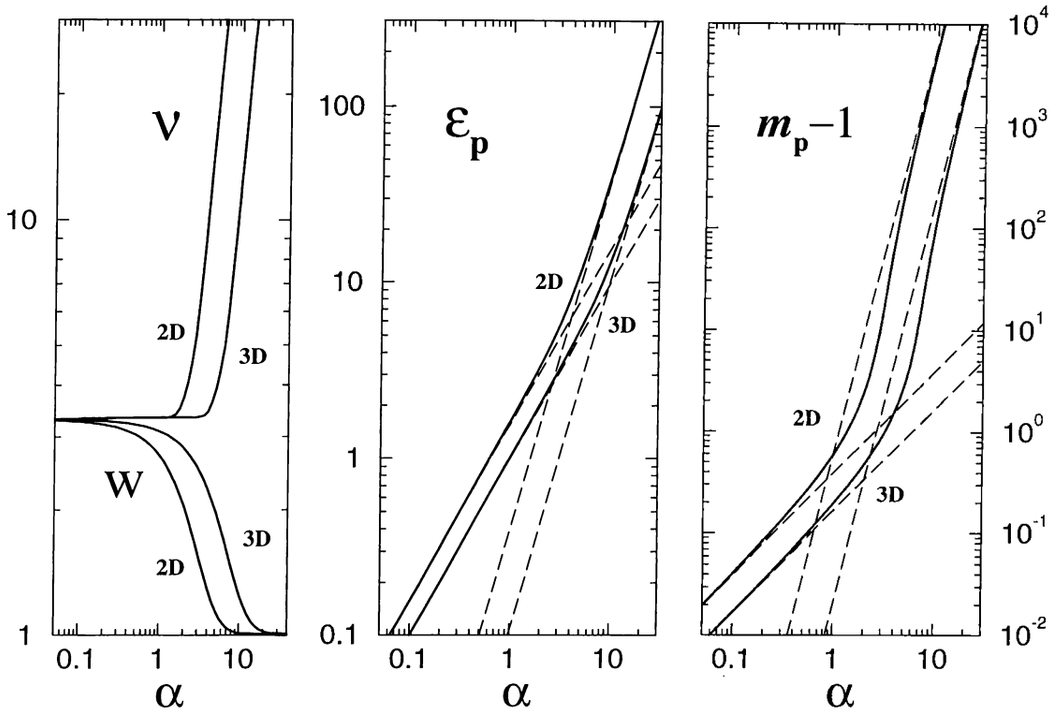

Figure 6.3: Polaron properties in three- and two-dimensions.
The variational parameters w and ν, the binding energy and mass for three and two dimensional polarons as functions of the coupling constant. The dashed lines refer to the perturbation and strong coupling theories.

and consequently, $\sigma_1(\eta) = \sigma(\eta)$ as given in Eq.(6.53), and $\sigma_2(\eta) \to \infty$. For the 2D binding energy we then obtain[73]

$$\mathcal{E}_p = -\left(E_g - \frac{1}{2}\Omega_2\right) = A - \frac{(\nu - w)^2}{2\nu}, \tag{6.60}$$

in which A is provided by the same expression (6.57) given for the bulk case except that the coefficient multiplying the η-integral is now $(\sqrt{\pi}/2)\alpha$. Similarly, the 2D - polaronic mass, $m_p^{(e)}$, is given by Eq.(6.58) where the corresponding factor multiplying the η–integral scales to $(\sqrt{\pi}/4)\alpha$.

For an extensive treatment of the polaron problem in (integer) N dimensions the reader is referred to [75]. Here (cf. Fig.6.3), we shall be content by only presenting the numerical displays of the variational parameters w and ν, the binding energy and the polaron mass for $N = 3$ and $N = 2$ over a wide range

of the coupling constant interpolating between the weak and strong coupling extremes.

Weak Coupling Limit

Since in the most commonly studied compound semiconductors the electron phonon coupling is rather weak, we would like to devote particular emphasis to the weak coupling regime. A discussion of the present model within the perturbation approach has already been provided in [35] with which we wish to make some correspondence here.

At weak coupling the parameters w and ν tend asymptotically to the same constant value (≈ 3.3) with the preservation of the intrinsic relation: $\nu > \mathrm{w}$ (cf. Fig.6.3 and [60]), and in the limit $\alpha \to 0$, one has $\nu - \mathrm{w} = \mathcal{O}(\alpha)$ regardless of the degree of confinement. Hence setting $\nu \approx \mathrm{w}$, we have

$$\left\{ \begin{array}{c} \xi_1(\Omega) \\ \xi_2(\Omega) \end{array} \right\} \approx \left\{ \frac{\Omega^2 + \mathrm{w}^2}{2} \mp \frac{|\Omega^2 - \mathrm{w}^2|}{2} \right\}^{\frac{1}{2}} \tag{6.61}$$

yielding the simplifications $E_0 = \Omega_1 + \frac{1}{2}\Omega_2$ and $B = 0$. In the weak - α regime, we thus readily obtain the binding energy to be given solely by A, Eq.(6.43), wherein $\sigma_{n=1,2}$ (6.46) reduces to exactly the same expression derived previously within the framework of second order perturbation theory,[35] i.e.,

$$\sigma_n(\eta) = \frac{\Omega_n \eta}{1 - e^{-\Omega_n \eta}} , \qquad n = 1, 2 . \tag{6.62}$$

An elaborate study of the weak-coupling polaron quantities as a function of Ω_1 and Ω_2 can be found in [35]. We, therefore, do not repeat the relevant results here, and readdress only to the three and two dimensional limits. In approaching the bulk case we assume a spherically symmetric isotropic confinement: $\Omega_1 = \Omega_2 = \Omega \ll 1$, and for the 2D limit we set $\Omega_1 = 0$ and let $\Omega_2 = \Omega \gg 1$. From Eqs.(6.31) and (6.52) we derive the binding energy and the polaron mass to lowest order contribution from Ω as

$$\mathcal{E}_\mathrm{p} = \left\{ \begin{array}{ll} \lim_{\Omega \to 0} \alpha(1 + \frac{\Omega}{8}) & 3\mathrm{D} \\ \lim_{\Omega \to \infty} \frac{\pi}{2}\alpha(1 - \frac{4}{\sqrt{\Omega}}) & 2\mathrm{D} \end{array} \right. \tag{6.63}$$

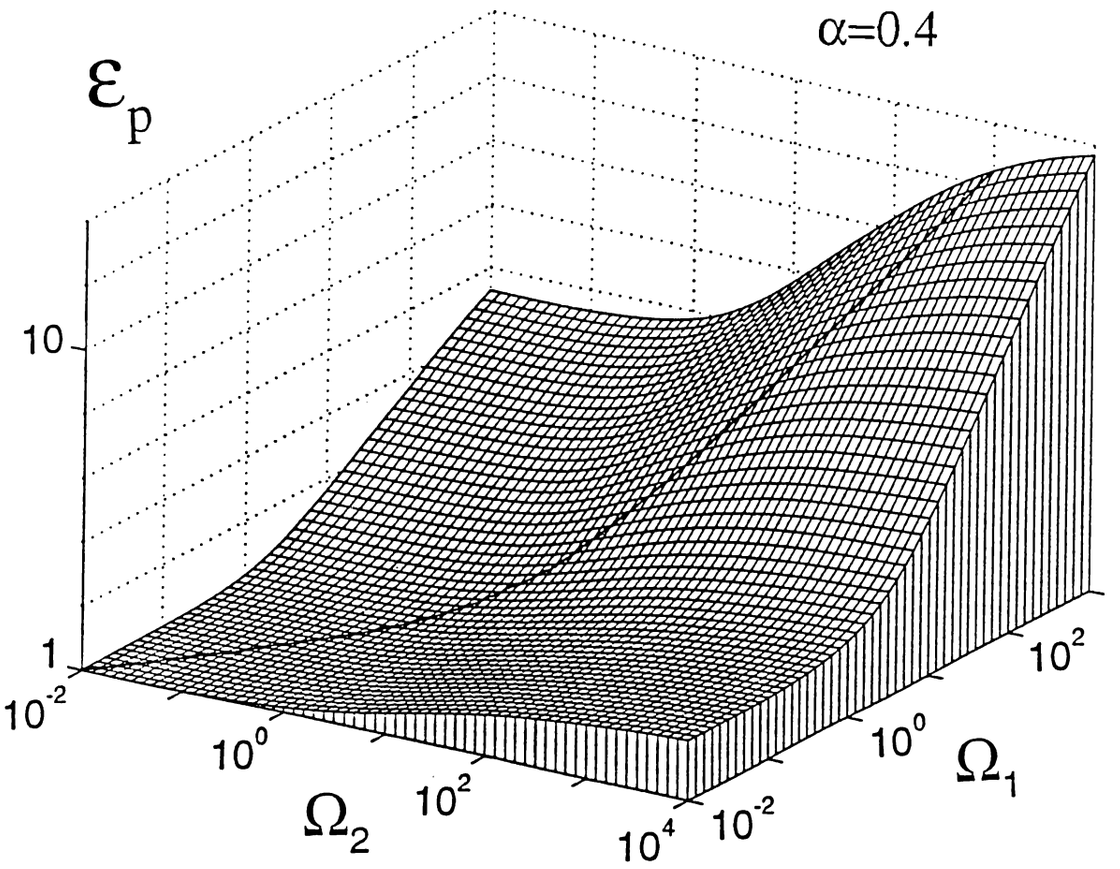

Figure 6.4: A global view of polaronic binding energy.
The binding energy (scaled relative to the bulk value) is given as a function of the confining parameters at weak coupling ($\alpha = 0.4$). The diagonal curve on the grid refers to the spherically symmetric configuration ($\Omega_1 = \Omega_2$).

$$m_{\rm p} = \begin{cases} \lim_{\Omega\to 0}\ 1 + \frac{1}{6}\alpha(1 + \frac{9}{8}\Omega) & \text{3D} \\ \lim_{\Omega\to\infty}\ 1 + \frac{\pi}{8}\alpha(1 - \frac{4}{\sqrt{\pi^3\Omega}}) & \text{2D} \end{cases} \tag{6.64}$$

Arbitrary dimensionality

For a total description interpolating between all possible extremes of the effective dimensionality and the coupling constant we refer back to the set of equations (6.40), (6.43) and (6.45), and minimize numerically the ground state energy (6.31) with respect to the variational parameters w and ν. In Fig.6.4 we select $\alpha = 0.4$

(appropriate for CdTe) and construct a unified physical image of the polaron binding over a reasonably broad range of Ω_1 and Ω_2 covering all interesting regimes of the effective dimensionality. Starting from the flat plateau at the bottom (corresponding to the bulk case) and following the inclination along increasing values of Ω_2, one arrives at a second plateau characterizing the two dimensionally confined nature of the polaron. Following the direction parallel to the Ω_1 – axis, however, $\mathcal{E}_\mathrm{p}$ is seen to increase steadily at a much faster rate and rapidly become much larger than in the Q2D configuration, which follows essentially from the fact that in the wire geometry the polaron becomes highly localized towards the wire axis due to confinement coming from all transverse directions. For instance, for the Q2D confinement with $\Omega = 10$ we obtain $\mathcal{E}_\mathrm{p}$ to be 1.16 times its bulk value, $\mathcal{E}_\mathrm{p}^{(3D)}$. For the case of a wire with the same parameter value the binding becomes stronger by a greater factor of about 1.45 over the 3D-energy. Lowering the dimensionality one further step down to the spherically symmetric QW-box – type localization of the polaron (displayed by the diagonal curve on the grid in Fig.6.4), the effective electron-phonon coupling is observed to be even much stronger ($\mathcal{E}_\mathrm{p}/\mathcal{E}_\mathrm{p}^{(3D)} = 2.02$), since now the polaron becomes radially squeezed in all directions. The corresponding values when Ω is set to 10^2, are 1.34, 2.27 and 5.70.

For completeness, we extend our considerations to the regime of strong phonon coupling and in Fig.6.5, with the confining parameter held fixed ($\Omega = 10^2$), we plot profiles of the polaronic binding as a function of growing α for the quasi-two, -one and -zero dimensional configurations; thus providing a comparison of the binding energy values in a succession of the effective dimensionalities pertaining to the slab, wire and box type geometries. The inset in the figure gives a complementary display of $\mathcal{E}_\mathrm{p}$ as a function of Ω where the coupling constant has been selected arbitrarily an order of magnitude larger than for CdTe. The general trend that the electron phonon coupling is inherently stronger in reduced dimensionalities is seen to reflect in the plots which we have generated insofar.

It should be mentioned that, the parameters α and Ω $\{= \Omega_1$ or $\Omega_2\}$ characterizing the model do not enter the problem in an independent way but

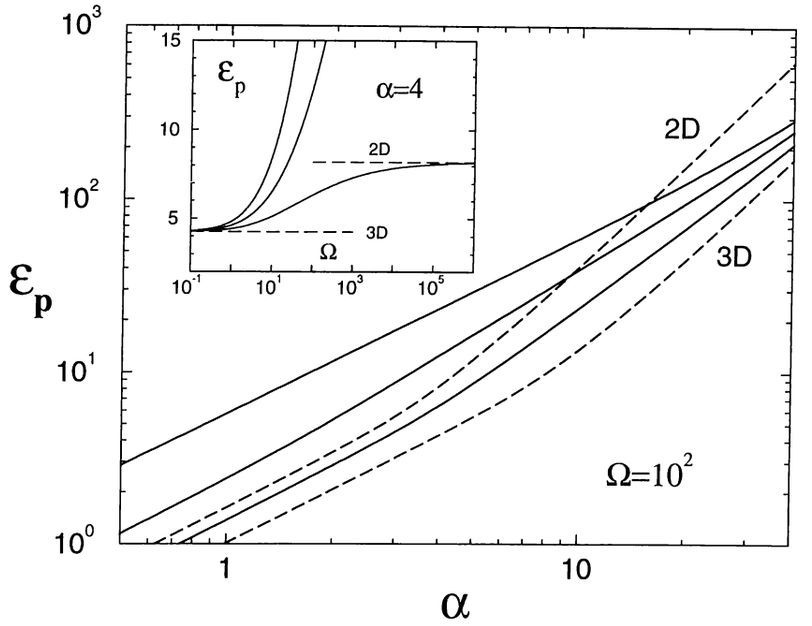

Figure 6.5: Comparison of different confinement geometries.
The binding energy as a function of the coupling constant with $\Omega (= \Omega_1$ and/or $\Omega_2)$ held fixed. The solid curves from bottom to top are respectively for the quasi-two, -one and -zero dimensional configurations, and the dashed curves give the bulk and strict-2D polaron energies. The inset provides an alternative view of the binding energy as a function of Ω in the strong coupling regime.

together take part in a related manner in the binding, dominating the effect of one another, and yet acting collaboratively in favor of stronger binding. Thus, a high degree of localization in reduced dimensionality is expected to lead to a pseudo–enhancement in the effective electron–phonon coupling. Even at weak coupling ($\alpha \ll 1$), when the polaron is in a delocalized state with a large spread, the influence of the geometric confinement on the polaron becomes immediate as Ω is turned on, and to first order in small Ω, the coupling constant is observed to scale as $\alpha \to \alpha[1 + \mathcal{O}(\Omega)]$ (cf. Eqs.(6.63) and (6.64), for instance).

For $\alpha \gg 1$, however, the situation is somewhat different. In this extreme the polaron is already in a highly localized state and a small sized polaron is not expected to feel the effect of the confining boundary except for too large Ω. This peculiar aspect can be seen clearly if the energy and mass of the confined polaron are displayed relative to their corresponding bulk values, $\mathcal{E}_p^{(3D)}$ and $m_p^{(3D)}$. On this

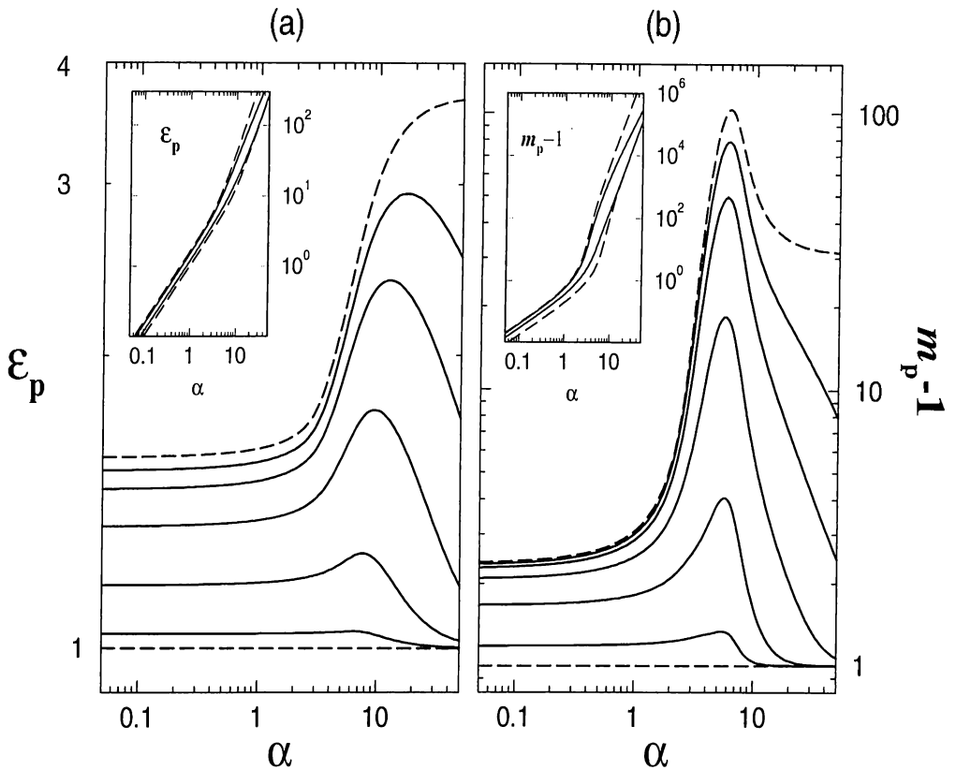

Figure 6.6: The scaling of polaron properties, in slab-like confinement. (a) The binding energy, $\mathcal{E}_p$, and (b) the polaron mass, $m_p - 1$, as functions of the coupling constant in the quasi-two dimensional configuration. All energy and mass values (except those in the insets) are scaled relative to the corresponding bulk values. The solid curves (from bottom to top) constrained by the lower (=3D) and upper (=2D) dashed curves are respectively for $\Omega \equiv \Omega_2 = 1, 10, 10^2, 10^3$ and 10^4. Similarly, the solid curves in the insets are for $\Omega = 10$ and 10^3.

purpose, we choose to refer to the slab - configuration and portray (cf. Fig.6.6) the variations of the binding energy and the mass (along the relevant free direction) as a function of the electron phonon coupling strength for a succession of different Ω values. In view of our results plotted in the figure we see that, starting from the weak-coupling extreme, the growth rates (with respect to α) of the binding energy and mass in low dimensional configurations ($\Omega > 0$) is not significantly different from that for the bulk polaron. However, as α is tuned to greater values the polaron goes into a more deeply bound state, and under the additional spatial constraint confining it, the binding becomes even much deeper since now the

intrinsic collaborative role which the geometric confinement plays on the effective phonon coupling becomes much more efficient and prominent. In the meantime, contrary to this trend, with growing α the polaron gets substantially localized and becomes unaffected by the boundary potential except for large values of Ω; thus, leading to a percentual reduction in the confinement – counterpart of the polaron binding. Clearly, in the extreme limit of an artificially large α dominating over the external confinement the problem should be characterized essentially by its bulk description. This salient feature is depicted in the plots for finite Ω by that the energy and mass profiles, after having displayed a maximum, start to fall off and eventually match with their bulk values as α is made stronger. A complementary remark in this regard is that for a large Ω one requires correspondingly a large α for the polaron to conform to its bulk characterization, and in particular, in the strict 2D-limit ($\Omega \rightarrow \infty$) of the slab-like confinement one should correspondingly have $\alpha \rightarrow \infty$. This feature can readily be seen from that the upper dashed curves in the figure tend to the two dimensional limiting values, $3\pi^2/8$ and $81\pi^4/256$, for the energy and mass, respectively.

In this chapter, we have retrieved the fundamental aspects of the polaron problem in a confined medium within a unifying scheme interpolating between the bulk and all low dimensional geometric configurations of general interest. The Feynman path integral theory suited to the "deformable potential box" - model allows us to achieve a simple and yet comprehensive review of the ground state polaron properties in structures with reduced dimensionality.

Chapter 7

MAGNETIC FIELD AS A MEANS OF CONFINEMENT

7.1 Introduction

We have seen that the effective electron-phonon coupling becomes enhanced with the increasing degree of confinement brought about by an external potential. For the case of a polaron under a magnetic field also, the binding gets deeper due to the additional degree of localization brought about by the magnetic field.[93-99] It has been noted that for intense magnetic fields the phonon part of the ground state energy grows at a rate $\sqrt{B}$, which is much faster than in 3D where the magnetic field dependence is $\ln B$.

In view of the innumerable amount of papers devoted to magneto-polarons, we see that the problem is not only interesting in laying out distinctive qualitative features in the different regimes of the magnetic field intensity and the electron - phonon coupling strength, but is as well attractive from a formal point of view. The visualization of the problem at large is not very immediate due to that the roles which the magnetic field and phonon coupling play in the polaron binding are not completely independent, but rather take part in an interrelated manner dominating over the effect of one another and yet act together in favor of enhanced phonon coupling. The qualitative aspects of the problem become simple, however,

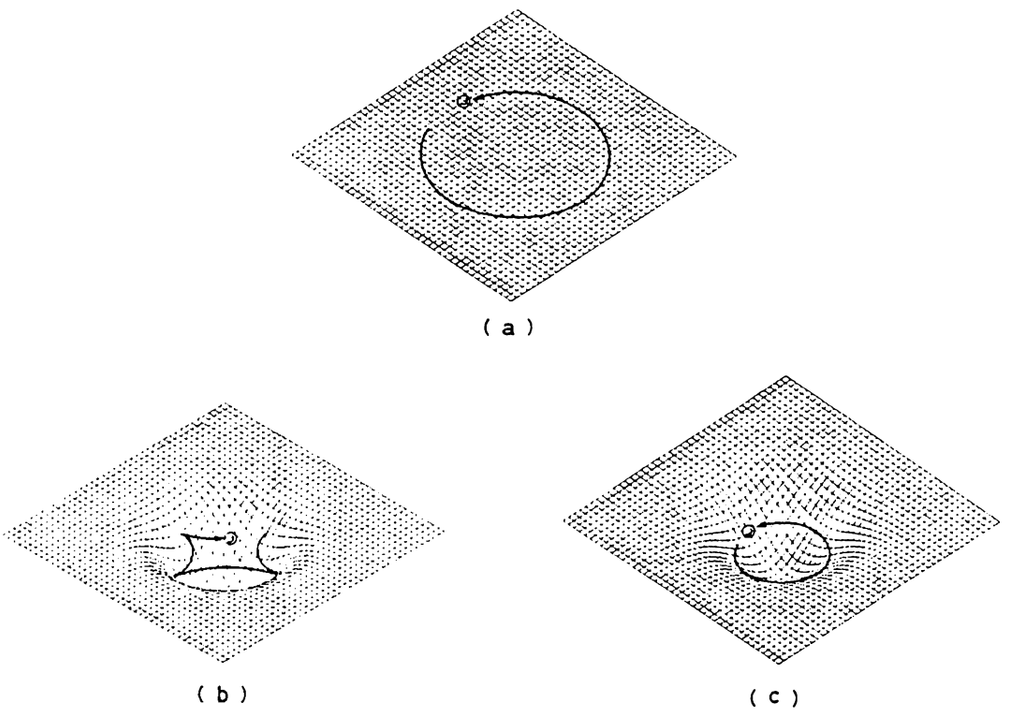

Figure 7.1: Sketch for the states of the 2D polaron in a uniform magnetic field. The electron is described by the small circle with its locus. (a) Free state for $\omega_c \ll 1$ and $\alpha \ll 1$, (b) self-trapped state for $\omega_c \ll 1$ and $\alpha \gg 1$, (c) magnetically trapped state for $\omega_c \gg 1$. (Taken from [100])

in some extremes.

Considering the sketch of tree distinctive states of the 2D polaron under a uniform perpendicular magnetic field, taken from [100] may help to visualize the situation.

For weak phonon coupling the most sensible approach is via the perturbation theory (see Larsen,[94,95] for instance), and moreover if the magnetic field is also weak, (cf. Fig.7.1(a)) the problem can be characterized as consisting of an electron orbiting together with its concomitant lattice deformation with an effective polaron mass rather than the band mass. In this limit the ground state energy can readily be written as the sum of the polaron self–energy

$-(\pi/2)\alpha\hbar\omega_{LO}$ and of the lowest Landau energy $eB/2m^*c$ in which m^*, corrected up to first order in the coupling constant, scales to $m^*(1+\frac{\pi}{8}\alpha)$. Introducing the dimensionless cyclotron frequency ω_c expressed in units of ω_{LO} (the LO–phonon frequency), the ground state energy (in usual polaron units: $\hbar = 2m^* = \omega_{LO} = 1$) is given approximately by

$$E_g \approx \frac{1}{2}\omega_c - \frac{\pi}{2}\alpha(1 + \frac{\omega_c}{8}). \tag{7.1}$$

A contrasting aspect to such a description of the polaron is the case where the electron goes into a bound state with a highly localized wave function in a deep self–induced potential well of the lattice polarization. A way to reach this totally distinctive aspect is either to imagine a rather strong coupling to the lattice or to go over to the high magnetic field limit where the lattice can only respond to the mean charge density of the rapidly orbiting electron and hence acquire a static deformation over the entire Landau orbit (see Fig.7.1(b)-(c)). Thus, one readily notes that, in spite of a small coupling constant, a pseudo–adiabatic condition can be attained when $\omega_c \gg 1$.

A complementary remark in this regard is that in the high field limit and at weak polar coupling ($\alpha \ll 1$), the usual adiabatic theory gives

$$E_g = \frac{1}{2}\omega_c - \frac{1}{2}\alpha\sqrt{\pi\omega_c/2} \tag{7.2}$$

for the ground state energy which differs from the perturbation theoretic estimate by a factor of $2^{-1/2}$ in the polaronic term.[95] The reason for the inconsistency lies in the fact that the most efficient coherent phonon state should not be taken as centered on the average electron position but instead on the orbit center[101] $\vec{\rho}_0 = x_0\hat{x} + y_0\hat{y}$, where

$$x_0 = \frac{1}{2}x - \frac{2}{\omega_c}p_y \qquad y_0 = \frac{1}{2}y + \frac{2}{\omega_c}p_x. \tag{7.3}$$

In fact, the role which the orbit center coordinates play in the theory and, for large ω_c, the necessity of imposing a coherent phonon state operator leading to a deformation centered at $\vec{\rho}_0$ were emphasized earlier in an elaborate discussion by Whitfield, Parker and Rona.[86]

In this chapter we retrieve the magneto–polaron problem within a generalized variational scheme and give all emphasis to the case where the effect of electron-phonon coupling is dominated over by the magnetic field counterpart of the problem. We shall totally disregard the phonon coupling – dominated ($\alpha \gg 1$) characterization of the polaron consisting of a deep self–induced potential well confining the rapidly fast random charge density fluctuations of the electron which is further under the influence of a relatively weak magnetic field. In the following we take the lattice deformation as centered essentially at $\vec{\rho}_0$ rather than at the mean electron position and think of the electron as rotating on a complete Landau orbit.

Even though for somewhat strong field intensities the problem shows a vague strong–coupling aspect, a pure adiabatic approach fails to reflect a correct description of the system except for infinitely large magnetic field strengths. On the other hand, a pure perturbation treatment may also be not perfectly appropriate except for too small α. We are therefore tempted to formulate the magnetic field – dominated regime of the magneto–polaron within the framework of a more convenient approach accounting for the fractional admixture of the weak– and strong–coupling aspects simultaneously. The formalism we follow in this work consists of the usage of a variational ansatz introduced previously by Devreese *et al.*[56] in their application to the bulk–optical polaron bound to a Coulomb potential. The procedure is to start with the standard canonical transformation of the strong–coupling formulation and then modify the adiabatic polaron state by a variationally determined perturbative extension serving for the theory to interpolate in the overall range of the coupling constant.

In fact, the problem that we refer here has already been discussed earlier within almost the same variational approach in a previous paper by Erçelebi and Saqqa.[99] The major distinction which sets the present concern apart from that given in the former paper is that the variational state derived here is of a more general content accounting for the magnetic field parameter ω_c not only in the electron part of the Hamiltonian, but also within the context of the part of the Hamiltonian describing the coupling of the electron to the phonon field.

Performing the two works separately under identical numerical precisions we have observed that one reaches significantly improved energy upper bounds in the present case and this consists of the motivation to re–address the same problem.

7.2 Application: 2D-Magneto-Polaron

7.2.1 Formal Preliminaries

Employing the symmetric gauge, $\vec{A} = \frac{B}{2}(-y, x, 0)$, for the vector potential, the Hamiltonian of a 2D electron immersed in the field of bulk LO–phonons is given by

$$H = H_e + \sum_Q a_Q^\dagger a_Q + \sum_Q V_Q[a_Q \exp(i\vec{q}\cdot\vec{\rho}) + a_Q^\dagger \exp(-i\vec{q}\cdot\vec{\rho})] \quad (7.4)$$

$$H_e = -\frac{\partial^2}{\partial x^2} - \frac{\partial^2}{\partial y^2} + \frac{1}{4}(\frac{1}{2}\omega_c\rho)^2 - \frac{i}{2}\omega_c(x\frac{\partial}{\partial y} - y\frac{\partial}{\partial x}) \quad (7.5)$$

in which a_Q ($a_Q^\dagger$) is the phonon annihilation (creation) operator, and $\vec{\rho} = (x, y)$ denotes the electron position in the transverse plane. The interaction amplitude is related to the electron–phonon coupling constant α and the phonon wave vector $\vec{Q} = \vec{q} + q_z\hat{z}$ through $V_Q = \sqrt{4\pi\alpha}/Q$. In the above all physical quantities and operators have been written in dimensionless form with $(\hbar/2m^*\omega_{\rm LO})^{1/2}$ being selected as unit of length and the phonon quantum $\hbar\omega_{\rm LO}$ as a unit of energy.

Electron Eigenstates

Before proceeding with our main theme we first put the electron part of the Hamiltonian and its eigenstates into a transparent and convenient form where the relevant algebra is well known and calculations are easily made. For this purpose we follow the representation advanced in the papers by Maĭkin and Man'ko,[102] Feldman and Kahn[103] and Whitfield, Parker and Rona.[86] Setting

$$z = \frac{1}{2}\sqrt{\frac{\omega_c}{2}}(x + iy),$$

and introducing the operators

$$\begin{aligned} u &= \frac{1}{\sqrt{2}}(\bar{z} + \frac{\partial}{\partial z}), \qquad u^\dagger = \frac{1}{\sqrt{2}}(z - \frac{\partial}{\partial \bar{z}}), \\ v &= \frac{1}{\sqrt{2}}(z + \frac{\partial}{\partial \bar{z}}), \qquad v^\dagger = \frac{1}{\sqrt{2}}(\bar{z} - \frac{\partial}{\partial z}) \end{aligned} \tag{7.6}$$

with

$$[u, u^\dagger] = [v, v^\dagger] = 1, \qquad [u, v] = [u, v^\dagger] = 0 \tag{7.7}$$

one obtains

$$H_e = (u^\dagger u + \frac{1}{2})\omega_c \ . \tag{7.8}$$

It is evident that $u^\dagger(u)$ steps up(down) both the energy and the angular momentum,

$$l_z = -i(x\frac{\partial}{\partial y} - y\frac{\partial}{\partial x}) = u^\dagger u - v^\dagger v.$$

On the other hand, $v^\dagger$ and v step only the angular momentum but not the energy. It thus follows that the energy eigenvalues of H_e are infinite–fold degenerate and, therefore, one is led to represent the corresponding eigenstates as

$$\mid n_u n_v\rangle = \chi_{n_u,n_v} \mid 00\rangle, \qquad n_u, n_v = 0, 1, 2, ... \tag{7.9}$$

where

$$\chi_{n_u,n_v} = (n_u!\ n_v!)^{-1/2}\ (u^\dagger)^{n_u}(v^\dagger)^{n_v} \ . \tag{7.10}$$

Displaced Oscillator Transformation

No matter how small α is, the starting idea in the foregoing approximation is to contemplate a highly strong magnetic field to which the lattice responds by acquiring a relaxed static deformation clothing the entire Landau orbit. The adiabatic polaron ground state thus formed can be written in a product ansatz consisting of the electron and lattice parts, i.e.,

$$\Psi_g = \mid 00\rangle e^S \mid 0_{ph}\rangle, \tag{7.11}$$

where $\mid 0_{ph}\rangle$ is the phonon vacuum and e^S is a unitary displacement operator changing the reference system of virtual particles by an amount $V_Q\sigma_{Q0}$. The

most appropriate lattice wave function corresponding to the relaxed state of the electron–lattice system is determined to be

$$\Phi_{\rm ph} = \exp[\sum_Q V_Q \sigma_{Q0}(a_Q e^{i\vec{q}\cdot\vec{\rho}_0} - {\rm hc})] \mid 0_{\rm ph}\rangle \tag{7.12}$$

with

$$\sigma_{Q0} \;=\; \langle 00 \mid e^{\pm i\vec{q}\cdot(\vec{\rho}-\vec{\rho}_0)} \mid 00\rangle \;=\; \exp(-q^2/2\omega_c). \tag{7.13}$$

Thus, having set up the most efficient coherent phonon state as centered on the orbit center the Hamiltonian transforms to

$$\begin{aligned} H' = e^{-S}He^{S} = H_{\rm e} \;+\; & \sum_Q a_Q^\dagger a_Q + \sum_Q V_Q^2\sigma_{Q0}^2 \\ - \; & \sum_Q V_Q^2\sigma_{Q0}[e^{i\vec{q}\cdot(\vec{\rho}-\vec{\rho}_0)} + {\rm cc}] + \sum_Q V_Q(\eta_Q a_Q + \eta_Q^* a_Q^\dagger) \end{aligned} \tag{7.14}$$

where

$$\eta_Q = e^{i\vec{q}\cdot\vec{\rho}_0}\{e^{i\vec{q}\cdot(\vec{\rho}-\vec{\rho}_0)} - \sigma_Q\}\ . \tag{7.15}$$

If what we would be interested in were the adiabatic – high field limit, all that remains would consist of calculating the expectation value of H' in the state $\mid 00\rangle \mid 0_{\rm ph}\rangle$ and we would readily obtain

$$E_{\rm g} = \frac{1}{2}\omega_c - \Lambda_0 \tag{7.16}$$

where

$$\Lambda_0 = \sum_Q V_Q^2\sigma_{Q0}^2 = \frac{1}{2}\alpha\sqrt{\pi\omega_c}\ , \tag{7.17}$$

which is identical to the perturbation result of Larsen[95] to leading order in α.

7.2.2 Theory

Obviously, for not too strong magnetic fields the adiabatic condition and hence Eq.(7.16) loses its validity, and one is tempted to consider the perturbation approach the applicability of which, however, is confined within $\alpha \ll 1$. A theory which is capable of yielding the effective phonon coupling, not restricted solely to the weak α limit, can be based on variational grounds. We thus choose to

continue from Eq.(7.14), and modify the state $\Phi_0 = \mid 00\rangle \mid 0_{\rm ph}\rangle$ accordingly by conforming it to a generalized form

$$\Phi_0 \rightarrow \Phi_0' = \Omega(\alpha, \omega_c)\Phi_0 \tag{7.18}$$

where the operator $\Omega(\alpha, \omega_c)$ is intended to interrelate the weak– and strong–coupling counterparts of the problem depending on the strength of phonon coupling and the magnetic field intensity.

The Variational Trial State

Taking an already small α and further shifting ω_c down to small values, the degree of localization of the electron becomes reduced in a significant manner, σ_{Q0} in Eq.(7.14) tends to become zero on the average and thus H' converts back to its original form as given by Eq.(7.4). In view of this reasoning one is led to treat the last term in Eq.(7.14) as a perturbation.[56]

In the perturbation treatment of the Fröhlich interaction, the first non-vanishing contribution to the ground-state energy comes from the term which is of second order in the interaction amplitude. Correspondingly, the leading correction to the ground state is of first order and is given by the sum

$$\Delta\Phi_0 = \sum_Q \sum_n \frac{1}{\varepsilon_n - \varepsilon_0 + 1} \mid \varphi_n\rangle \mid 1_Q\rangle \langle\varphi_n \mid \langle 1_Q \mid \sum_{Q'} V_{Q'} \eta^*_{Q'} a^\dagger_{Q'} \mid \Phi_0\rangle \tag{7.19}$$

in which the index n refers to the intermediate states consisting those of the electron and one–phonon with wave vector $\vec{Q}$. In the above, φ_n and ε_n are to be thought of as the eigenstates and the eigenvalues of the unperturbed part of the transformed Hamiltonian (7.14). In order to calculate the perturbation sum (7.19) one needs to know the explicit functional forms of φ_n and the energies ε_n which however is a rather difficult task since now they depend in general on α and the lattice coordinates in involved manners. Nevertheless, for the energy correction to be retained up to first order in α, we choose φ_n as the set of eigenfunctions of the bare electron problem and ignore any α – dependence in either φ_n or ε_n, i.e., we take

$$\varphi_n \equiv \chi_{n_u, n_v} \mid 00\rangle, \qquad \varepsilon_n = (n_u + \frac{1}{2})\omega_c. \tag{7.20}$$

Making a correspondence with the perturbation treatment of the problem one readily notes that the only thing we should do is account for the momentum conservation of the scattered electron–phonon system. We are thus tempted to write the energy difference as

$$\varepsilon_n - \varepsilon_0 \approx n_u\omega_c + \delta_n(Q) \tag{7.21}$$

where $\delta_n(Q)$ is introduced as to bear any necessary phonon–wave vector dependence.

Using the identity $s^{-1} = \int_0^\infty d\xi e^{-s\xi}$, we set

$$\frac{1}{\varepsilon_n - \varepsilon_0 + 1} \approx g_Q \ \mathrm{J}(\omega_c, n_u) \tag{7.22}$$

where

$$\mathrm{J}(\omega_c, n_u) \equiv \int_0^\infty d\xi \ e^{-\xi} \exp(-\omega_c n_u \xi) \tag{7.23}$$

and g_Q stands for the exponential $e^{-\delta_n(Q)\xi}$ factored out as an averaged quantity which, in the calculation, will be determined variationally. Substituting (7.15) and (7.22) into Eq.(7.19) we obtain

$$\Delta\Phi_0 = \sum_Q V_Q g_Q \sum_n \ \mathrm{J}(\omega_c, n_u) \ \tilde{\sigma}_{Qn} \ \{\sigma_{Qn} - \sigma_{Q0}\delta_{n_u,0}\} \ \chi_{n_u,n_v} a_Q^\dagger \Phi_0 \tag{7.24}$$

where

$$\begin{aligned} \sigma_{Qn} &= \langle \Phi_n \mid e^{-i\vec{q}\cdot(\vec{\rho}-\vec{\rho}_0)} \mid \Phi_0 \rangle \\ &= (n_u!)^{-1/2}[-i(q_x - iq_y)\omega_c^{-1/2}]^{n_u}\sigma_{Q0}, \end{aligned} \tag{7.25}$$

$$\begin{aligned} \tilde{\sigma}_{Qn} &= \langle \Phi_n \mid e^{-i\vec{q}\cdot\vec{\rho}_0} \mid \Phi_0 \rangle \\ &= (n_v!)^{-1/2}[-i(q_x + iq_y)\omega_c^{-1/2}]^{n_v}\sigma_{Q0} \end{aligned} \tag{7.26}$$

Using Eqs.(7.10), (7.25) and (7.26) we see that the extended state $\Phi_0' = c\Phi_0 + \Delta\Phi_0$ can indeed be written in the form (7.18) with

$$\Omega(\alpha, \omega_c) = c + \sum_Q V_Q g_Q \lambda_Q^* a_Q^\dagger \tag{7.27}$$

in which c is a constant to serve for normalization, and

$$\lambda_Q = \sigma_{Q0}^2 \sum_{n_u}\sum_{n_v} \frac{(-i\omega_c^{-1/2})^{n_u+n_v}}{n_u!\, n_v!}\, \mathrm{J}(\omega_c, n_u) \times\{(q_x - iq_y)^{n_u} - (q_x + iq_y)^{n_v}\delta_{n_u,0}\}\ (u^\dagger)^{n_u}(v^\dagger)^{n_v}\ . \quad (7.28)$$

Projecting out the quantum numbers n_u and n_v, and, for notational convenience, writing

$$\vec{q}(\xi) = \vec{q}\exp(-\omega_c\xi), \quad (7.29)$$

we find that λ_Q takes the compact form

$$\lambda_Q = \int_0^\infty d\xi\ e^{-\xi}\ \eta_{Q(\xi)}\varrho_{Q(\xi)} \quad (7.30)$$

where

$$\eta_{Q(\xi)} = e^{i\vec{q}\cdot\vec{\rho}_0}\{e^{i\vec{q}(\xi)\cdot(\vec{\rho}-\vec{\rho}_0)} - \sigma_{Q(\xi)}\} \quad (7.31)$$

and

$$\varrho_{Q(\xi)} = \frac{\sigma_{Q0}}{\sigma_{Q(\xi)}} = \exp\{-\frac{q^2 - q^2(\xi)}{2\omega_c}\} \quad (7.32)$$

in which

$$\sigma_{Q(\xi)} = \exp(-q^2(\xi)/2\omega_c)\ . \quad (7.33)$$

It should be remarked that the two individual contributions to the binding coming from the electron–phonon coupling alone and the magnetic field alone are fundamentally incorporated by the operator $\Omega(\alpha,\omega_c)$ and, in particular, by the variational parameter g_Q which as well governs the detailed admixture of the strong– and weak–coupling counterparts of the problem.

Due to the complicated nature of Eq.(7.27) where yet, at this stage, g_Q remains undetermined, simple concise predictions are not readily tractable except in the high field limit where one expects the theory to impart most dominance to the strong–coupling aspect. In this extreme, $\varrho_{Q(\xi)} \to 1$, $\eta_{Q(\xi)} \to 0$, and consequently λ_Q in (7.27) becomes zero, and hence $\Omega(\alpha,\omega_c)$ conforms to the identity operator where we recover back the strong–coupling theory.

Formulation

In order to reach the optimal fit to g_Q one has to minimize the expectation value of H' in the trial state $\Phi_0' = \Omega(\alpha, \omega_c)\Phi_0$ subject to the constraint that Φ_0' is normalized:

$$\begin{aligned} F(c, g_Q) &\equiv \langle \Phi_0' \mid \Phi_0' \rangle - 1 \\ &= c^2 + \sum_Q V_Q^2 g_Q^2 h_Q^{(1)} - 1 \;=\; 0 \end{aligned} \tag{7.34}$$

where

$$h_Q^{(1)} = \langle \Phi_0 \mid \lambda_Q \lambda_Q^* \mid \Phi_0 \rangle \; . \tag{7.35}$$

The variational procedure thus requires

$$\frac{\partial}{\partial g_Q}\{E(c, g_Q) - \Lambda F(c, g_Q)\} = 0 \tag{7.36}$$

where Λ is a Lagrange multiplier, and $E(g_Q, c)$ refers to the ground state energy given as

$$\begin{aligned} E(c, g_Q) \;=\; \langle \Phi_0' \mid H' \mid \Phi_0' \rangle \;&=\; \frac{1}{2}\omega_c - \Lambda_0 + 2c \sum_Q V_Q^2 g_Q h_Q^{(0)} \\ &+ \sum_Q V_Q^2 g_Q^2 [e_Q + h_Q^{(1)}(1 + 2\Lambda_0) - \delta_Q] \end{aligned} \tag{7.37}$$

in which

$$h_Q^{(0)} \;=\; \langle \Phi_0 \mid \eta_Q \lambda_Q^* \mid \Phi_0 \rangle \tag{7.38}$$

$$e_Q \;=\; \omega_c \langle \Phi_0 \mid \lambda_Q u^\dagger u \lambda_Q^* \mid \Phi_0 \rangle \tag{7.39}$$

and

$$\delta_Q = \sum_{Q'} V_{Q'}^2 \sigma_{Q'0} \; \langle \Phi_0 \mid \lambda_Q \{\exp[i\vec{q}\,' \cdot (\vec{\rho} - \vec{\rho}_0)] + \mathrm{cc}\} \lambda_Q^* \mid \Phi_0 \rangle \; . \tag{7.40}$$

The corresponding analytic expressions for $h_Q^{(0)}$, $h_Q^{(1)}$, e_Q and δ_Q are rather lengthy to give here, and therefore we provide them in the Appendix 7.2.4.

Carrying out the Lagrange–multiplier minimization technique we find that the optimal fits to g_Q and Λ can be derived through the set of equations:

$$\Lambda = \sum_Q V_Q^2 \, [g_Q/c] \, h_Q^{(0)}, \tag{7.41}$$

$$\frac{g_Q}{c} = -\frac{h_Q^{(0)}}{e_Q - \delta_Q + (1 + 2\Lambda_0 - \Lambda) h_Q^{(1)}}, \tag{7.42}$$

and further, for the ground state energy, we obtain

$$E_g = \frac{1}{2}\omega_c - \Lambda_0 + \Lambda \; . \tag{7.43}$$

7.2.3 Remarks and Conclusions

In the energy expression (7.43), the additive term Λ, by means of which the adiabatic theory goes over to the weak coupling regime, depends implicitly on the magnetic field and phonon coupling strengths through the transcendental equation (41). For a large value of the cyclotron frequency, $h_Q^{(0)}$ in Eqs.(7.41) and (7.42) tends to zero, thereby $\Lambda \approx 0$, and hence the strong–coupling limit is readily attained even for $\alpha \ll 1$. As however ω_c is decreased to lower values, parameter Λ starts to interfere in the theory and strongly modify the results of the adiabatic approximation. In particular, for somewhat small field intensities and weak phonon coupling, the role Λ plays becomes very prominent and the polaron binding is effectively determined by this term. In this limit it is easy to see that the terms δ_Q, Λ_0 and Λ in Eq.(7.42) are all proportional to α in leading order and thus become far too small to yield any significant contribution to the summand in the transcendental Eq.(7.41). Therefore, retaining only $h_Q^{(0)}$, $h_Q^{(1)}$ and e_Q, and expanding the summand in a power series up to first order in ω_c, we have

$$\frac{g_Q}{c} h_Q^{(0)} \approx \frac{[h_Q^{(0)}]^2}{e_Q + h_Q^{(1)}} \approx \frac{1}{1+q^2} + \omega_c \{ 4\frac{q^2}{(1+q^2)^3} - 3\frac{q^2+q^4}{(1+q^2)^4} \} - \sigma_{Q0}^2 \; . \tag{7.44}$$

Finally, projecting out the wave vector sum in (7.41), we achieve

$$\Lambda \approx -\alpha \int_0^\infty dq \frac{[h_Q^{(0)}]^2}{e_Q + h_Q^{(1)}} \approx -\frac{\pi}{2}\alpha(1 + \frac{\omega_c}{8}) + \Lambda_0 \tag{7.45}$$

which, when inserted in Eq.(7.43), yields the approximate effective–mass argument – based energy expression as given in Eq.(7.1); thus exemplifying the essential role which Λ plays in conforming the adiabatic approximation over to the results derived from the perturbation theory.[94]

It is instructive to remark that when the binding is somewhat deep ($\omega_c \gg 1$), one expects the energy eigenvalues of the bare electron Hamiltonian and hence the differences in them to be significantly larger than the LO-phonon energy, which we take to be unity in our dimensionless units. If what we really applying was ordinary perturbation theory the only significant contribution in the perturbation sum would come from the leading term $n_u = 0$, for this term has the smallest energy denominator. Dropping all terms except $n_u = 0$, we arrive at exactly the same expression obtained by the present calculation with $\Lambda = 0$. We thus note that in the extreme regime of highly localized configurations with shrinking cyclotron size the perturbation and strong coupling theories match and are equally valid. On the other hand, as the magnetic field strength is made smaller, the adiabatic approach rapidly loses its validity since now the Landau levels are closer and even tend to coalesce towards the ground level. The corresponding perturbation series thus becomes slowly convergent and one needs to include the remaining terms, other than $n_u = 0$ as well. This however is accomplished in the present formalism by simply solving the transcendental equation (7.41) for the Lagrange multiplier Λ. Obviously, due to the analytic complexity the optimal fit to Λ (and to g_Q) can only be done by numerical techniques.

Alternative Approach

Before presenting a general display of our numerical results we would like to make a small digression on an alternative approach and set up some correspondence with the variational bound–polaron state which has been proposed previously by Devreese *et al.*,[56] and later, in [99], adapted to the two dimensional magneto-polaron problem. The basic distinction which sets the present formulation apart from that advanced in papers [56] and [99], stems essentially from the manner the perturbation expression (7.19) is treated in deriving the variational extension

to the adiabatic polaron state Φ_0.

A more straightforward and less tedious approach in obtaining an analogous form for the variational state Φ_0', or equivalently for the operator $\Omega(\alpha, \omega_c)$ as defined in Eq.(7.18), can be achieved by treating the reciprocal of the total energy denominator "$\varepsilon_n - \varepsilon_0 + 1$" in Eq.(7.19) as some average c–value, g_Q, and then setting $\sum_n \mid \varphi_n\rangle\langle\varphi_n \mid$ to the identity operator. Thus, in complete form, one obtains a more simple structure for the operator Ω as introduced in [56] or [99], i.e.

$$\Omega(\alpha, \omega_c) = c + \sum_Q V_Q g_Q \eta_Q^* a_Q^\dagger \tag{7.46}$$

in which the ω_c–dependence is provided only implicitly through the parameter g_Q.

In the present treatment of the problem, however, we have found necessary to conserve the track of the magnetic field parameter ω_c all throughout the computational steps in reaching the extended variational state Φ_0', Eq.(7.18), thus accounting for this parameter not solely in the bare electron part of the Hamiltonian, but also within the context of the part of the Hamiltonian describing the coupling of the electron to the phonon field. A glance at Eq.(7.30) reveals that the way this is accomplished is through the ξ–integrals involving the modified wave vector $\vec{q}(\xi) = \vec{q}e^{-\omega_c\xi}$ which imposes a detailed link incorporating the cyclotron frequency and the electron–phonon coupling. More peculiar in concern with the weight $e^{-\omega_c\xi}$ is that it further takes part in determining the variational parameter g_Q which sets up the detailed interbalance between the strong and weak coupling counterparts of the coupled electron–phonon system. The passage from the form (7.27) derived in this work to that given in Eq.(7.46) can readily be attained by simply deleting the exponential factor $e^{-\omega_c\xi}$ in Eq.(7.29), thus replacing $\vec{q}(\xi)$ by $\vec{q}$ in the set of Eqs.(7.30–7.33). The ground state energy can similarly be derived through Eqs.(7.41–7.43), where now the parameters $h_Q^{(0)}$, $h_Q^{(1)}$, e_Q and δ_Q simplify to

$$\begin{aligned} h_Q^{(0)} = h_Q^{(1)} &= 1 - \sigma_{Q0}^2, \\ e_Q &= q^2 \end{aligned}$$

ω_c	(a)	(b)	(III)	(IV)
0.1	0.03435	0.03420	0.04802	0.04720
0.2	0.08427	0.08399	0.09720	0.09604
0.5	0.23388	0.23336	0.24557	0.24373
1	0.48301	0.48233	0.49373	0.49114
2	0.98109	0.98036	0.99114	0.98747
5	2.47582	2.47520	2.48599	2.48018
10	4.96880	4.96830	4.98018	4.97198
20	9.95808	9.95772	9.97198	9.96037

Table 7.1: The ground state energy versus the cyclotron frequency for at weak coupling ($\alpha = 0.01$).
The columns (a) and (b) display $E_g^{(a)}$ and $E_g^{(b)}$, and the third and fourth columns are the adiabatic results obtained from Eqs.(7.2) and (7.16–7.17), respectively.

$$\delta_Q = 2\Lambda_0\sigma_{Q0}^2 - 2\Lambda_0\sigma_{Q0}I_0(q^2/8\omega_c), \tag{7.47}$$

and this facilitates the numerical computations greatly. On the contrary however, the usage of this simplified version (7.46) is expected to yield somewhat larger energy upper bounds due to that the variational parameter g_Q is now introduced to replace the energy denominator as an *average* quantity factored out away from the intermediate Landau level index n_u, thus containing only an *average* of the detailed content of the Fröhlich interaction interrelated to each of the Landau levels involved in the perturbation sum in Eq.(7.19).

Hereafter, in our foregoing discussions we shall refer to the variational ground state energy values by $E_g^{(a)}$ and $E_g^{(b)}$, respectively for the cases where either the form (7.46) or (7.27) is adopted. In order to provide a clear insight into the improvement achieved by the present formulation we display our results for both approaches computed under identical numerical precisions.

Numerical Results

We first refer to the regime of extreme weak coupling and tabulate E_g versus ω_c for $\alpha = 0.01$. An immediate glance at the respective columns for $E_g^{(a)}$

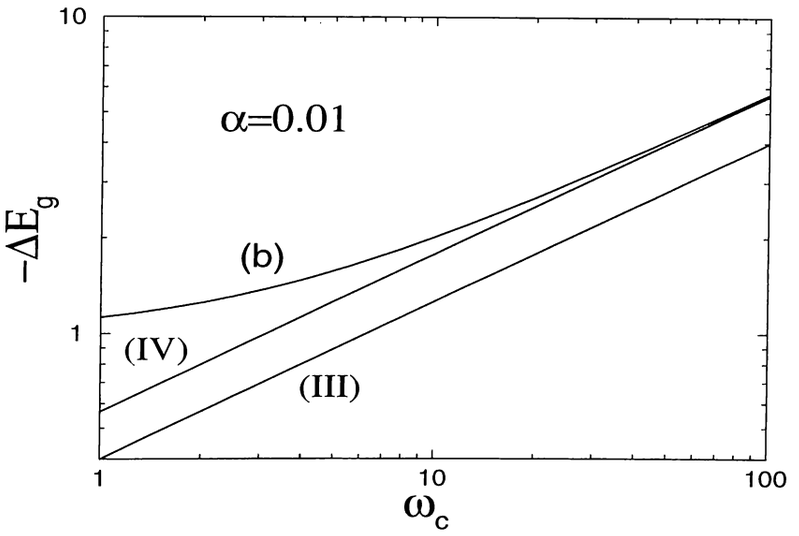

Figure 7.2: Polaron induced shift in the ground state energy at high magnetic field limit, for $\alpha = 0.01$.
Curve (b) displays the results of the improved version in the present calculation. The straight lines (III) and (IV) are the strong–coupling results plotted from Eqs.(7.2) and (7.16–7.17), respectively. The energies are expressed in terms of the free–polaron binding energy, $(\pi/2)\alpha$.

and $E_g^{(b)}$ in Table 7.1 reveals that the improved trial state (7.27) derived in this work yields significantly lowered energy upper bounds, and moreover, we find that the numerical values led by the present treatment of the problem are in perfect agreement with those obtained from the second order perturbation approximation[94]:

$$\Delta E_g^{(\mathrm{pert})} = -\frac{\pi}{2}\alpha\sqrt{\omega_c}\,\frac{\Gamma(1+1/\omega_c)}{\Gamma(\frac{1}{2}+1/\omega_c)}\,. \tag{7.48}$$

We should redraw attention to that, in spite of a small α, a pseudo–adiabatic condition is reached for large ω_c and that the adiabatic limit considered here is the case where the lattice distortion is thought as centered on the orbit center coordinates (7.3) as characterized by Eqs.(7.16 – 7.17) rather than by Eq.(7.2). It is only then the adiabatic approximation (and hence the present variational approach) fit the second order perturbation theory for $\alpha \ll 1$ and $\omega_c \gg 1$. Indeed, a careful examination of the numerical values in Table 7.1 confirms that the energies in columns (b) and (IV) (those obtained from Eqs.(7.16 – 7.17)) tend

to approach to one another and eventually join as the magnetic field is made stronger. The energy values obtained from Eq.(7.2), however, remain deviated from the correct high field limit due to that the electronic wave function in the x–y plane does not have to be as broad as depicted under when the lattice displacement is set at $\vec{\rho} = 0$ (cf. section III in [86]). This feature has been made more explicit in Fig.7.2 where $\Delta E_{\rm g}$ is displayed for large cyclotron frequencies.

In order to provide a pictorial view of the asymptotic energy profile of the system in the low field limit, and in particular, to give somewhat more impact to the limiting expression for parameter Λ as derived in Eq.(7.45), we also display the polaron–induced shift, $\Delta E_{\rm g} = E_{\rm g} - E_{\rm g}(\alpha = 0)$, in the lowest Landau level calculated from both approaches, (a) and (b), over a reasonably broad range of small ω_c values. A remarkable feature pertaining to the set of energy values (a) and (b) in Fig.7.3 is that as ω_c tends to become small, $\mid \Delta E_{\rm g}^{(a)} \mid$ approaches the free–polaron binding energy, $\frac{\pi}{2}\alpha$, from slightly below, which clearly is an incorrect description at least from a qualitative viewpoint that the binding should inherently be stronger under an external magnetic field. The deficiency encountered here, however, gets cured under utilizing the improved version (b). Within the framework of the modified trial state (7.27) we observe that $\mid \Delta E_{\rm g}^{(b)} \mid$ displays instead a monotonically decreasing profile approaching the asymptotic value $\frac{\pi}{2}\alpha$ from above, thus being totally consistent with the description implied by Eq.(7.1) or equivalently, by (7.48).

Going over to stronger coupling constants a clear and concise description of the polaron state may no more be readily tractable owing to the combined effect of the magnetic field and the Fröhlich interaction. Depending on the strengths of the parameters ω_c and α there takes place two competitive contributions coming from the magnetic field alone and the phonon coupling alone, yet however, acting in an interrelated manner, thus leading to rather involved and distinguishing characterizations of the magneto-polaron. The treatment of the problem is relatively simple, however, in the extreme regimes where either the magnetic field counterpart or the phonon coupling dominates over the other. It is worthwhile to remind that our present considerations have been focused to the regime in which

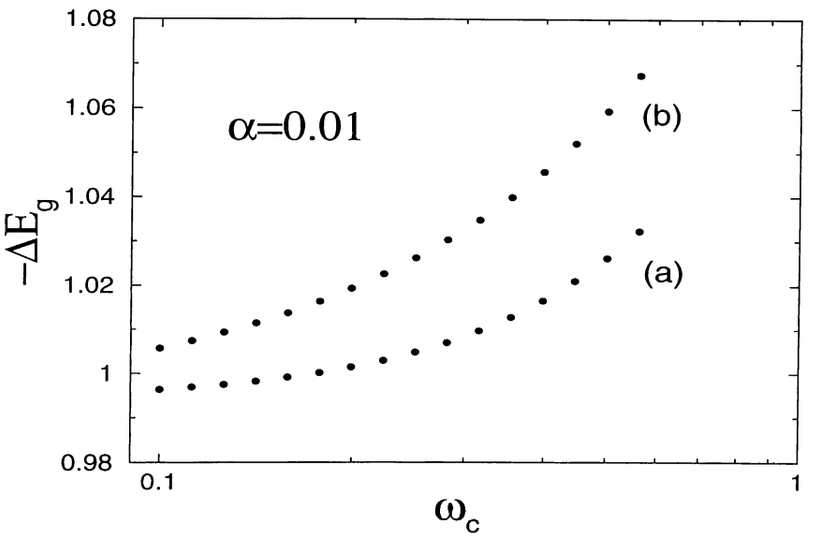

Figure 7.3: ΔE_g versus ω_c in the low field regime.
The set of dark circles (a) and (b) display the results of the present formalism for the cases where either the form (7.46) or (7.27) is adopted. The energies are expressed in terms of the free–polaron binding energy, $(\pi/2)\alpha$.

the magnetic field has the dominating strength over the coupled electron–phonon system where the relevant coherent phonon state is most appropriately structured so as to clothe the entire Landau orbit (with center at $\vec{\rho}_0$) rather than the mean electron position at the origin.

In Fig.7.4 we select the coupling constant as larger by an order of magnitude, $\alpha = 0.1$, and provide plots of the phonon–induced shift in the energy against ω_c together with the available data (cf., dark circles in the figure) taken from the generalized path–integral formalism of Xiaoguang, Peeters and Devreese[96] (henceforth denoted XPD). At this point it should be mentioned that the validity of the XPD–theory has remained an open question over almost a decade (since the pioneering conjecture of Larsen[104]) from the formal viewpoint in the sense that their high–field estimates might lie below the actual ground state energy.[98,104–106] The controversy in the literature on the applicability of path–integral formalism for the systems with non–zero magnetic fields has been resolved recently,[107] and it is pointed out that ordinary path–integral treatment does not –*a priori*– provide an upper bound for the free energy of

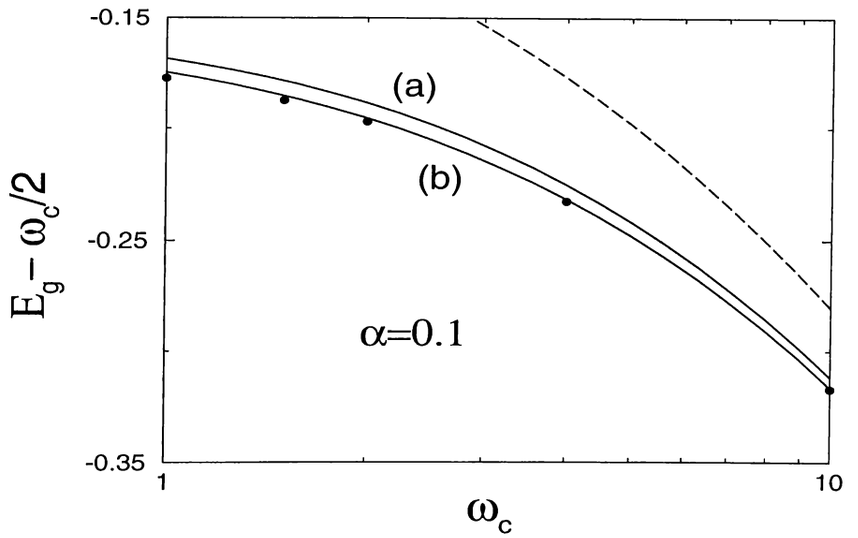

Figure 7.4: The phonon-induced shift in the lowest Landau level energy as function of ω_c.
Curves (a) and (b) are respectively for the cases where either the form (7.46) or (7.27) is used for $\Omega(\alpha, \omega_c)$. The dark circles display the generalized path-integral results of the XPD-theory,[96] and the dashed line refers to the results of the strong coupling approximation (7.17).

the Fröhlich polaron in a magnetic field.[108] Nevertheless, we still choose to make correspondence with the XPD-results and compare them with those derived from the present approximation which has a conventional variational framework free of any mathematical curiosities as inquired in concern with the XPD-formulation.

Referring first to the present results (a) and (b) derived within the variational polaron states given through equations (7.46) and (7.27), we infer that $E_g^{(b)}$ drops significantly below $E_g^{(a)}$ and that the usage of the improved trial state (b) gives by far more satisfying energy upper bound values. Comparing our results with those of XPD we find that even though $E_g^{(b)}$ lies consistently above the XPD-energies, the discrepancy does not seem to be strikingly prominent especially for large magnetic field strengths. For $\omega_c = 4$, for instance, we obtain $\Delta E_g^{(b)} = -0.2310$ which is fairly close (within only 0.6%) to the value -0.2324 derived by XPD. Using the form (7.46) for $\Omega(\alpha, \omega_c)$ however, we obtain $\Delta E_g^{(a)} = -0.2250$ yielding a percentual discrepancy as large as 3.2%. We thus see explicitly that approach

(b) gives far better results than (a) and further that the values reached by (b) are in fairly close agreement with those of XPD.

As the adiabatic limit ($\omega_c \gg 1$) is approached, we observe that the present formulation and the XPD–theory match and give almost identical results, e.g. for $\omega_c = 10$ we have $\Delta E_g^{(b)} = -0.3170$ and $\Delta E_g^{(\mathrm{XPD})} = -0.3173$. For even larger values of ω_c the theory puts comparatively less weight to the role which parameter Λ plays in Eq.(7.43), thus imparting somewhat most dominance to the strong coupling counterpart of the problem. Therefore, in the limit of intense magnetic fields, one readily expects all theories (a, b and XPD) to duplicate asymptotically the strong coupling results given by Eq.(7.17). Similar conclusions hold true for even stronger values of the coupling constant provided the magnetic field is sufficiently large so as to preserve the validity of the displaced oscillator transformation applied to the starting strong–coupling ansatz in the derivation of the present variational formalism. Setting $\omega_c = 10$, we obtain $\Delta E_g^{(b)} = -3.1472$ and -12.4171 for $\alpha = 1$ and $\alpha = 4$, respectively, whereas the corresponding XPD–values have been reported to be -3.1737 and -12.7004 which lie below (b) by not more than 0.8% and 2.2%.

In order to provide a comprehensive insight into the extent of applicability of the present approach in the large – α regime we display our results together with some of the available XPD – data (dark circles) for two different magnetic field strengths (cf., Fig.7.5). We note that as far as the magnetic field is strong enough to dominate over phonon–coupling – induced self–localization of the polaron, the agreement is fairly well in that all the XPD points for $\alpha = 0.1, 1$ and 4 lie only slightly below our calculations plotted for $\omega_c = 10$ and $\omega_c = 4$, except the one for $\alpha = 4$ and $\omega_c = 4$ which is seen to lie drastically deviated below the present theory ($\Delta E_g^{(\mathrm{XPD})} = -10.0090$, $\Delta E_g^{(b)} = -8.7823$). The reason for the fault lies in that the transformed Hamiltonian (7.14) involves the coherent phonon state centered on the orbit center $\vec{\rho}_0$ which obviously is misleading since for strong phonon coupling but not large enough ω_c, the polaronic aspect over compensates the magnetic field counterpart of the problem – this particular situation being beyond the limit of applicability of the present approximation. A way to overcome

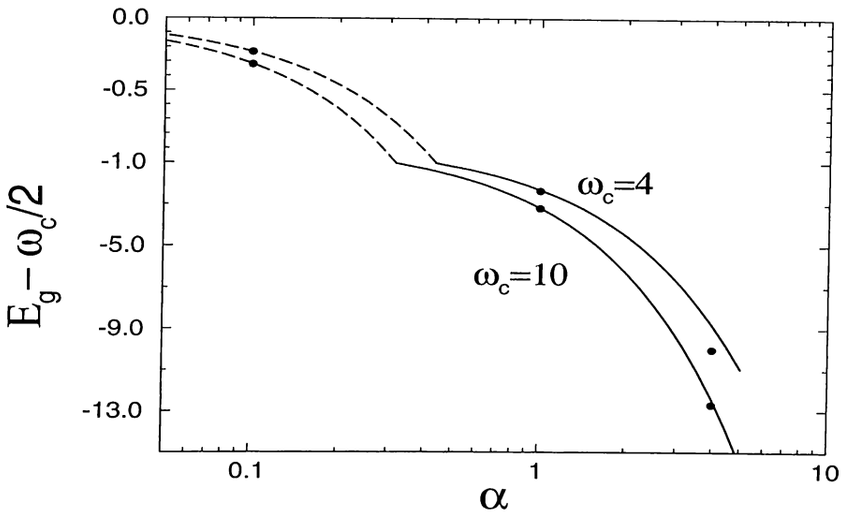

Figure 7.5: The phonon-induced shift in the lowest Landau level energy as a function of α.
The dark circles display the generalized path-integral results of the XPD-theory.[96] The plot is expanded in the energy region between -1 and 0, and to avoid confusion the curves are dashed in that region.

the drawback encountered here can readily be achieved by making reference to the extreme limit of $\alpha \gg 1$ and $\omega_c \ll 1$ where now the lattice deformation should be thought as surrounding the mean charge density of the electron itself rather than its overall motion in a complete Landau orbit (cf., [99]). The discussions pertaining to this totally distinctive aspect of the magneto-polaron is beyond the scope of our present interest.

In summary, this work revises the problem of a polaron in a magnetic field within an improved version of the extended variational scheme of Devreese *et al.*[56] proposed for the bulk bound-polaron. Although most of the formulation that we have adopted applies to a polaron in any dimensionality, for the present we have restricted our considerations to the 2D-model of a magneto-polaron so as to eliminate any complications comprised by the third dimension and have attributed most emphasis to the formal viewpoint of the problem. In view of our numerical results and the asymptotic analytic forms (7.16) and (7.45) achieved for $\omega_c \gg 1$ and $\omega_c \ll 1$, we reach the conclusion that the improved

trial state introduced through Eqs.(7.27, 7.29 – 7.33) is rather promising in that it conveniently sets up a weighted admixture of the strong and weak coupling counterparts of the problem and thus enables the adiabatic results to conform satisfactorily to those attained from second order perturbation theory.

7.2.4 Appendix

Referring to the set of Eqs.(7.30–7.33) and using the integral transform

$$\int_0^\infty d\xi \int_0^\infty d\xi' \; f(\xi,\xi') = \frac{1}{2}\int_0^\infty dt \int_{-t}^{t} dt' \; f(\frac{t+t'}{2}, \frac{t-t'}{2}) \tag{7.49}$$

we obtain the following functional forms for the parameters $h_Q^{(0)}$, $h_Q^{(1)}$, e_Q and δ_Q defined in Eqs.(7.35) and (7.38–7.40):

$$h_Q^{(n)} = \int_0^\infty dt \; t^n e^{-t} \exp[-\frac{q^2}{\omega_c}(1-e^{-\omega_c t})] \; - \; \sigma_{Q0}^2, \qquad n = 0, 1 \tag{7.50}$$

$$e_Q = q^2 \int_0^\infty dt \; t \; e^{-t} e^{-\omega_c t} \exp[-\frac{q^2}{\omega_c}(1-e^{-\omega_c t})] \tag{7.51}$$

and

$$\begin{aligned}\delta_Q &= 2\Lambda_0\sigma_{Q0}^2 \; - \; 2\Lambda_0 \int_0^\infty dt \; e^{-t} \int_0^t dt' \; [G(t+t') + G(t-t')] \\ &+ \; 2\Lambda_0 \int_0^\infty dt \; e^{-t} \exp[\frac{q^2}{\omega_c}(1-e^{-\omega_c t})] \int_0^t dt' \; F[\frac{q^2}{4\omega_c} e^{-\omega_c t}(1-\cosh\omega_c t')]\end{aligned} \tag{7.52}$$

where

$$G(t \pm t') = \exp[-\frac{q^2}{\omega_c}(1-e^{-\omega_c(t\pm t')})] \; F[\frac{q^2}{8\omega_c} e^{-\omega_c(t\pm t')}] \tag{7.53}$$

and

$$F(x) = e^{-x} I_0(x)$$

with I_0 denoting the modified Bessel function of order zero.

Chapter 8

CONCLUSIONS

We have presented five different formal approaches to polaron problem and have considered their applications to low dimensionally confined polarons. Among them perturbation theory, adiabatic strong-coupling approximation and the variational scheme of LLP are shown to have restricted domain of validity in both the electron-phonon coupling strength and the degree of confinement. Nevertheless, they are essential for the qualitative understanding of the polaron at some special cases, where the characterization of the problem is distinctively different. Moreover, they form the checking criteria for other more powerful and interpolating approximations. In this work, the path-integral formalism and the perturbative variational approach have been considered as examples of such unifying and comprehensive theoretical tools of the study of polarons, the former being the superior to all the others.

The visualization of the polaron ground state at large, is not immediate in its most general context. Depending on the strength of the electron-phonon coupling, the situation is more transparent in the two extremes, weak- and strong-coupling regimes. At weak coupling the polaron is in a delocalized state along the free spatial directions and if there exists any, the character of the localization is governed by the external potential. The phonon coupling is a perturbation to the electron ground state, leading to small corrections to the effective mass and the ground state energy in the order of α. In the opposite extreme, however, the

electron goes into a bound state with a highly localized wave function in the self-induced potential, which is built up by the phonon field. In view of the conclusion arrived at, with the elegant work of Gerlach and Löwen,[10] the transition from the quasi-free to the self-trapped state of the polaron as the coupling strength is increased, should take place in a smooth and continuous way. Consequently, in every case, the polaron state should be viewed as a weighted admixture of quasi-free and localized parts, the relative weights of which depend on the value of α, as well as the degree of confinement of the electron. This statement has been explicitly demonstrated in this work, as such, it is shown that the roles which the external confining potential (or in the case of magneto-polaron, the external field) and the phonon coupling play in the formation of the polaron state, are not completely independent, but rather take part in an interrelated manner, determining the localization character of the electron. For example, in the case of an infinite boundary wire configuration, we have seen in Chapter 4 that, in spite of a weak polar coupling, a pseudo-adiabatic condition can be reached due to the high degree of confinement achieved in thin wires.

Regarding the effect of confinement, there are two competing trends in the polaron binding. In highly anisotropic systems, as the degree of confinement is increased, there comes about a competitive interrelation between whether the charge density fluctuations of the electron will condense on the polaron center or will expand to relax itself in the free directions. The former enhances the effective coupling, leading to a deeper binding, whereas the latter is in favor of a more delocalized state with a less binding. This salient feature is observed for the wire geometry in the weak-coupling regime in Chapter 5.

In the general scope of this thesis work, we have presented an overview to the single-polaron properties in low dimensionally confined media. Giving most emphasis to the formal structure of the problem, we have demonstrated the bulk phonon effects on the confined electron.

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