

DOKUZ EYLÜL UNIVERSITY
GRADUATE SCHOOL OF NATURAL AND APPLIED SCIENCES

THE BOUND EXCITON
TO AN IONIZED DONOR IMPURITY IN
SEMICONDUCTOR SPHERICAL
QUANTUM DOT

by

Bahadır Ozan AKTAŞ

July, 2009

İZMİR

**THE BOUND EXCITON
TO AN IONIZED DONOR IMPURITY IN
SEMICONDUCTOR SPHERICAL
QUANTUM DOT**

**A Thesis Submitted to the
Graduate School of Natural and Applied Sciences of
Dokuz Eylül University
In Partial Fulfillment of the Requirements for
the Degree of Master of Science in Physics**

by

Bahadır Ozan AKTAŞ

**July, 2009
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M.Sc. THESIS EXAMINATION RESULT FORM

We have read the thesis entitled “**THE BOUND EXCITON TO AN IONIZED DONOR IMPURITY IN SEMICONDUCTOR SPHERICAL QUANTUM DOT**” completed by **BAHADIR OZAN AKTAŞ** under supervision of **ASSIST. PROF. DR. HAKAN EPİK** and we certify that in our opinion it is fully adequate, in scope and in quality, as a thesis for the degree of Master of Science.

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Bahadır Ozan AKTAŞ

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ABSTRACT

The effects of quantum confinement on the ground state energy of a bound correlated electron-hole pair as an exciton to an hydrogenic ionized donor impurity which placed at the center of an infinite spherical microcrystal in interior dielectric medium have been investigated constitutively as a function of quantum dot size. Most of formulas and results obtained are compared for cases with and without impurity or have been checked for accuracy in a number of special case. A mathematically rigorous study confirms, in a unified and simpler manner, several results obtained earlier in the literature but not necessarily in the same contexts. Unlike the conventional procedure, the Fourier transforms have been used for evaluating three-particle integrals terms including interparticle distance \mathbf{r}_{ij} in Hylleraas coordinates are given formulae are obtained for the Hamiltonian matrix elements of various operators arising in Hylleraas-type variational calculations for states of arbitrary angular momenta.

The integrals have been generated from Hamiltonian matrix are well suited to computer implementation. To construct an exact analytical expression for the expectation value of the Hamiltonian have been used a numerically fast and well stable algorithm for the calculation of the relevant integrals with high powers of interparticle coordinates. The optimum value of the variational parameter have been vary in the range of $\lambda = [0.055, 0.300]$.

The behaviors of the complexes X and D^+, X are similar cause of the values of the two additional interparticle interaction integral terms I_{G_1} and I_{G_2} are completely the same by a difference opposite notation. Consequently the main inference is that injecting a donor impurity to the X complex would not change the stationary state of the system.

Keywords: Quantum Dot, Exciton, Hylleraas-type wave function, Rayleigh-Ritz's variational method.

YARIİLETKEN KÜRESEL KUANTUM NOKTASINDA İYONİZE OLMUŞ BİR VERİCİ SAFSIZLIĞINA BAĞLI EGZİTON

ÖZ

Bir dielektrik ortam içerisinde sonsuz küresel mikrokristal merkezinde konumlanmış olan hidrojenik verici safsızlığına bağlı egziton görüngüsünde ilintili elektron-deşik çiftinin kuantum kuşatma altında taban durum enerjisine kuantum noktasının boyutunun etkisi incelenmiştir. Birçok eşitlik ve sonuç verici safsızlığının mevcut olduğu ve olmadığı durumlar için karşılaştırılmış ya da kesinlik açısından bir özel duruma indirgenerek kontrol edilmiştir. Matematiksel olarak özenli çalışma, literatürde önceleri elde edilmiş olan sonuçlar ile birebir örtüşmese dahi, şeklen bütünleştirici ve daha basitçe gerçekleyici sonuçların eldesini mümkün kılar. Geleneksel izlekten farklı olarak, keyfi açısal momentum durumları için Hylleraas-tipi varyasyonel hesabında çeşitli işlemciler bütünü biçiminde Hamiltonyan matris elemanlarından elde edilen, eşitlikte verilmiş olan Hylleraas koordinatlarında parçacıklar arası \mathbf{r}_{ij} uzaklığını içeren üç-parçacık integrallerinin hesaplanmasında Fourier dönüşümü kullanılmıştır.

Hamiltonyan matrisinden türemiş integraller bilgisayar uygulamasına oldukça elverişlidir. Hamiltonyan'ın beklenen değerine ait kesin analitik ifadesinin inşası için, parçacıklar arası koordinatların yüksek mertebeden kuvvetlerini içeren integrallerin hesaplanmasında nümerik olarak hızlı ve kararlı bir algoritma kullanıldı. Varyasyonel parametresinin optimum değeri $\lambda = [0.055, 0.300]$ aralığına yayılmaktadır.

İki ek I_{G_1} ve I_{G_2} parçacıklar arası etkileşim integral terimlerinin bir işaret farkı ile tamamen aynı olmasından ötürü, X ve D^+, X yapılarının davranışları benzerdir. Dolayısıyla temel çıkarımsama, X yapısına bir verici safsızlığı enjekte etmenin sistemin dingin durumunda bir değişikliğe neden olmayacağıdır.

Anahtar sözcükler: Kuantum Nokta, Egziton, Hylleraas-tipi dalga fonksiyonu, Rayleigh-Ritz varyasyonel yöntemi.

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CHAPTER ONE

PROLOGUE

During the past few years, research in semiconductors has taken on, quite literally, new dimensions. Their numbers are two, one and zero. Electrons in recently developed devices can be confined to planes, lines or mathematical points- *quantum dots*. The QD¹ concept is 21st century theory of atomic reductionism.

Microchip manufacturers have developed a toolbox of nanofabrication technologies capable of creating structures almost atom by atom. These techniques have opened up a new realm of fundamental physics and chemistry as workers make and study artificial analogues of atoms, molecules and crystals. Experimenters are no longer limited by the atomic shapes, sizes and charge distributions available in nature (Reed, 1993).

New research directions are emerging. One that is now in embryonic stage is the combination of QD molecules. Many of the QD systems currently being studied have the potential to be combined into molecular complexes with one-, two- or three-dimensional structures. One can imagine growing this *solid-state atoms* or molecules within structures containing electronic or magnetic gates and optical cavities, perhaps all connected together by *quantum wires* (Gammon, 2000).

QDs have great flexibility because their properties can be artificially engineered, but this comes at a price. Nature has given atoms; scientists must make QDs. Further advances in this exciting field of science and technology will depend heavily on the creativity of physicists, chemists and materials scientists who make this tiny structures.

¹Quantum dot

CHAPTER TWO

QUANTUM DOT PHENOMENA

2.1 A Brief Overview: Designer Atoms

With dimensions of only 1 to 100 nanometers and containing somewhere between 10^3 and 10^6 atomic nuclei in a crystalline lattice, semiconductor QDs are often described as *solid-state, artificial atoms* (MRS Bull, 1998) or *designer atoms* (Reed, 1993) by some experts. In this sense, most experts would concur that a QD is a semiconductor whose excitons are confined in all three spatial dimensions. As a result, they have properties that are between those of bulk semiconductors and those of discrete molecules. They were discovered by Louis E. Brus, who was then at Bell Labs. The term QD was coined by Mark A. Reed.

Researchers have studied QDs in transistors, solar cells (Hanna et al., 2005), LEDs², diode lasers and many other areas. They have also investigated QDs as agents for medical imaging (Nie et al., 2007) and hope to use them as qubits (Loss, & DiVincenzo, 1998).

2.2 Exciting The Electrons In Pointlike Structures

If photons of energy comparable to the band gap are incident on a semiconductor, then they can be absorbed by the electrons forming atomic bonds between neighboring atoms, and so provide them with enough energy to break free and move around in the body of the crystal. Within the band theory of solids, this would be described as *exciting an electron from the valence band across the*

²evidot LEDs

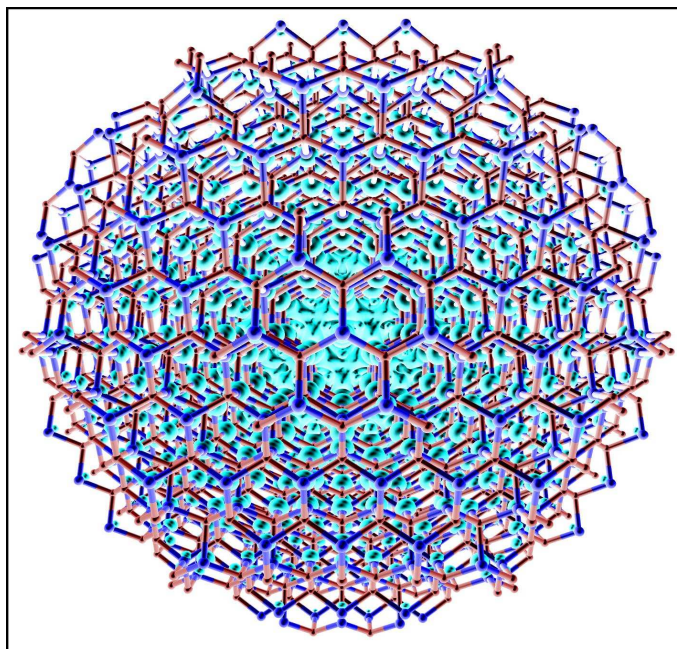


Figure 2.1 Fluorescence from CdSe QD solids in environments varying from stable to high unstable show that small deviations from uniform stress distribution greatly affect the electronic properties. In the *VMD-Visual Molecular Dynamics* picture, the red represents cadmium, the blue represents selenium and the green represents a cloud of electrons in their excited state. Image by Sebastien Hamel/LLNL.

band gap into the conduction band. If the energy of the photon is larger than the band gap, then a free electron is created and an empty state is left within the valence band.³ The empty state within the valence band behaves very much like an air bubble in a liquid and rises to the top-the lowest energy state. This hole behaves as though it were positively charged and hence often forms a bond with a conduction-band electron.⁴ The attractive potential leads to a reduction⁵ in the total energy of the electron and hole. This bound electron-hole pair is known as an *exciton*. Photons of energy just below the band gap can be absorbed, thus

³*High energy excitation*

⁴*Exciton formation*

⁵by an amount E_X

creating excitons directly.

As the hole mass is generally much greater than the electron mass, then the two-particle system resembles a hydrogen atom, with the negatively charged electron orbiting the positive hole. The exciton is quite stable and can have a relatively long lifetime, of the order of hundreds of ps to ns. Exciton recombination is an important feature of low, temperature photoluminescence, although as the binding energies are relatively low, i.e. a few meV to a few tens of meV, they tend to dissociate at higher temperatures.

Eventual, in an unconfined (bulk) semiconductor, an electron-hole pair is typically bound within a characteristic length called the *Bohr exciton radius*. If the electron and hole are constrained further, then the semiconductor's properties change. This effect is a form of *quantum confinement*, and it is a key feature in many emerging electronic structures (Greenemeier, 2008; NY Times Science Watch, 1991).

2.3 Modern Nanofabrication Techniques

Conventionally fabrication of QDs proceeds through a series of masking and etching steps. First, an electron beam scans the surface of a semiconductor containing a buried layer of *quantum well* material. Resist is removed where the beam has drawn a pattern. A metal layer is deposited on the resulting surface, and then a solvent removes the remaining resist, leaving metal only where the electron beam exposed the resist. Reactive ions etch away the chip except where it is protected by metal, leaving a QD.⁶

An alternative fabrication method lays down a pattern of electrodes above a

⁶see in Figure 2.2

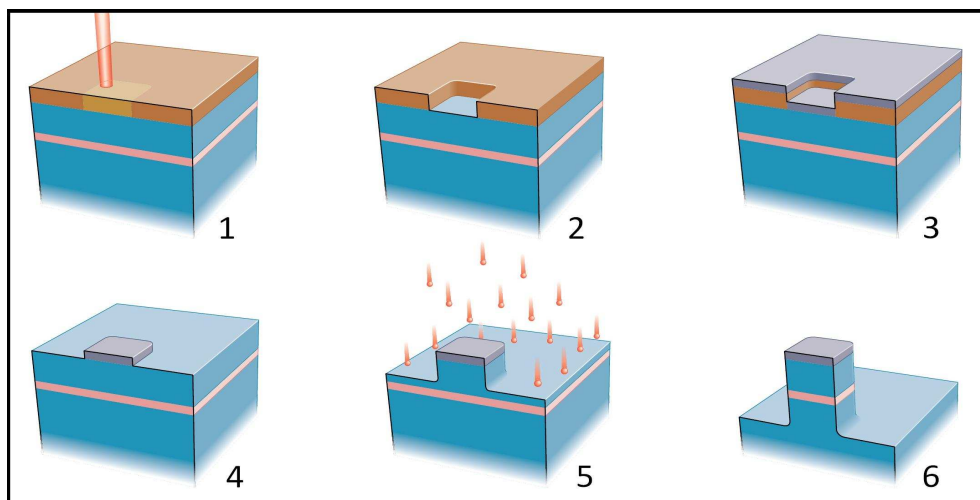


Figure 2.2 Building a QD conventionally in zero dimensions in rows in shapes.

buried QW⁷ layer. When a voltage is applied to the electrodes, the resulting field expels electrons from the layer except in certain small regions. The degree of quantum confinement in those regions can be manipulated by changing the electrode voltages.⁸

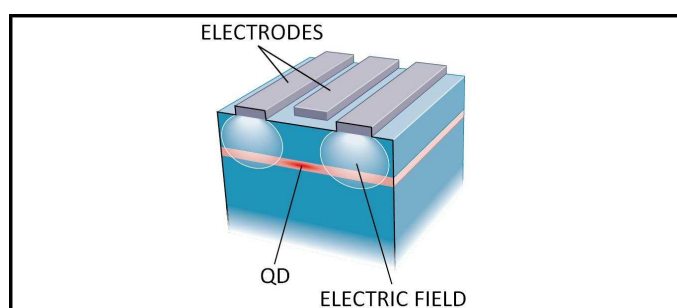


Figure 2.3 Schematically an alternative fabrication method of QD.

As a description, QDs possess unique properties that could potentially revolutionize existing optical and electronic technologies as well as open up new technologies. Conventional QD fabrication techniques, however, have several

⁷Quantum well

⁸see in Figure 2.3

drawbacks, such as large recombination velocities and surface depletion, that arise from having the surface exposed while patterning the substrate before or after growth.

As an applications, the reliable production of QDs offers outstanding opportunities for optical and electronic technologies as well as the development of new technologies. Devices that use the unique properties and advantages of QDs, such as improved vertical cavity surface emitting lasers and individual electron counters, thus become feasible.

There are several ways to confine excitons in semiconductors, resulting in different methods to produce QDs. In general, *quantum wires*, QWs and QDs are grown by advanced *epitaxial techniques* in nanocrystals produced by chemical methods or by ion implantation, or in nanodevices made by state-of-the-art *lithographic techniques* (Delerue, & Lannoo, 2004).

2.3.1 Lithographic Techniques

Method frequently used to create quantum confinement in a semiconductor heterostructure is the lithographic patterning of gates, i.e. nanoscale electrodes are created on the surface of a heterostructures (Mlinar, 2007). The widely used lithographic techniques are, optical lithography and holography, X-ray lithography, electron and focused ion beam lithography, and scanning tunneling microscopy (Şakiroğlu, 2009).

Self-assembled QDs are typically between 10 and 50 nm in size. QDs defined by lithographically patterned gate electrodes, or by etching on two-dimensional electron gases in semiconductor heterostructures can have lateral dimensions exceeding 100 nm. Some QDs are small regions of one material buried in

another with a larger band gap. These can be so-called core-shell structures, e.g., with CdSe in the core and ZnS in the shell or from special forms of silica called ormosil.

2.3.2 Epitaxial Growth

Epitaxy is used in nanotechnology and in semiconductor fabrication. Indeed, epitaxy is the only affordable method of high crystalline quality growth for many semiconductor materials, including technologically important materials as silicon-germanium, gallium nitride, gallium arsenide and indium phosphide.

Epitaxial growth techniques are currently the best choice to grow high-quality crystalline-films (Bianucci, 2007). An epitaxial layer can be doped during deposition by adding impurities to the source gas, such as arsine, phosphine or diborane. The concentration of impurity in the gas phase determines its concentration in the deposited film. As in CVD, impurities change the deposition rate.

CHAPTER THREE

THEORETICAL BASIS AND METHOD

3.1 Understanding The Problem

To choose the right model for a particular problem is not always straightforward, and often different models yield complimentary information. However, more often the computational resources are the limiting factor in determining which model can be used (Şakiroğlu, 2009). The aim of all the quantum mechanical many particle system methods is to solve the relevant Schrödinger⁹ equation. To get good enough powerful approach to solve the Coulombic quantum *three-body problem*¹⁰ (or *three-particle system*), usually impersonal passive to begin some approximations and most common structural nature which are the problem is obtained within and based on it.

3.1.1 *Further Confinement*

The reduction in dimensionality produced by confining electrons (or holes) to a thin semiconductor layer leads to dramatic change in their behaviour. This principle can be developed by further reducing the dimensionality of the electron's environment from a two-dimensional QW to a one-dimensional QWR¹¹ and eventually to a zero-dimensional QD (Harrison, 2005). In this monograph, of course, the dimensionality refers to the number of degrees of freedom in the electron momentum; in fact, within a QWR, the electron is confined across two directions, rather than just the one in a QW, and, so, therefore, reducing the degrees of freedom to one. In a QD, the electron is confined in all three-dimensions,

⁹Erwin Rudolf Josef Alexander Schrödinger (1887-1961)

¹⁰As well-known as non-chaotic flows, the classical one- and two-body problems have deterministic analytical solutions. These problems are most easily visualized, but extending to higher dimensions prompts to exhibit chaos.

¹¹Quantum wire

Table 3.1 The number of degrees of freedom F_f in the electron motion, together with the extent of the confinement F_c , for the four basic dimensionality systems.

System	F_c	F_f
Bulk	0	3
Quantum Well	1	2
Quantum Wire	2	1
Quantum Dot	3	0

thus reducing the degrees of freedom to zero. If the number of degrees of freedom are labeled as F_f and number of directions of confinement are labeled as F_c , then clearly:

$$F_f + F_c = 3 \quad (3.1.1)$$

for all the solid state systems. These values are highlighted for the four possibilities shown in Table 3.1. Tradition has determined that the reduced-dimensionality systems are labeled by the remaining degrees of freedom in the electron motion, i.e. F_f , rather than the number of directions with confinement F_c .

3.1.2 The Born-Oppenheimer Approximation

To describe the various motions of the quantum mechanical many-particle system which contain electrons and two *nucleilike* holes, have to begin with the Schrödinger equation. The Hamiltonian is given by

$$\mathbf{H} = T_e + T_h + V_{ee} + V_{eh} + V_{hh}, \quad (3.1.2)$$

where

$$T_e = \sum_{i=1}^N \frac{p_i^2}{2m}, \quad (3.1.3)$$

represents the kinetic energy of the electrons and

$$T_h = \sum_{\nu=1}^2 \frac{p_{\nu}^2}{2M}, \quad (3.1.4)$$

is the kinetic energy of the holes. V_{eh} represents the attractive electron-hole potential. V_{ee} describes the repelling electron-electron interaction. V_{hh} indicates the repelling Coulomb interaction between the holes. Since the masses of the hole are relatively large, T_h can be neglected. This step is called the *Born*¹²-*Oppenheimer*¹³ *approximation*.

If be neglected the kinetic energy T_h of the hole¹⁴, the relative distance R between hole only occurs as a parameter. The Schrödinger equation becomes,

$$[T_e + V_{ee}(\mathbf{r}) + V_{eh}(\mathbf{r}, \mathbf{R})]\varphi_n(\mathbf{r}, \mathbf{R}) = [\varepsilon_n(\mathbf{R}) - V_{hh}(\mathbf{R})]\varphi_n(\mathbf{r}, \mathbf{R}). \quad (3.1.5)$$

Here r indicates the position of the electron. The solutions $\varphi_n(\mathbf{r}, \mathbf{R})$ depend parametrically on the distance between the holes. The energy of this state is given by the electronic energy $\varepsilon_n(\mathbf{R})$ lowered by $V_{hh}(\mathbf{R})$. The solutions $\varphi_n(\mathbf{r}, \mathbf{R})$ represent a complete set of functions. The true wave function $\psi(\mathbf{r}, \mathbf{R})$ can be expanded within this set:

$$\psi(\mathbf{r}, \mathbf{R}) = \sum_m \phi_m(\mathbf{R})\varphi_m(\mathbf{r}, \mathbf{R}). \quad (3.1.6)$$

The coefficients $\phi_m(\mathbf{R})$ are to be found and, in general, depend on \mathbf{R} . $\psi(\mathbf{r}, \mathbf{R})$ is the solution of the full Schrödinger equation, which takes into consideration the kinetic energy T_h of the hole, i.e.

$$(T_e + T_h + V_{ee} + V_{eh} + V_{hh})\psi(\mathbf{r}, \mathbf{R}) = E\psi(\mathbf{r}, \mathbf{R}). \quad (3.1.7)$$

¹²Max Born (1882-1970)

¹³Julius Robert Oppenheimer (1904-1967)

¹⁴*Static approximation*: Fixed distance R of the hole

Inserting (3.1.6) into (3.1.7) and using (3.1.5), we obtain,

$$\sum_m (\varepsilon_m(\mathbf{R}) + T_h) \phi_m(\mathbf{R}) \varphi_m(\mathbf{r}, \mathbf{R}) = E \sum_m \phi_m(\mathbf{R}) \varphi_m(\mathbf{r}, \mathbf{R}). \quad (3.1.8)$$

Multiply from the left-hand side with $\psi_n^\dagger(\mathbf{r}, \mathbf{R})$, integrate over the full space, and get

$$\sum_m \int d^3r \psi_n^\dagger(\mathbf{r}, \mathbf{R}) T_h \phi_m(\mathbf{R}) \varphi_m(\mathbf{r}, \mathbf{R}) + \varepsilon_n(\mathbf{R}) \phi_n(\mathbf{R}) = E \phi_n(\mathbf{R}). \quad (3.1.9)$$

Here we have used the orthogonality of the functions $\varphi_n(\mathbf{r}, \mathbf{R})$ and T_h is proportional to the Laplace operator Δ_R , which acts on $\phi_m \varphi_m$. It holds that,

$$\Delta_R(\phi\varphi) = (\Delta_R\phi)\varphi + 2\nabla_R\Phi \cdot \nabla_R\varphi + \phi\Delta_R\varphi. \quad (3.1.10)$$

The index R indicates the action of the operators in R space. The first term in (3.1.10) is proportional to $T_h\phi_n$. The rest is brought to the right-hand side of (3.1.9). The result reads,

$$[T_h + \varepsilon_n(\mathbf{R})]\phi_n(\mathbf{R}) = E\phi_n(\mathbf{R}) - \sum_m C_{n,m}\phi_m(\mathbf{R}) \quad (3.1.11)$$

with

$$\begin{aligned} C_{n,m}\phi_m(R) &= -\hbar^2 \sum_\alpha \frac{1}{2M_\alpha} \int d^3r \varphi_n^\dagger(r, R) \\ &\times [2\nabla_{R_\alpha}\phi_m(\mathbf{R}) \cdot \nabla_{R_\alpha}\varphi_m(\mathbf{r}, \mathbf{R}) + \phi_m(\mathbf{R})\Delta_{R_\alpha}\varphi_m(\mathbf{r}, \mathbf{R})]. \end{aligned} \quad (3.1.12)$$

The sum over α comes from T_h and ∇_{R_α} acts only on the coordinate \mathbf{R}_α of the hole α , which appears in $R = \sqrt{(\mathbf{R}_2 - \mathbf{R}_1)^2}$. Now, the order of magnitude of $C_{n,m}$ is $(m/M)^{1/2}$ times smaller than the electronic kinetic energy. The order of magnitude of the term $\sim \hbar^2 \Delta_{R_\alpha}\varphi_m/2M_\alpha$ (the kinetic energy of the holes) is proportional to $-(m/M_\alpha)\hbar^2(\Delta_r\varphi_m/2m)$; we have simply replaced Δ_{R_α} by Δ_r

and introduced the electronic kinetic energy $-\hbar^2 \Delta_r \varphi_m / 2m$. The factor m/M_α indicates that the contribution of Δ_{R_α} to $C_{n,m}$ is smaller by this factor than the kinetic energy of the electron.

The first term in (3.1.12) remains to be estimated. For this approximate ϕ_m by a harmonic oscillator wave function: $\phi_m \approx \exp([-(\mathbf{R} - \mathbf{R}_0)^2 M\omega/2\hbar])$, R_0 being the equilibrium position of the holes α . Be had,

$$\nabla_{R_\alpha} \phi_m \approx |\mathbf{R} - \mathbf{R}_0| \frac{M\omega}{\hbar} \phi_m \approx \frac{(\delta R)M\omega}{\hbar} \phi_m. \quad (3.1.13)$$

δR indicates the shift from the equilibrium position. The factor M is canceled by $1/M$ in (3.1.12) and the contribution is proportional to the vibrational energy $\hbar\omega$. As noted earlier, this goes like $\sim (m/M)^{1/2}$. As a summary, the $C_{n,m}$ term can be neglected with the help of perturbation theory. Without the $C_{n,m}$ term, (3.1.11) reduced to

$$[T_h + \varepsilon_n(\mathbf{R})]\phi_n(\mathbf{R}) = E\phi_n(\mathbf{R}). \quad (3.1.14)$$

This equation has an interesting interpretation: the energy of the electron states $\varepsilon_n(R)$ acts like an effective potential in R . Imagine that the electrons build a medium in which the hole move. This medium acts as an elastic band. If the hole try to leave the equilibrium position, they will be drawn back. There is an equilibrium position where $\varepsilon(R)$ has a minimum deep enough to generate binding. The elastic ban behavior is then nothing other than the expansion up to the order $(\mathbf{R} - \mathbf{R}_0)^2$.

The $C_{n,m}$ produce a mixing between different states φ_n and φ_m . This mixing between the $\varphi_n(\mathbf{R})$ states can be neglected in lowest order, because the $C_{n,m}$ are small (of order $(m/M)^{1/2}$, as explained previously). Accordingly the wave function is approximately given by

$$\psi_{n,\nu}(\mathbf{r}, \mathbf{R}) = \phi_{n\nu}(\mathbf{R})\varphi_n(\mathbf{r}, \mathbf{R}). \quad (3.1.15)$$

Here ν stands for all quantum numbers of level n . $E_{n,\nu}$ indicates the energy of the system, which is calculated from (3.1.14).

In order to describe vibrations and rotations of the system $\varepsilon_n(\mathbf{R})$ is expanded in coordinates describing vibration and rotation, respectively. The expansion in $\delta R = |R - R_0|$ up to the squared order leads to a harmonic vibrational potential. $\varepsilon_h(R)$ does not depend on the angles¹⁵. Hence the rotations of the system are free. An excitation of the system is a combination of excitations of the harmonic vibrational oscillator and of the rotations.

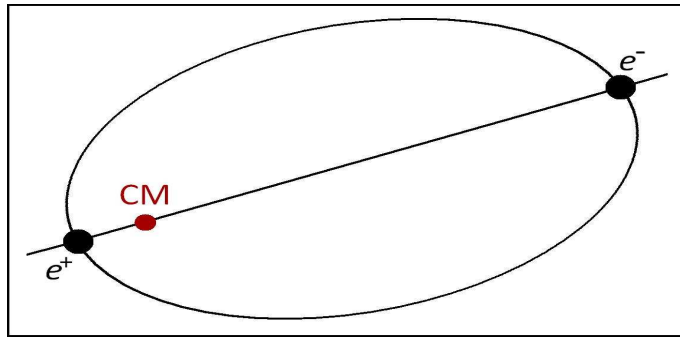


Figure 3.1 Semiquantum mechanical Kepler orbit with the center of gravity CM located in one of the foci of the ellipse.

Summary: In the Born-Oppenheimer approximation, first the energy levels of the electrons are determined for fixed distance \mathbf{R} of the holic centers. The electron energy $\varepsilon_n(R)$ plays the role of a potential, in which the holes are moving. If this potential has one or several deep enough minima, one or several bound states of the system can exist. If the minima are only weak or do not exist at all, then the system is not bound (Greiner, 1998).

¹⁵*Euler angles*

3.1.3 The *Effective Mass Approximation*

Therefore the crystal potential is complex; however using the principle simplicity¹⁶ imagine that it can be approximated by a constant. Then the Schrödinger equation derived for an electron in a vacuum would be applicable. Clearly though, a crystal isn't a vacuum so allow the introduction of an empirical fitting parameter called the *effective mass*, m^* . Thus the time-independent Schrödinger equation becomes:

$$-\frac{\hbar^2}{2m^*}\nabla^2\psi = E\psi,$$

and energy solutions follow as:

$$E = \frac{\hbar^2 k^2}{2m^*}$$

This is known as the *effective mass approximation* and has been found to be very suitable for relatively low electron momenta as occur with low electric fields. Indeed, it is the most widely used parameterisation in semiconductor physics. Experimental measurements of the effective mass have revealed it to be anisotropic as might be expected since the crystal potential along say the [001] axis is different than along the [111] axis. Adachi (Adachi, 1994) collates reported values for GaAs and its alloys; the effective mass in other materials can be found in Landolt and Börnstein (Landolt, & Börnstein, 1987).

In GaAs, the reported effective mass is around $0.067m_0$, where m_0 is the rest mass of an electron (Harrison, 2005).

¹⁶Choose the simplest thing first; if it works use it, and if it doesn't, then try the next simplest.

3.1.4 *Central Coulombic Potential*

If the potential energy is rotationally invariant, and thus dependent only on the distance r from a center of force, chosen as the coordinate origin, orbital angular momentum is conserved. This constant of the motion enables to reduce the three dimensional Schrödinger equation to an ordinary differential equation, the radial equation, analogous to the reduction of a central force problem in classical mechanics to a dynamical problem for the radial coordinate r alone, provided that angular momentum conservation is used and the inertial centrifugal force introduced. Probably the best known example of central potential is the attractive Coulomb potential (the one-electron atom, AKA the hydrogen atom).

The hydrogen atom, the simplest atomic system in nature, provided historically the first important test for the *quantum theory*, initially in the form of the *old quantum theory* of Bohr¹⁷ and Sommerfeld¹⁸, and subsequently for Schrödinger's, with later refinements by Dirac¹⁹ and by Feynman²⁰, Schwinger²¹ and Tomonaga²², the first owing to relativity and the second to *quantum electrodynamics*.

As a first step in the treatment of this two-particle problem that separate out the center of mass motion, after which the wave function of the relative coordinates of the electron with respect to the nucleus has to satisfy a one-particle Schrödinger equation with the reduced mass $\mu = Mm/(m + M)$, if denote the masses of the electron and the nucleus, respectively, by m and M , and the electric charged of the nucleus by Ze (allowing for the possibility of $Z \neq 1$, say, in the

¹⁷Niels Henrik David Bohr (1885-1962)

¹⁸Arnold Johannes Wilhelm Sommerfeld (1868-1951)

¹⁹Paul Adrien Maurice Dirac (1902-1984)

²⁰Richard Phillips Feynman (1918-1988)

²¹Julian Seymour Schwinger (1918-1994)

²²Shin'ichiro Tomonaga (1906-1979)

case of a helium ion):

$$-\frac{\hbar^2}{2\mu}\nabla^2\psi - \frac{Ze^2}{r}\psi = E\psi, \quad (3.1.16)$$

where the reduced mass μ of the electron differs from its actual mass by only 0.05%. The potential being rotationally invariant, next be separated out the angular dependence, writing $\psi = r^{-1}R_l(r)Y_l^m(\theta, \phi)$, so that R_l must satisfy the radial equation,

$$-R_l'' + \left[\frac{l(l+1)}{r^2} - \frac{2\mu Ze^2}{\hbar^2 r} \right] R_l = \frac{2\mu E}{\hbar^2} R_l. \quad (3.1.17)$$

The coulomb potential has two special characteristics to be recognized immediately: It is singular as r^{-1} , at infinity. The first does not cause any serious difficulties, but the slow decrease at large distance has important consequences. This physically important potential does not belong to the class (of potentials decreasing faster than r^{-2} at infinity) to which all of the mathematical statements are applicable (Newton, 2002).

3.2 Meta-Information About Calculations

In the following, we would like to present some of the mathematical based necessary details to obtain the results of the main problem. The relevant coordinate system, therefore trial wave function and finally, the variational method that relies heavily on it in the analytical calculation.

3.2.1 *On The Hylleraas Coordinates*

Hylleraas²³ in 1929 carried out a variational computation on the Schrödinger equation for the helium atom which gave, for the first time, a ground-state energy in essential agreement with experimental results. Coolidge and James in 1933 (James, & Coolidge, 1933), likewise did the first accurate computation for the hydrogen molecule. These are considered epoch-making contributions in the development of *ab initio* quantum mechanics, since they provided definitive evidence for the validity of the multiple-particle Schrödinger equation for atoms and molecules. Before then, exact solutions had been obtained only for one-electron hydrogenlike atoms. The helium and hydrogen work was done long before the advent of electronic computers and required many months of drudgery, using hand-cranked calculating machines.

The explicitly correlated Hylleraas basis set is one of the most efficient representation of a few-electron wave function. Thus while *Hylleraas coordinates* facilitate accurate calculations for the helium and lithium atoms or atomlike many partical systems, the idea of using an electron-electron distance as a coordinate is not extendable to atoms with more than two electrons. Other, special coordinates (similar to Hylleraas coordinates) used for two-electron atoms include perimetric coordinates (Hylleraas, 1964) and hyperspherical coordinates (Morse, & Feshbach, 1953).

3.2.2 *Hylleraas-Type Trial Wave Function*

The methodology of calculating of the energy states, in the many-electron case using a *Hylleraas-type trial wave function* is a variational method that introduces the correlation effects, including explicitly the interelectronic distances

²³Egil Andersen Hylleraas (1898-1965)

in the wave function. The Hylleraas-type wave functions are linear expansions of basis functions that are constructed with Slater orbitals and whose coefficients are determined variationally. The difficulties with these calculations remain essentially of the mathematical kind but are, in principle, solvable. To demonstrate this, Hylleraas began with the next problem, the helium atom. In the work (Slater, 1928), one can find Slater's early ideas concerning the introduction of the interelectronic coordinate in the coordinate wave function, but he did not develop them analytically.

To construct the wave function, Hylleraas (Hylleraas, 1928) chose the three independent variables that determine the form and the size of a triangle, r_1 , r_2 , and r_{12} , instead of r_1 and r_2 . The first Hylleraas wave function was chosen to be linear in r_{12} , instead of r_1 , r_2 , and θ , with θ being the angle between r_1 and r_2 . The first Hylleraas wave function was chosen to be linear in r_{12} and was built up with Slater orbitals. Hylleraas obtained an expression of the Hamiltonian in the coordinates r_1 , r_2 , and r_{12} by performing the derivatives of the wave function with respect to the cartesian coordinates.²⁴ In this thesis, also the chain rule of derivation will be used to transform the Hamiltonian into polar and interpartical coordinates.

A Hylleraas-type wave function expansion is (Hylleraas, 1964):

$$\psi(s, u, t) = N e^{-(1/2)s} \sum_{l,m,n} C_{l,m,n} s^l u^m t^n, \quad (3.2.1)$$

where n , m , l , are positive integers and N is a normalization constant. The results for the helium atom differed from the experiment only in the relativistic corrections and corrections due to the motion of the nucleus or nucleilike partical. However, this expansion is not a formal solution of the Schrödinger equation

²⁴To solve the eigenvalue equation, Hylleraas used the elliptic coordinates $s = r_1 + r_2$, $t = r_2 - r_1$ and $u = r_{12}$. The coordinates s , u , t satisfy the relation $s \geq u \geq |t|$.

because it does not contain negative powers of the variables s and u (Fock, 1954; Hylleraas, 1960; Bartlett et al., 1935). In the method of Kinoshita (Kinoshita, 1957, 1959) the values of the exponents of s and u are allowed to be negative. The expansion is a formal solution and can be written as:

$$\psi(s, u, t) = Ne^{-(1/2)s} \sum_{l,m,n} C_{l,m,n} s^{l-m} u^{m-n} t^n. \quad (3.2.2)$$

(3.2.2) is then a subseries with $l \geq m \geq n$. The energy differences were not significant (Hylleraas, & Midthall, 1958). Fractional values of the exponents l and m were included, improving the convergence of the Hylleraas expansion (Schwartz, 1960, 1962). As the Hylleraas wave function expansion is not a formal solution of the Schrödinger equation, one needs a larger number of terms in the wave function.

Breit (Breit, 1930) had to introduce Euler angles and polar coordinates into the wave function, to separate the eigenvalue equation in the study of P states of two-electron systems. This shows the necessity to introduce angles in the Hamiltonian in case the wave function depends on them explicitly, e.g., employing Slater orbitals.

James and Coolidge (James, & Coolidge, 1933, 1935) used a wave function depending on the elliptical coordinates of the two electrons and on r_{12} and performed the first *ab initio* calculation of molecules. They investigated the ground state of the lithium atom (James, & Coolidge, 1936) constructing the wave function as a antisymmetrized product of Slater orbitals and all interpartical distances r_{ij} .

3.2.3 Rayleigh-Ritz's Variational Method

The one state that did not fare too well with the conventional *WKB approximation* (Wentzel²⁵, Kramers²⁶, Brillouin²⁷) is, not surprisingly, the lowest energy state, which has a wave function without oscillations. Here is a method directed specifically at the state. Consider any Hamiltonian for which the spectrum is bounded below:

$$H' = E \geq E_0. \quad (3.2.3)$$

In the present circumstance, $H = p^2/(2M) + F|x|$, it is clear that $H' > 0$; there is a lowest energy state. Generally be had,

$$(H - E_0)' = E - E_0 \geq 0, \quad (3.2.4)$$

so that, for any state $|\ \rangle$, the expectation value of $H - E_0$ is positive,

$$\langle (H - E_0) \rangle = \sum_E (E - E_0)p(E) \geq 0, \quad (3.2.5)$$

where the equal sign holds only if $|\ \rangle = |H' = E_0\rangle$. Equivalently,

$$\langle H \rangle \geq E_0, \quad (3.2.6)$$

so that, for any state $|\ \rangle$, $\langle H \rangle$ provides an upper limit to E_0 . One then tries to minimize $\langle H \rangle$ to get a good value. In the quantum literature, this is known as the *Rayleigh*²⁸-*Ritz's*²⁹ *variational method*.

It's often convenient to write a normalized (real) wave function as

²⁵Gregor Wentzel (1898-1978)

²⁶Hendrik Anthony Kramers (1894-1952)

²⁷Léon Brillouin (1889-1969)

²⁸John William Strutt, AKA Lord Rayleigh (1842-1919)

²⁹Walther Ritz (1878-1909)

$\psi(x)/\sqrt{\int dx' [\psi(x')]^2}$. Here then

$$\left\langle \frac{1}{2M} p^2 + F|x| \right\rangle = \frac{\int dx \left[\frac{1}{2M} \left(-\frac{\hbar}{i} \frac{\partial}{\partial x} \psi \right) \left(\frac{\hbar}{i} \frac{\partial}{\partial x} \psi \right) + \psi F|x| \psi \right]}{\int dx \psi^2} \geq E_0. \quad (3.2.7)$$

Writing

$$x = \left(\frac{\hbar^2}{2MF} \right)^{\frac{1}{3}} q$$

and

$$E_0 = \left(\frac{\hbar^2 F^2}{2M} \right)^{\frac{1}{3}} \varepsilon_0$$

converts this into

$$\frac{\int dq \left[\left(\frac{d\psi}{dq} \right)^2 + |q| \psi^2 \right]}{\int dq \psi^2} \geq \varepsilon_0 \quad (3.2.8)$$

where the range of q is, say, $0 \rightarrow \infty$ and $(d\psi/dq)(0) = 0$.

Now we had to pick a suitable trial wave function $\psi(q)$. It should be a maximum at $q = 0$, and it must decrease rapidly for large q . Suppose try (having some knowledge of its shape)

$$\psi(q) = e^{-\frac{2}{3}\lambda q^{\frac{3}{2}}}, \quad (3.2.9)$$

where λ is an adjustable parameter. Then get

$$\frac{\int_0^{\infty} dq (\lambda^2 q + q) e^{-\frac{4}{3}\lambda q^{\frac{3}{2}}}}{\int_0^{\infty} dq e^{-\frac{4}{3}\lambda q^{\frac{3}{2}}}} \geq \varepsilon_0 \quad (3.2.10)$$

or, with

$$q = \left(\frac{3}{4\lambda}\right)^{\frac{2}{3}} s^{\frac{2}{3}}, \quad (3.2.11)$$

$$(\lambda^2 + 1) \left(\frac{3}{4\lambda}\right)^{\frac{2}{3}} \frac{\int_0^{\infty} ds s^{\frac{1}{3}} e^{-s}}{\int_0^{\infty} ds s^{-\frac{1}{3}} e^{-s}} = \left(\frac{3}{4}\right)^{\frac{2}{3}} \frac{\left(\frac{1}{3}\right)!}{\left(-\frac{1}{3}\right)!} \left(\lambda^{\frac{4}{3}} + \lambda^{-\frac{2}{3}}\right) \geq \varepsilon_0, \quad (3.2.12)$$

where $\left(\frac{1}{3}\right)! = 0.892980$, $\left(-\frac{1}{3}\right)! = 1.354118$, and $\left(\frac{1}{3}\right)! \left(-\frac{1}{3}\right)! = \frac{1}{3}\pi / \sin\left(\frac{1}{3}\pi\right) = 2\pi/3^{\frac{3}{2}}$ illustrates a property of the factorial function. Now pick λ to minimize this:

$$\frac{d}{d\lambda} \left(\lambda^{\frac{4}{3}} + \lambda^{-\frac{2}{3}}\right) = \frac{4}{3}\lambda^{\frac{1}{3}} - \frac{2}{3}\lambda^{-\frac{5}{3}} = 0 \quad (3.2.13)$$

or

$$\lambda^2 = \frac{1}{2}, \quad \lambda^{\frac{4}{3}} + \lambda^{-\frac{2}{3}} = \frac{3}{2^{\frac{2}{3}}}. \quad (3.2.14)$$

Therefore

$$\varepsilon_0 \geq \frac{3^{\frac{5}{3}}}{4} \frac{\left(\frac{1}{3}\right)!}{\left(-\frac{1}{3}\right)!} = 1.0288 \quad [= 1.0188 \times 1.0098]. \quad (3.2.15)$$

The approximation is correctly in excess and remarkably close considering the simplicity of the trial wave function. Any more general choice will yield a lower and better answer (Schwinger, 2001).

CHAPTER FOUR

ANALYTICAL SOLUTIONS

4.1 Building The System In Three Dimensions

Consider a case in which a particle (or i particles) is confined by walls to a region of space of radius \mathbf{R} . The walls are represented by a potential energy that is zero inside the region and which rises abruptly to infinity at the edges. This system is called a *three-dimensional infinite spherical QD*. The sphericity in the former name refers to the steepness with which the potential energy goes infinity at the inner surfaces of the sphere.³⁰ Because the particle is confined, its energy is quantized, and the boundary conditions determine which energies are permitted. So, essentially it is perhaps easier to deal with a finite barrier QD with spherical rather than *any other symmetry*.

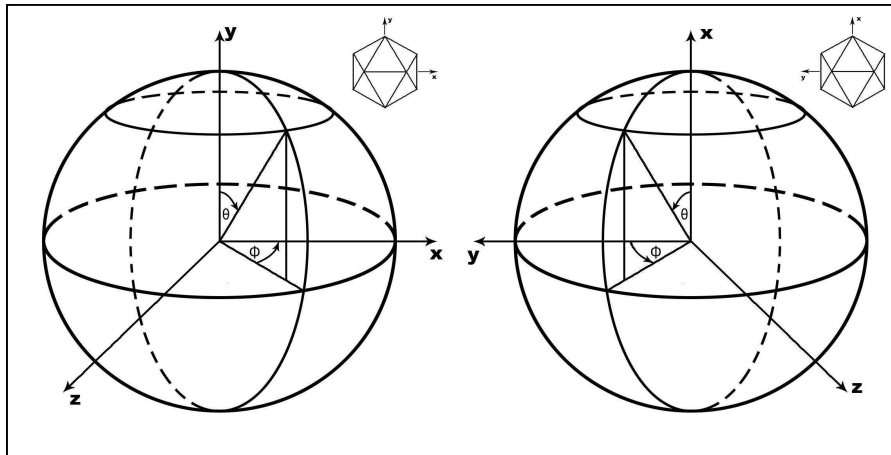


Figure 4.1 Relevant direction of the unit vectors depends on *solid angles* in three-dimensional right-handed or left-handed infinite spherical QD as mentioned above.

³⁰seen in Figure 4.1

4.1.1 An Electron In An Infinite Spherical Quantum Dot

The system which be contemplated is a particle (*as an electron*) in an three-dimensional infinite³¹ spherical QD.³² Given the spherical symmetry of the potential, then the wave function would also be expected to have spherical symmetry and the Hamiltonian for a particle could be written with a constant effective mass,

$$\mathbf{H} = \sum_i \left[-\frac{\hbar^2}{2m_i^*} \nabla_i^2 + V(\mathbf{r}_i) \right], \quad i = 1 \vee e. \quad (4.1.1)$$

Here m_i^* and \mathbf{r}_i are isotropic effective mass of i^{th} particle and position

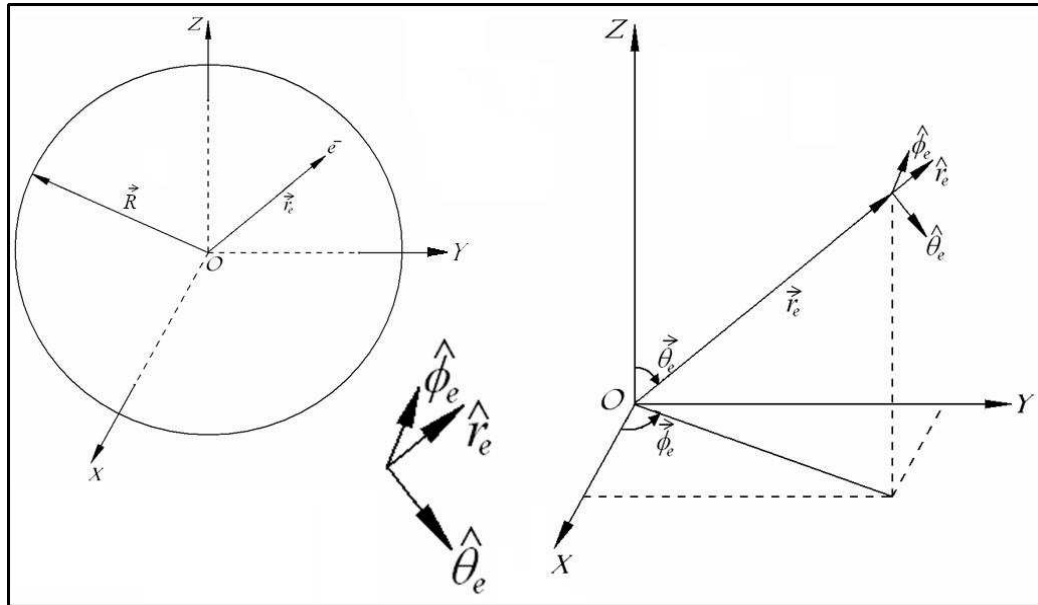


Figure 4.2 Relevant unit and position vectors in the system which contains an electron in the form of three-dimensional infinite spherical QD.

vectors. $V(\mathbf{r}_i)$ is the confinement potential with radius \mathbf{R} for the particle has been considered as spherical. The Hamiltonian in (4.1.1) includes three independent spherical coordinates. Hence the main Schrödinger equation, as be generalized

³¹in an three-dimensional *dielectric medium*

³²see in Figure 4.2

could be written,

$$\left[-\frac{\hbar}{2m^*} \nabla^2 + V(\mathbf{r}, \varphi) \right] \psi_e = E_{\mathbf{r}, \varphi} \psi_e, \quad (4.1.2)$$

and the confinement potential,

$$V(\mathbf{r}, \varphi) = \begin{cases} \infty & \text{if } |\mathbf{r}| \geq |\mathbf{R}| \\ 0 & \text{if } |\mathbf{r}| < |\mathbf{R}| \end{cases}.$$

Essentially $\psi(\mathbf{r}, \varphi)$ is spherical symmetric wave function depends on relevant three independent coordinates are made up of two parts as radial $R(\mathbf{r})$, and as spherical $Y(\varphi)$. So that the form of the wave function is,

$$\psi_e(\mathbf{r}, \varphi) = R(\mathbf{r})Y(\varphi). \quad (4.1.3)$$

The square of the operator del in spherical polar coordinates in the form of

$$\nabla^2 = \frac{1}{r^2} \frac{\partial}{\partial r} \left(r^2 \frac{\partial}{\partial r} \right) + \frac{1}{r^2 \sin \theta} \frac{\partial}{\partial \theta} \left(\sin \theta \frac{\partial}{\partial \theta} \right) + \frac{1}{r^2 \sin^2 \theta} \frac{\partial^2}{\partial \phi^2}. \quad (4.1.4)$$

Inserting (4.1.3) and (4.1.4) into the main Schrödinger equation in (4.1.2) yields with *Spherical Harmonics* $Y(\varphi)$ cause rotational symmetry of the Hamiltonian,

$$Y(\varphi) \left[\frac{1}{r^2} \frac{\partial}{\partial r} \left(r^2 \frac{\partial}{\partial r} \right) \right] R(r) + R(r) \left[\frac{1}{r^2 \sin \theta} \frac{\partial}{\partial \theta} \left(\sin \theta \frac{\partial}{\partial \theta} \right) + \frac{1}{r^2 \sin^2 \theta} \frac{\partial^2}{\partial \phi^2} \right] \times Y(\varphi) + R(r)Y(\varphi) \left[\frac{2m^* E_{r, \varphi}}{\hbar^2} \right] = 0,$$

then rewriting

$$\frac{1}{R(r)} \left[\frac{\partial}{\partial r} \left(r^2 \frac{\partial}{\partial r} \right) \right] R(r) + \frac{2m^* E_r}{\hbar^2} r^2 = -\frac{1}{Y(\varphi)} \times \left[\frac{1}{\sin \theta} \frac{\partial}{\partial \theta} \left(\sin \theta \frac{\partial}{\partial \theta} \right) + \frac{1}{\sin^2 \theta} \frac{\partial^2}{\partial \phi^2} \right] Y(\varphi). \quad (4.1.5)$$

Where the index on E_r has been added just indicate that this energy is associated with the confinement along the radius. Presetting both sides of the (4.1.5) a

constant like Λ gives two differential equations,

$$\frac{1}{R(r)} \left[\frac{d}{dr} \left(r^2 \frac{d}{dr} \right) \right] R(r) + \frac{2m^* E_r}{\hbar^2} r^2 = \Lambda \quad (4.1.6a)$$

$$-\frac{1}{Y(\varphi)} \left[\frac{1}{\sin \theta} \frac{\partial}{\partial \theta} \left(\sin \theta \frac{\partial}{\partial \theta} \right) + \frac{1}{\sin^2 \theta} \frac{\partial^2}{\partial \phi^2} \right] Y(\varphi) = \Lambda \quad (4.1.6b)$$

$$\left[\frac{d}{dr} \left(r^2 \frac{d}{dr} \right) \right] R(r) + \left[\frac{2m^* E_r}{\hbar^2} r^2 - \Lambda \right] R(r) = 0 \quad (4.1.7a)$$

$$\left[\frac{1}{\sin \theta} \frac{\partial}{\partial \theta} \left(\sin \theta \frac{\partial}{\partial \theta} \right) + \frac{1}{\sin^2 \theta} \frac{\partial^2}{\partial \phi^2} \right] Y(\varphi) + [\Lambda] Y(\varphi) = 0 \quad (4.1.7b)$$

In actual fact, the spherical part of the wave function $Y(\varphi)$ is made up of two independent coordinates too. As, $\Theta(\theta)$ and $\Phi(\phi)$. The notation is chosen in the form of

$$Y(\varphi) = \Theta(\theta)\Phi(\phi).$$

By using this form, (4.1.7b) becomes,

$$\frac{1}{\Phi(\phi)} \left[\frac{\partial^2}{\partial \phi^2} \right] \Phi(\phi) = \frac{1}{\Theta(\theta)} \left[\sin \theta \frac{\partial}{\partial \theta} \left(\sin \theta \frac{\partial}{\partial \theta} \right) \right] \Theta(\theta) + \Lambda \sin^2 \theta \quad (4.1.8)$$

then assigning with some pre-cognition both sides again a constant like m_l^2 gives two new independent *subODEs*³³,

$$\frac{1}{\Phi(\phi)} \left[\frac{d^2}{d\phi^2} \right] \Phi(\phi) = m_l^2 \quad (4.1.9a)$$

$$\frac{1}{\Theta(\theta)} \left[\sin \theta \frac{d}{d\theta} \left(\sin \theta \frac{d}{d\theta} \right) \right] \Theta(\theta) + \Lambda \sin^2 \theta = m_l^2 \quad (4.1.9b)$$

$$\left[\frac{d^2}{d\phi^2} \right] \Phi(\phi) + [m_l^2] \Phi(\phi) = 0 \quad (4.1.10a)$$

$$\left[\sin \theta \frac{d}{d\theta} \left(\sin \theta \frac{d}{d\theta} \right) \right] \Theta(\theta) + \left[\Lambda - \frac{m_l^2}{\sin^2 \theta} \right] \Theta(\theta) = 0. \quad (4.1.10b)$$

³³sub Ordinary differential equations

Table 4.1 The cases for the equation which comes the spherical part, depends on θ of the main Schödinger equation.

Case	Equation	Solution
$m_l = 0$	Legendre ODE	Legendre Polynomials
$m_l \neq 0$	General Legendre ODE	Associated Legendre Polynomials

Phenomenologically (4.1.10a) is similar with *the harmonic oscillator*³⁴ and the solution of this equation³⁵,

$$\Phi_{m_l}(\phi) = A_l \exp(im_l\phi), \quad m_l = 0, \pm 1, \pm 2, \pm 3, \dots \quad (4.1.11)$$

Defining a new parameter $\mu = \cos \theta$ and then with relevant mapping (4.1.10b) becomes,

$$\begin{aligned} \left[(1 - \mu^2) \frac{d^2}{d\mu^2} \right] \Theta(\arccos \mu) - \left[2\mu \frac{d}{d\mu} \right] \Theta(\arccos \mu) \\ + \left[\Lambda - \frac{m_l^2}{(1 - \mu^2)} \right] \Theta(\arccos \mu) = 0. \end{aligned} \quad (4.1.12)$$

There exist two case as is seen from (4.1). In mathematics, the *Associated Legendre*³⁶ *Polynomials* are the canonical solutions of the *General Legendre ODE*. Since the Legendre ODE is a second-order ordinary differential equation, it has two linearly independent solutions. Thus, for the stationary state $m_l = 0$ rewriting (4.1.12) in the form,

$$\left[(1 - \mu^2) \frac{d^2}{d\mu^2} \right] P_l(\mu) - \left[2\mu \frac{d}{d\mu} \right] P_l(\mu) + [\Lambda] P_l(\mu) = 0. \quad (4.1.13)$$

As mentioned above, this equation is The Legendre ODE where, $P_l(\mu)$ is Legendre

³⁴The harmonic oscillator differential equation generally in the form of $x'' + a_0x = 0$.

³⁵see in Appendix for values of *magnetic quantum number* m_l

³⁶Adrien-Marie Legendre (1752-1833)

Polynomials. So, the solution of the (4.1.10b) is³⁷,

$$\Theta_l(\theta) = B_l P_l^{m_l}(\cos \theta), \quad l = 0, 1, 2, 3, \dots \quad (4.1.14)$$

Then the total solution of the spherical part which is called Spherical Harmonics as mentioned above,

$$Y_l^{m_l}(\varphi) = N_{l,m_l} P_l^{m_l}(\cos \theta) \exp(im_l \phi), \quad \begin{cases} l & = 0, 1, 2, 3, \dots \\ m_l & = -l, \dots, l \end{cases} \quad (4.1.15)$$

where N_{l,m_l} is the normalization coefficient. For normalization this spherical part in all space,

$$\int_0^\pi \int_0^{2\pi} d\tau_\varphi |Y_l^{m_l}(\varphi)|^2 = 1, \quad (d\tau_\varphi = \sin \theta d\theta d\phi) \quad (4.1.16)$$

$$\implies N_{l,m_l} = (-1)^{m_l} \left[\frac{2l+1}{4\pi} \frac{(l-|m_l|)!}{(l+|m_l|)!} \right]^{1/2}. \quad (4.1.17)$$

The solution to the above radial part of the main Schrödinger equation, by reorganizing (4.1.7a), defining new parameters $\Lambda = n(n+1)$, $k^2 = 2m^*E/\hbar^2$, $\rho = kr$ and substituting³⁸,

$$\left[2r \frac{d}{dr} + r^2 \frac{d^2}{dr^2} \right] R(r) + [k^2 r^2 - n(n+1)] R(r) = 0. \quad (4.1.18)$$

These new definitions lead to dimensionless radial equation of the system to be

$$\left[\rho^2 \frac{d^2}{d\rho^2} \right] R_n + [2\rho^2] R_n + [\rho^2 - n(n+1)] R_n = 0. \quad (4.1.19)$$

³⁷see in Appendix for *series solution of Legendre ODE*

³⁸seen in Appendix for *scaling*

To convert (4.1.19) to the Standard Bessel's³⁹ ODE⁴⁰ with (4.1.20),

$$R_n = U(\rho)/(\rho^{1/2}) \quad (4.1.20)$$

$$\rho(\rho U'(\rho))' + [\rho^2 - v^2] U(\rho) = 0. \quad (4.1.21)$$

(4.1.21) is the Standard Bessel's ODE and arises when finding separable solutions to Laplace's⁴¹ equation and the Helmholtz⁴² equation in cylindrical or spherical coordinates. Since this is a second-order ODE, there must be two linearly independent solutions.⁴³ Solution includes Bessel functions but it is not the solution of the original radial equation. By inverse mapping,

$$U(\rho) = J_v(\rho),$$

$$R_n = \left(\frac{1}{\rho}\right)^{1/2} J_v(\rho),$$

$$R_n = \left(\frac{1}{\rho}\right)^{1/2} J_{n+1/2}(\rho), \quad J_{n+1/2}(\rho) = \left(\frac{2}{\pi}\right)^{1/2} J_n(\rho),$$

$$\implies R_n = \left(\frac{2}{\pi\rho}\right)^{1/2} J_n(\rho).$$

Depending upon the circumstances, however, various formulations of these solutions are convenient, and the different variations are described below. Bessel functions of the first kind, denoted as $J_v(\rho)$, are solutions of Bessel's ODE that are finite at the origin⁴⁴ for non-negative integer v , and diverge as ρ approaches zero for negative non-integer v . With a normalization coefficient,

$$R_n = C_n \left(\frac{2}{\pi\rho}\right)^{1/2} J_n(\rho), \quad n = s, p, d, \dots \quad (4.1.22)$$

³⁹Friedrich Wilhelm Bessel (1784-1846)

⁴⁰see in Appendix for the relevant transformation

⁴¹Pierre-Simon, marquis de Laplace (1749-1827)

⁴²Hermann Ludwig Ferdinand von Helmholtz (1821-1894)

⁴³see in Appendix for *series solution of Standard Bessel's ODE*

⁴⁴ $\rho = 0$

As a result the solution of the radial part obviously,

$$R_n = C_n \left(\frac{2}{\pi\rho} \right)^{1/2} \left[\left(\frac{\rho}{2} \right)^n \sum_{p=0}^{\infty} \frac{(-1)^p}{p! \Gamma(n+p+1)} \left(\frac{\rho}{2} \right)^{2p} \right] \quad (4.1.23)$$

As a natural consequence, the corresponding result for the total wave function which is solution of the main Schrödinger equation of relevant system in (4.1.2) can be obtained by permuting the (4.1.22) and (4.1.15), in the form of

$$\psi(r, \theta\phi)_{n,l,m_l} = R_n(r) Y_l^{m_l}(\theta, \phi) = R_n(r) \Theta_l(\theta) \Phi_{m_l}(\phi), \quad (4.1.24)$$

$$\psi(r, \theta\phi)_{n,l,m_l} = C_n N_{l,m_l} \left(\frac{2}{\pi\rho} \right)^{1/2} J_n(\rho) P_l^{m_l}(\cos\theta) \exp(im_l\phi). \quad (4.1.25)$$

Accordingly the boundary condition,

$$\psi(r = |\mathbf{R}|, \theta, \phi) = \underbrace{R_n(r = |\mathbf{R}|)}_0 Y_l^{m_l}(\theta, \phi) = 0$$

so,

$$R(r = |\mathbf{R}|) = C_n \left(\frac{2}{\pi\rho} \right)^{1/2} J_n(\rho) = 0, \quad \text{iff} \quad J_n(k|\mathbf{R}|) = 0.$$

Hence, be obtained infinite solutions from these which will be independent, apart, possibly, from the case when all roots differ by an integer, i.e., when n is an integer. As the stationary state for a particle ($i = 1$, be mentioned above) the ground state energy (*for an electron* $i = e$ and in the index e , in another statement) be generated from the Bessel's function's first root.⁴⁵ For each Bessel's function which has relevant index,

$$k_{e_n,l} |\mathbf{R}| = \rho_{e_n,l}$$

$$E_{e_n,l} = \frac{\hbar^2 k_{e_n,l}^2}{2m_e} = \frac{\hbar^2}{2m_e |\mathbf{R}|^2} \rho_{e_n,l}^2 \quad (4.1.26)$$

⁴⁵see in Figure 4.3

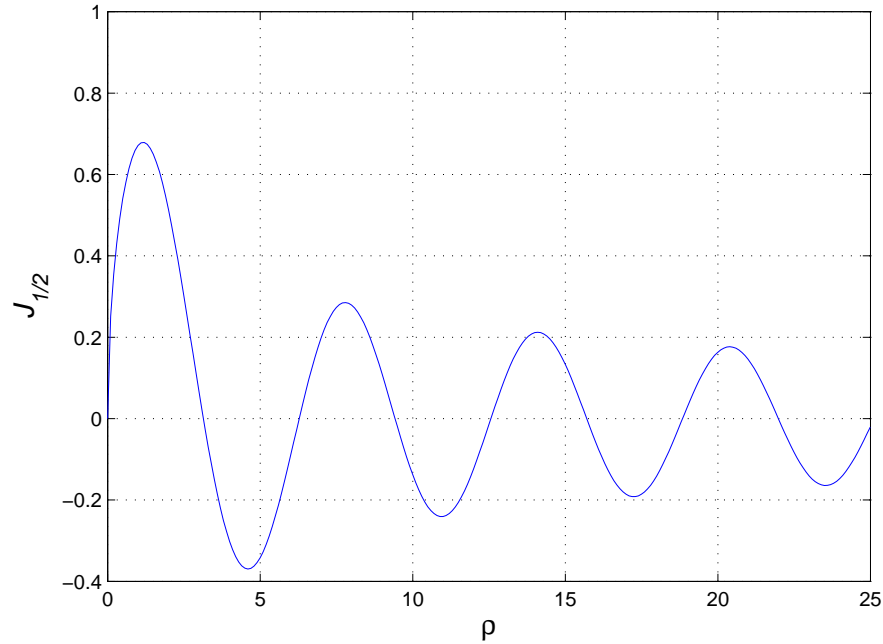


Figure 4.3 Plot of Bessel's function of the first kind for $n = 1/2$.

As control, radial ODE in (4.1.18) transform to the one-dimensional Schrödinger equation for S -ground states and then wave number for the solutions of well as n is the positive set of zahlen,

$$k_{e_{n,l}}|\mathbf{R}| = n\pi, \quad n \in \mathbb{Z}^+. \quad (4.1.27)$$

In this case, the *orbitals* be formed on integer order of π .

4.1.2 An Exciton In An Infinite Spherical Quantum Dot

In nonrelativistic classical mechanics the motion of two-body system with a central interaction separates into the free motion of the center of mass and the motion of a single fictitious particle in a central field. The same simplification holds in quantum mechanics. The problem is then reduced to finding the eigenvalues and eigenfunctions for the radial motion of one

particle in a central field, because the angular eigenfunctions are already known from *the theory of orbital angular momentum*. In short, what is called *separation of variables* in the theory of differential equations is done by exploiting the symmetry of the problem (Gottfried, & Tung-Mow, 2008).

Within the framework the effective mass Hamiltonian for an interacting pair of two particles (*as an electron and a hole*) confined in a QD by an infinite potential⁴⁶ is given as

$$\mathbf{H} = \sum_i \left[-\frac{\hbar^2}{2m_i^*} \nabla_i^2 + V(\mathbf{r}_i) \right] + \frac{ZQ^2}{r_{12}}, \quad i = 1, 2 \vee e, h. \quad (4.1.28)$$

Here m_i^* and \mathbf{r}_i are isotropic effective mass of i^{th} particle and position vec-

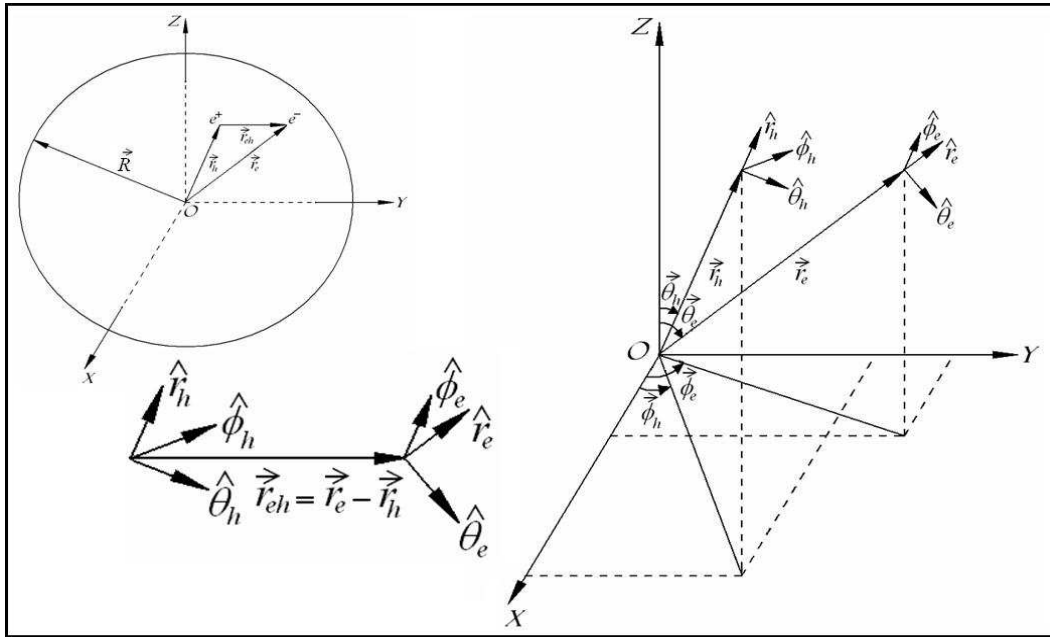


Figure 4.4 Relevant unit and position vectors in the system which contains an electron and a hole in the form of three-dimensional infinite spherical QD.

tors. $V(\mathbf{r}_i)$ is the confinement potential with radius \mathbf{R} for the particle has been considered as spherical. In a condition of ϵ is the dielectric constant of the medium where the particles move, $Z = 1/4\pi\epsilon$. Q is the charge of each particles and it's

⁴⁶see in Figure 4.4

value is $-e$ for an electron e for a hole. The location of each particle, with effective mass m_i^* , relative to the center of QD is labeled by \mathbf{r}_i for the first and second particle, respectively (Şakiroğlu, 2009). In order to express the Hamiltonian dimensionless form, by defining new parameters, $\mu = 1/(m_e^{*-1} + m_h^{*-1})$ as the reduced effective mass, $\sigma_i = m_i^*/\mu$ as the dimensionless effective mass of electron ($i = e$) and hole ($i = h$), be chosen effective Bohr radius $a^* = 4\pi\epsilon\hbar^2/\mu e^2$ as the length scale and effective Hartree⁴⁷ energy $E_H^* = \hbar^2/\mu a^{*2}$ as the energy scale be obtained the dimensionless form of the Hamiltonian in (4.1.28),

$$\tilde{\mathbf{H}} = \sum_i \left[-\frac{1}{2\sigma_i} \nabla_{\tilde{r}_i}^2 + \tilde{V}(\tilde{r}_i) \right] - \frac{1}{\tilde{r}_{eh}}, \quad i = e, h, \quad (4.1.29)$$

where $\tilde{V}(\tilde{r}_i)$ and \tilde{r}_i ($i = e, h$) is dimensionless confinement potential and dimensionless coordinates respectively. \tilde{r}_{eh} represents the dimensionless interparticle distance. The Hamiltonian in (4.1.29) includes six independent spherical coordinates. Hence the main Schrödinger equation, as be generalized could be written,

$$\left[-\frac{1}{2\sigma_e} \nabla_{\tilde{r}_e}^2 - \frac{1}{2\sigma_h} \nabla_{\tilde{r}_h}^2 + \tilde{V}(\tilde{r}_e) + \tilde{V}(\tilde{r}_h) - \frac{1}{\tilde{r}_{eh}} \right] \psi_X = \tilde{E}_X \psi_X, \quad (4.1.30)$$

and the confinement potential,

$$V(\tilde{r}_i) = \begin{cases} \infty & \text{if } \tilde{r}_i \geq |\mathbf{R}| \\ 0 & \text{if } \tilde{r}_i < |\mathbf{R}| \end{cases}, \quad i = e, h.$$

Using Hylleraas coordinate system which explicitly includes \tilde{r}_{eh} interparticle distance is very convinient for this problem (Kayanuma, 1988). One of the most important point in the variational works on two electron systems is the choice of appropriate wave function (Aquino et al., 2006). In the light of this information, ansatz for wave function describing the ground state of the electron-hole QD

⁴⁷Douglas Rayner Hartree (1897-1958)

confined by spherical potential is chosen in the form of,

$$\psi_X(\tilde{r}_e, \tilde{r}_h, \tilde{r}_{eh}, \Omega_e, \Omega_h; \lambda) = \psi_e^S(\tilde{r}_e, \Omega_e) \psi_h^S(\tilde{r}_h, \Omega_h) F(\tilde{r}_{eh}; \lambda), \quad (4.1.31)$$

where $\psi_e^S(\tilde{r}_e, \Omega_e)$, $\psi_h^S(\tilde{r}_h, \Omega_h)$ are independent S -type wave functions belonging to an electron and a hole respectively. $F(\tilde{r}_{eh}; \lambda)$ term is hydrogenic binding function which contains variation parameter λ and obviously with a normalization coefficient,

$$F(\tilde{r}_{eh}; \lambda) = N_b \exp(-\lambda \tilde{r}_{eh}). \quad (4.1.32)$$

For potentials that fall off faster than a Coulomb field, bound-state radial wave functions for any angular momentum have the universal asymptotic form of an exponential decrease determined solely by the binding energy. As mentioned S -type wave functions separately,

$$\psi_e^S(\tilde{r}_e, \Omega_e) = R_{n_e, l_e=0}(\tilde{r}_e) Y_{l_e=0, m_{l_e}=0}(\Omega_e) \quad (4.1.33a)$$

$$\psi_h^S(\tilde{r}_h, \Omega_h) = R_{n_h, l_h=0}(\tilde{r}_h) Y_{l_h=0, m_{l_h}=0}(\Omega_h). \quad (4.1.33b)$$

The wave function expanded in terms of generalized Hylleraas basis set has been used in variational treatment of three-body Coulomb systems with optimization techniques chosen according to the desired accuracy (Aquino et al., 2006). Using the definition of operator nabla expressed in Hylleraas-type coordinates as

$$\nabla_i = \hat{r}_i \frac{\partial}{\partial \tilde{r}_i} + \sum_{j \neq i} \hat{r}_{ij} \frac{\partial}{\partial \tilde{r}_{ij}} \quad (4.1.34)$$

general procedure for the coulombic interaction potential $-1/\tilde{r}_{eh}$,

$$\tilde{\mathbf{r}}_{eh} = \tilde{\mathbf{r}}_e - \tilde{\mathbf{r}}_h, \quad (4.1.35)$$

$$\tilde{r}_{eh}^2 = (\tilde{\mathbf{r}}_e - \tilde{\mathbf{r}}_h)^2 = \tilde{r}_e^2 + \tilde{r}_h^2 - 2\tilde{\mathbf{r}}_e \tilde{\mathbf{r}}_h, \quad (4.1.36)$$

$$\tilde{\mathbf{r}}_{eh}^2 - \tilde{\mathbf{r}}_e^2 - \tilde{\mathbf{r}}_h^2 = -2\tilde{\mathbf{r}}_e\tilde{\mathbf{r}}_h, \quad (4.1.37)$$

$$\tilde{\mathbf{r}}_e\tilde{\mathbf{r}}_h = \frac{1}{2}(\tilde{\mathbf{r}}_e^2 + \tilde{\mathbf{r}}_h^2 - \tilde{\mathbf{r}}_{eh}^2), \quad (4.1.38)$$

$$\hat{r}_e\hat{r}_{eh} = \frac{\tilde{\mathbf{r}}_e\tilde{\mathbf{r}}_e - \tilde{\mathbf{r}}_h}{\tilde{r}_e\tilde{r}_{eh}} = \frac{\tilde{\mathbf{r}}_e^2 - \tilde{\mathbf{r}}_e\tilde{\mathbf{r}}_h}{\tilde{\mathbf{r}}_e\tilde{\mathbf{r}}_{eh}}, \quad (4.1.39a)$$

$$\hat{r}_h\hat{r}_{eh} = \frac{\tilde{\mathbf{r}}_h\tilde{\mathbf{r}}_e - \tilde{\mathbf{r}}_h}{\tilde{r}_h\tilde{r}_{eh}} = \frac{\tilde{\mathbf{r}}_e\tilde{\mathbf{r}}_h - \tilde{\mathbf{r}}_e^2}{\tilde{\mathbf{r}}_h\tilde{\mathbf{r}}_{eh}}. \quad (4.1.39b)$$

By inserting (4.1.38) into (4.1.39a) and (4.1.39b) in relevant site respectively,

$$\hat{r}_e\hat{r}_{eh} = \frac{\tilde{\mathbf{r}}_e^2 - 1/2(\tilde{\mathbf{r}}_e^2 + \tilde{\mathbf{r}}_h^2)}{\tilde{\mathbf{r}}_e\tilde{\mathbf{r}}_{eh}} = \frac{\tilde{\mathbf{r}}_e^2 - \tilde{\mathbf{r}}_h^2 + \tilde{\mathbf{r}}_{eh}^2}{2\tilde{\mathbf{r}}_e\tilde{\mathbf{r}}_{eh}}, \quad (4.1.40a)$$

$$\hat{r}_h\hat{r}_{eh} = \frac{1/2(\tilde{\mathbf{r}}_e^2 + \tilde{\mathbf{r}}_h^2) - \tilde{\mathbf{r}}_h^2}{\tilde{\mathbf{r}}_h\tilde{\mathbf{r}}_{eh}} = \frac{\tilde{\mathbf{r}}_h^2 - \tilde{\mathbf{r}}_e^2 + \tilde{\mathbf{r}}_{eh}^2}{2\tilde{\mathbf{r}}_h\tilde{\mathbf{r}}_{eh}}. \quad (4.1.40b)$$

Then the terms in left hand side of the Schrödinger equation⁴⁸ in (4.1.30),

$$\begin{aligned} \tilde{\mathbf{H}} &= \\ &- \psi_h^S \frac{1}{2\sigma_e} \left[F \nabla_e^2 \psi_e^S + 2 \left(\frac{\tilde{r}_e^2 - \tilde{r}_h^2 + \tilde{r}_{eh}^2}{2\tilde{r}_e\tilde{r}_{eh}} \right) \left(\frac{\partial^2}{\partial \tilde{r}_e \partial \tilde{r}_{eh}} \right) \psi_e^S F + F \left(\frac{2}{\tilde{r}_e} \frac{\partial}{\partial \tilde{r}_e} + \frac{\partial^2}{\partial \tilde{r}_e^2} \right) \psi_e^S \right] \\ &+ \psi_h^S \left[\tilde{V}_c^e(\tilde{r}_e) \right] \psi_e^S F \\ &- \psi_e^S \frac{1}{2\sigma_h} \left[F \nabla_h^2 \psi_h^S + 2 \left(\frac{\tilde{r}_h^2 - \tilde{r}_e^2 + \tilde{r}_{eh}^2}{2\tilde{r}_h\tilde{r}_{eh}} \right) \left(\frac{\partial^2}{\partial \tilde{r}_h \partial \tilde{r}_{eh}} \right) \psi_h^S F + F \left(\frac{2}{\tilde{r}_h} \frac{\partial}{\partial \tilde{r}_h} + \frac{\partial^2}{\partial \tilde{r}_h^2} \right) \psi_h^S \right] \\ &+ \psi_e^S \left[\tilde{V}_c^h(\tilde{r}_h) \right] \psi_h^S F \\ &- \left[\frac{1}{\tilde{r}_{eh}} \right] \psi_e^S \psi_h^S F \\ &= \tilde{E}_X \psi_e^S \psi_h^S F \end{aligned} \quad (4.1.41)$$

The square of the radial part of the the operators del in spherical polar coordinates which appertain to electron and hole respectively in the form of,

$$\nabla_{e\tilde{r}_e}^2 = \frac{1}{\tilde{r}_e} \frac{\partial}{\partial \tilde{r}_e} \left(\tilde{r}_e^2 \frac{\partial}{\partial \tilde{r}_e} \right) \quad (4.1.42a)$$

$$\nabla_{h\tilde{r}_h}^2 = \frac{1}{\tilde{r}_h} \frac{\partial}{\partial \tilde{r}_h} \left(\tilde{r}_h^2 \frac{\partial}{\partial \tilde{r}_h} \right). \quad (4.1.42b)$$

⁴⁸see in Appendix for internal operations

Thus the terms of the Hamiltonian in (4.1.41) clearly without wave functions,

$$\begin{aligned}
& \blacksquare - \frac{1}{2\sigma_e} \left[\frac{1}{\tilde{r}_e} \left(2\tilde{r}_e \frac{\partial}{\partial \tilde{r}_e} + \tilde{r}_e^2 \frac{\partial^2}{\partial \tilde{r}_e^2} \right) + \left(\frac{\tilde{r}_e^2 - \tilde{r}_h^2 + \tilde{r}_{eh}^2}{2\tilde{r}_e \tilde{r}_{eh}} \right) \left(\frac{\partial^2}{\partial \tilde{r}_e \partial \tilde{r}_{eh}} \right) + \left(\frac{2}{\tilde{r}_e} \frac{\partial}{\partial \tilde{r}_e} + \frac{\partial^2}{\partial \tilde{r}_e^2} \right) \right], \\
& \blacksquare \tilde{V}_c^e(\tilde{r}_e), \\
& \blacksquare - \frac{1}{2\sigma_h} \left[\frac{1}{\tilde{r}_h} \left(2\tilde{r}_h \frac{\partial}{\partial \tilde{r}_h} + \tilde{r}_h^2 \frac{\partial^2}{\partial \tilde{r}_h^2} \right) + \left(\frac{\tilde{r}_h^2 - \tilde{r}_e^2 + \tilde{r}_{eh}^2}{2\tilde{r}_h \tilde{r}_{eh}} \right) \left(\frac{\partial^2}{\partial \tilde{r}_h \partial \tilde{r}_{eh}} \right) + \left(\frac{2}{\tilde{r}_h} \frac{\partial}{\partial \tilde{r}_h} + \frac{\partial^2}{\partial \tilde{r}_h^2} \right) \right], \\
& \blacksquare \tilde{V}_c^h(\tilde{r}_h), \\
& \blacksquare - \frac{1}{\tilde{r}_{eh}}.
\end{aligned} \tag{4.1.43}$$

Again, by taking a look to the total wave function's $\psi_X(\tilde{r}_e, \tilde{r}_h, \tilde{r}_{eh}, \Omega_e, \Omega_h; \lambda)$ parts with appropriate normalization coefficients obviously,

$$\begin{aligned}
& \blacksquare \psi_e^S(\tilde{r}_e, \Omega_e) = N_e R_{n_e, l_e=0}(\tilde{r}_e) Y_{l_e=0, m_{l_e}=0}(\Omega_e), \\
& \blacksquare \psi_h^S(\tilde{r}_h, \Omega_h) = N_h R_{n_h, l_h=0}(\tilde{r}_h) Y_{l_h=0, m_{l_h}=0}(\Omega_h), \\
& \blacksquare F(\tilde{r}_{eh}; \lambda) = N_b \exp(-\lambda \tilde{r}_{eh}).
\end{aligned} \tag{4.1.44}$$

$$\psi_X(\tilde{r}_e, \tilde{r}_h, \tilde{r}_{eh}, \Omega_e, \Omega_h; \lambda) = \underbrace{N_e N_h N_b}_{N_T} R_e(\tilde{r}_e) Y_e(\Omega_e) R_h(\tilde{r}_h) Y_h(\Omega_h) \exp(-\lambda \tilde{r}_{eh})$$

Hence the total wave function with a *total normalization coefficient*,

$$\psi_X(\tilde{r}_e, \tilde{r}_h, \tilde{r}_{eh}, \Omega_e, \Omega_h; \lambda) = N_T R_e(\tilde{r}_e) Y_e(\Omega_e) R_h(\tilde{r}_h) Y_h(\Omega_h) \exp(-\lambda \tilde{r}_{eh}). \tag{4.1.45}$$

The procedure for evaluation of integrals in order to determine ground state energy by using the Rayleigh-Ritz's variational method. In this method, as mentioned above in a system's which is in *any state*, for Hamiltonian's expected value, always could be written accurately this inequality,

$$\tilde{E}_X = \langle \tilde{\mathbf{H}}_X \rangle = \frac{\langle \psi_X | \tilde{\mathbf{H}}_X | \psi_X \rangle}{\langle \psi_X | \psi_X \rangle} \geq \tilde{E}_{X_0}. \tag{4.1.46}$$

The nonlinear variation parameter λ in the wave function are defined to minimize

the expected value of the energy:

$$\tilde{E}_X(\lambda) = \frac{\langle \psi_X | \tilde{\mathbf{H}}_X | \psi_X \rangle}{\langle \psi_X | \psi_X \rangle}. \quad (4.1.47)$$

Optimization with respect to variation parameter,

$$\frac{\partial \tilde{E}_X(\lambda)}{\partial \lambda} = 0 \quad (4.1.48)$$

and by getting *the optimum* λ_0 value from (4.1.48) yields the exact numerical ground state energy of the system in the form of

$$\tilde{E}_{X_0} = \tilde{E}_X(\lambda_0). \quad (4.1.49)$$

The asymptotic form of the continuum states also depends on whether the condition in (4.1.32) is met. In the work (Şakiroğlu et al., 2009), Fourier transforms have been used for the terms including interparticle distance \tilde{r}_{eh} . The Fourier transform for three-dimensional spherical QD are defined as (Deb, 1994; Bhattacharyya et al., 1994),

$$\frac{\exp(-\tilde{r}_{eh}\lambda)}{\tilde{r}_{eh}} = \frac{2}{(2\pi)^2} \int d\mathbf{q} \frac{\exp(i\mathbf{q} \cdot \tilde{\mathbf{r}}_{eh})}{(q^2 + \lambda^2)^2}. \quad (4.1.50)$$

By taking the derivative both sides for λ ,

$$\begin{aligned} \frac{\partial}{\partial \lambda} \frac{\exp(-\tilde{r}_{eh}\lambda)}{\tilde{r}_{eh}} &= \frac{2}{(2\pi)^2} \frac{\partial}{\partial \lambda} \int d\mathbf{q} \frac{\exp(i\mathbf{q} \cdot \tilde{\mathbf{r}}_{eh})}{(q^2 + \lambda^2)^2}, \\ -\exp(-\tilde{r}_{eh}\lambda) &= \frac{2}{(2\pi)^2} \int \frac{\partial}{\partial \lambda} d\mathbf{q} \frac{\exp(i\mathbf{q} \cdot \tilde{\mathbf{r}}_{eh})}{(q^2 + \lambda^2)^2}, \\ -\exp(-\tilde{r}_{eh}\lambda) &= \frac{2}{(2\pi)^2} \int d\mathbf{q} \frac{2\lambda \exp(i\mathbf{q} \cdot \tilde{\mathbf{r}}_{eh})}{(q^2 + \lambda^2)^2}. \end{aligned} \quad (4.1.51)$$

For $\lambda \longrightarrow 2\lambda$ (4.1.51) becomes,

$$-\exp(-2\tilde{r}_{eh}\lambda) = \frac{2}{(2\pi)^2} \int d\mathbf{q} \frac{4\lambda \exp(i\mathbf{q} \cdot \tilde{\mathbf{r}}_{eh})}{(q^2 + 4\lambda^2)^2}, \quad (4.1.52)$$

and

$$-\exp(-2\tilde{r}_{eh}\lambda) = \frac{2}{(2\pi)^2} \int d\mathbf{q} \frac{4\lambda}{(q^2 + 4\lambda^2)^2} (\exp(i\mathbf{q} \cdot \tilde{\mathbf{r}}_e) \exp(i\mathbf{q} \cdot \tilde{\mathbf{r}}_h)). \quad (4.1.53)$$

In the references (Brandsen, & Joachain, 2000; Arfken, & Weber, 2005), according to Jacobi-Anger expansion for $\tilde{\mathbf{r}}_e$ ve $\tilde{\mathbf{r}}_h$ plane wave's exponential statements's may be expanded in a series of cylindrical waves and with Spherical Harmonics in the form of,

$$\exp(i\mathbf{q} \cdot \tilde{\mathbf{r}}_e) = 4\pi \sum_{l'_e=0}^{\infty} (i)^{l'_e} J_{l'_e}(\mathbf{q} \cdot \tilde{\mathbf{r}}_e) \sum_{m_{l'_e}=-l'_e}^{l'_e} Y_{l'_e, m_{l'_e}}^*(\Omega_{\mathbf{q}}) Y_{l'_e, m_{l'_e}}(\Omega_e), \quad (4.1.54a)$$

$$\exp(i\mathbf{q} \cdot \tilde{\mathbf{r}}_h) = 4\pi \sum_{l'_h=0}^{\infty} (-i)^{l'_h} J_{l'_h}(\mathbf{q} \cdot \tilde{\mathbf{r}}_h) \sum_{m_{l'_h}=-l'_h}^{l'_h} Y_{l'_h, m_{l'_h}}(\Omega_{\mathbf{q}}) Y_{l'_h, m_{l'_h}}^*(\Omega_h). \quad (4.1.54b)$$

Insert (4.1.54a) and (4.1.54b) into the (4.1.53),

$$\begin{aligned} -\exp(-2\tilde{r}_{eh}\lambda) &= \frac{2}{(2\pi)^2} \int d\mathbf{q} \frac{4\lambda}{(q^2+4\lambda^2)^2} \\ &\times 4\pi \sum_{l'_e=0}^{\infty} (i)^{l'_e} J_{l'_e}(\mathbf{q} \cdot \tilde{\mathbf{r}}_e) \sum_{m_{l'_e}=-l'_e}^{l'_e} Y_{l'_e, m_{l'_e}}^*(\Omega_{\mathbf{q}}) Y_{l'_e, m_{l'_e}}(\Omega_e) \\ &\times 4\pi \sum_{l'_h=0}^{\infty} (-i)^{l'_h} J_{l'_h}(\mathbf{q} \cdot \tilde{\mathbf{r}}_h) \sum_{m_{l'_h}=-l'_h}^{l'_h} Y_{l'_h, m_{l'_h}}(\Omega_{\mathbf{q}}) Y_{l'_h, m_{l'_h}}^*(\Omega_h) \end{aligned} \quad (4.1.55)$$

where Ω_i , ($i = e, h$) are solid angles describing spatial orientation of electron and hole.

The Rayleigh equation states that a plane wave may be expanded in a series of spherical waves (Arfken, & Weber, 2005; Abramowitz, & Stegun, 1972),

$$\exp(i\mathbf{q} \cdot \mathbf{r} \cos \varphi) = \sum_{n=0}^{\infty} i^n (2n+1) J_n(qr) P_n(\cos \varphi) \quad (4.1.56)$$

where $J_n(qr)$ is Bessel function and $P_n(\cos \varphi)$ is Legendre polynomial.

The spherical integrals in the form of,

$$\int d\Omega_e Y_{l_e, m_{l_e}}^2(\Omega_e) Y_{l'_e, m'_{l'_e}}(\Omega_e) \quad (4.1.57a)$$

$$\int d\Omega_h Y_{l_h, m_{l_h}}^*(\Omega_h) Y_{l'_h, m'_{l'_h}}^2(\Omega_h) \quad (4.1.57b)$$

For ground state, have to be the equalities which refers electron and hole quantum number sets $n_e = n_h = 1$, $l_e = l_h = 0$ and $m_{l_e} = m_{l_h} = 0$. For the integrals in (4.1.56) and (4.1.57a) could be differ from 0, *iff* $l'_e = l'_h = 0$ and $m'_{l'_e} = m'_{l'_h} = 0$. The orthogonality relations between spherical harmonics would lead to,

$$\int d\Omega_e Y_{0,0}^2(\Omega_e) Y_{0,0}(\Omega_e) = \frac{1}{2\sqrt{\pi}} \quad (4.1.58a)$$

$$\int d\Omega_h Y_{0,0}^*(\Omega_h) Y_{0,0}^2(\Omega_h) = \frac{1}{2\sqrt{\pi}} \quad (4.1.58b)$$

$$\int d\Omega_{\mathbf{q}} Y_{0,0}^2(\Omega_{\mathbf{q}}) Y_{0,0}(\Omega_{\mathbf{q}}) = 1. \quad (4.1.58c)$$

Then the radial parts for the ground state,

$$R(\tilde{r}_e) = R_{n_e=1, l_e=0}(\tilde{r}_e) \quad (4.1.59a)$$

$$R(\tilde{r}_h) = R_{n_h=1, l_h=0}(\tilde{r}_h) \quad (4.1.59b)$$

Utilization of this transform leads to the general integral representations for the

terms in the form of $\exp(-\lambda\tilde{r}_{eh})$ which avoid the use of general integration technique for Hylleraas coordinates. This approach provides the calculation of the integrals in (4.1.60). By these expansion, the integral representations separate coordinates of electron and hole from each other, the integrations over \tilde{r}_e and \tilde{r}_h as be given below lead to the integrals in similar form from each carrier. The integrals have been generated from Hamiltonian matrix and as be labeled,

$$\begin{aligned}
\blacksquare I_{A_1} &= \left\langle \psi_X \left| \frac{d^2}{d\tilde{r}_{eh}^2} \right| \psi_X \right\rangle \\
\blacksquare I_{A_2} &= \left\langle \psi_X \left| \frac{2}{\tilde{r}_{eh}} \frac{d}{d\tilde{r}_{eh}} \right| \psi_X \right\rangle \\
\blacksquare I_{A_3} &= \left\langle \psi_X \left| \frac{1}{\tilde{r}_{eh}} \right| \psi_X \right\rangle \\
\blacksquare I_{B_1} &= \left\langle \psi_X \left| \tilde{V}_c^e(\tilde{r}_e) \right| \psi_X \right\rangle \\
\blacksquare I_{B_2} &= \left\langle \psi_X \left| \tilde{V}_c^h(\tilde{r}_h) \right| \psi_X \right\rangle \\
\blacksquare I_{C_1} &= \left\langle \psi_X \left| \frac{\tilde{r}_e}{\tilde{r}_{eh}} \frac{\partial^2}{\partial \tilde{r}_e \partial \tilde{r}_{eh}} \right| \psi_X \right\rangle \\
\blacksquare I_{C_2} &= \left\langle \psi_X \left| -\frac{\tilde{r}_h^2}{\tilde{r}_e \tilde{r}_{eh}} \frac{\partial^2}{\partial \tilde{r}_e \partial \tilde{r}_{eh}} \right| \psi_X \right\rangle \\
\blacksquare I_{C_3} &= \left\langle \psi_X \left| \frac{\tilde{r}_{eh}}{\tilde{r}_e} \frac{\partial^2}{\partial \tilde{r}_e \partial \tilde{r}_{eh}} \right| \psi_X \right\rangle \\
\blacksquare I_{D_1} &= \left\langle \psi_X \left| \frac{\tilde{r}_h}{\tilde{r}_{eh}} \frac{\partial^2}{\partial \tilde{r}_h \partial \tilde{r}_{eh}} \right| \psi_X \right\rangle \\
\blacksquare I_{D_2} &= \left\langle \psi_X \left| -\frac{\tilde{r}_e^2}{\tilde{r}_h \tilde{r}_{eh}} \frac{\partial^2}{\partial \tilde{r}_h \partial \tilde{r}_{eh}} \right| \psi_X \right\rangle \\
\blacksquare I_{D_3} &= \left\langle \psi_X \left| \frac{\tilde{r}_{eh}}{\tilde{r}_h} \frac{\partial^2}{\partial \tilde{r}_h \partial \tilde{r}_{eh}} \right| \psi_X \right\rangle \\
\blacksquare I_{E_1} &= \left\langle \psi_X \left| \frac{d^2}{d\tilde{r}_e^2} \right| \psi_X \right\rangle \\
\blacksquare I_{E_2} &= \left\langle \psi_X \left| \frac{2}{\tilde{r}_e} \frac{d}{d\tilde{r}_e} \right| \psi_X \right\rangle \\
\blacksquare I_{F_1} &= \left\langle \psi_X \left| \frac{d^2}{d\tilde{r}_h^2} \right| \psi_X \right\rangle \\
\blacksquare I_{F_2} &= \left\langle \psi_X \left| \frac{2}{\tilde{r}_h} \frac{d}{d\tilde{r}_h} \right| \psi_X \right\rangle
\end{aligned} \tag{4.1.60}$$

Since (4.1.47),

$$\tilde{E}_X(\lambda) = -\frac{1}{2\sigma_e} \sum_i \frac{I_i}{I_N} - \frac{1}{2\sigma_h} \sum_j \frac{I_j}{I_N} + \sum_k \frac{I_k}{I_N} \tag{4.1.61}$$

where $i = C_1, C_2, C_3, E_1, E_2$, $j = D_1, D_2, D_3, F_1, F_2$, $k = A_1, A_2, A_3, B_1, B_2$ and $I_N = \langle \psi_X || \psi_X \rangle$.

4.1.3 Additional Donor Impurity Placed At The Center

In this subsection, will be concentrate the study on the D^+, X complex. They result, from the binding of an exciton to an ionized hydrogenic donor impurity. Consider an exciton X bound to an ionized hydrogenic donor impurity D^+ placed at the center of an infinite spherical microcrystal embedded in a glassy matrix by assuming that the electron and the hole are completely confined in the microcrystal by an infinite potential barrier.⁴⁹ In the case of the effective mass approximation the dimensionless Hamiltonian in the form of,

$$\tilde{\mathbf{H}} = \sum_i \left[-\frac{1}{2\sigma_i} \nabla_{\tilde{r}_i}^2 + \tilde{V}(\tilde{r}_i) \right] + \frac{1}{\tilde{r}_h} - \frac{1}{\tilde{r}_e} - \frac{1}{\tilde{r}_{eh}}, \quad i = e, h, \quad (4.1.62)$$

where \tilde{r}_e and \tilde{r}_h is the position length and also represents the dimensionless inter

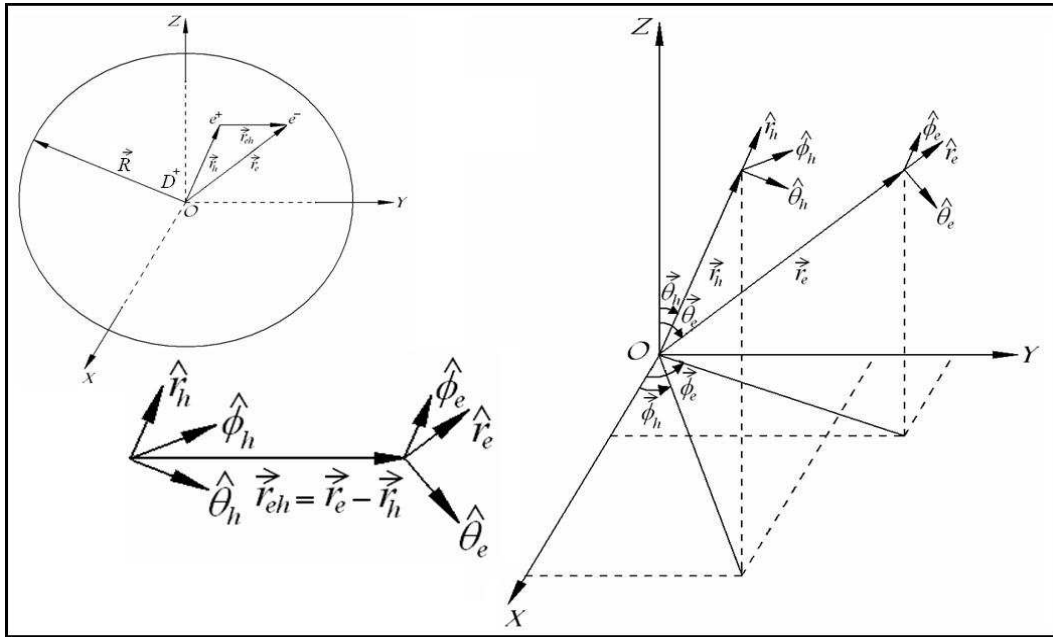


Figure 4.5 Relevant unit and position vectors in the system which contains a donor impurity placed at the center and an exciton in the form of three-dimensional infinite spherical microcrystal.

electron-impurity and hole-impurity distance at the same time. The energy and

⁴⁹see in Figure 4.4

the envelope wave function are solutions of the effective Schrödinger equation,

$$\left[-\frac{1}{2\sigma_e} \nabla_{\tilde{r}_e}^2 - \frac{1}{2\sigma_h} \nabla_{\tilde{r}_h}^2 + \tilde{V}(\tilde{r}_e) + \tilde{V}(\tilde{r}_h) + \frac{1}{\tilde{r}_h} - \frac{1}{\tilde{r}_e} - \frac{1}{\tilde{r}_{eh}} \right] \psi_{D^+,X} = \tilde{E}_{D^+,X} \psi_{D^+,X}, \quad (4.1.63)$$

and the confinement potential,

$$V(\tilde{r}_i) = \begin{cases} \infty & \text{if } \tilde{r}_i \geq |\mathbf{R}| \\ 0 & \text{if } \tilde{r}_i < |\mathbf{R}| \end{cases}, \quad i = e, h.$$

The simplest trial wave function as given so far describes each particle by a hydrogenic binding term with an effective nuclear charge which allows for screening by the other particle and the impurity at the same time. The procedure similar to the system contains an electron and a hole so all the transforms and operations can be applied to the relevant system. Thus, additionally there may come two new integrals into the set as labeled above in (4.1.60),

$$\begin{aligned} \blacksquare I_{G_1} &= \left\langle \psi_X \left| \frac{1}{\tilde{r}_h} \right| \psi_X \right\rangle \\ \blacksquare I_{G_2} &= \left\langle \psi_X \left| -\frac{1}{\tilde{r}_e} \right| \psi_X \right\rangle \end{aligned} \quad (4.1.64)$$

then the energy spectra depends on λ by this means,

$$\tilde{E}_{D^+,X}(\lambda) = -\frac{1}{2\sigma_e} \sum_i \frac{I_i}{I_N} - \frac{1}{2\sigma_h} \sum_j \frac{I_j}{I_N} + \sum_k \frac{I_k}{I_N} \quad (4.1.65)$$

where additionally $k = A_1, A_2, A_3, B_1, B_2, G_1, G_2$. Thus, could be evaluated the minima in the λ spectrum for ground state energy in (4.1.61):

$$\frac{\partial}{\partial \lambda} \left[-\frac{1}{2\sigma_e} \sum_i \frac{I_i}{I_N} - \frac{1}{2\sigma_h} \sum_j \frac{I_j}{I_N} + \sum_k \frac{I_k}{I_N} \right] = 0. \quad (4.1.66)$$

4.2 The Main Problem

Nowadays, students of physics can carry out these computations in a matter of hours, or even minutes, using relatively straightforward *MatLab & Simulink*[®] or any other high level routines in comparison with a low level routine like *previously FORTRAN*[®], *Fortran*[®] or *C/C++*[®]. Moreover, the results can be easily improved far beyond the capabilities of the original workers. In light of these information, could be told that the main problem is computing the optimum λ value corresponding to the ground state energy with by using one or more routines, maybe by combining them becomingly. Thus, the routines well-known have to be supposed to flexible approach to the system. The requisite formulas and equations are fairly lengthy and been calculated the details but could not appended *Wolfram Mathematica*[®] printout. It is impossible to determine the eigenfunctions of (4.1.60) exactly and analytically. Hence, test wave functions are constructed and the energy is minimized by variation.

CHAPTER FIVE

COMPUTATION AND RESULTS

5.1 Numerical Estimates

The goal of a good theoretical understanding should be the ability to predict or to explain, at least *semi-quantitatively*, the observed rates of convergence for systematic variational calculations with different basis sets. Be concluded that theoretical understanding of variational calculations on the two- or three-particle system is far outstripped by the raw computing power of available machinery.

Have been investigated three system which be made up of one- two- or three-particle and resemble each other in QD with following aspects: Electron, exciton (as an electron-hole pair) and the bound exciton to an donor impurity. Following theoretical studies on infinite spherical QDs, be used the material parameters of GaAs for the inner core, because it's basic physical properties such as effective masses and dielectric constants are better known (Adachi, 1985). The parameters of more realistic structures can easily be used with the present numerical estimates (Tomak, & Şahin, 2005).

Have been used atomic units throughout the calculations. Effective Bohr radius $a^* = 100\text{\AA}$ and effective Hartree energy $E_H^* = 11\text{meV}$. And be take electron effective mass $m_e = 0.067m_0$, and hole effective $m_{lh} = 0.090m_0$ for light hole (LH) and $m_{hh} = 0.377m_0$ for heavy hole (HH) where m_0 indicates free electron mass. At this place, notice that the effective masses of electron and hole inside GaAs as m_i^* , ($i = e, h$) is similarly (Jaziri, & Bennaceur, 1995; Halonen et al., 1992).

This thesis is organized as follows. The exact analytical solution describing

Table 5.1 First eight actual values comparison with the numerical values and additionally ground state energies with regard to roots of the Bessel function for the first kind for $n = 1, 1/2$ respectively with any quantum states $|n_e, l_e\rangle$.

ρ	Actual	$J_1(\rho)$	$n_e l_e$	$J_{1/2}(\rho_{n_e, l_e})$	E_e
1.00	0.4400506	0.4400506	1s	3.141592653589793	181.2513657418906
2.00	0.5767248	0.5767248	2p	6.283185307179586	725.0054629675623
3.00	0.3390590	0.3390590	1d	9.424777960769379	1631.262291677016
4.00	-0.0660433	-0.0660433	2s	12.566370614359172	2900.021851870249
5.00	-0.3275791	-0.3275791	1f	15.707963267948966	4531.28.4143547266
6.00	-0.2766839	-0.2766839	2p	18.849555921538759	6525.049166708062
7.00	-0.0046828	-0.0046828	1g	21.991148575128552	8881.316921352639
8.00	0.2346364	0.2346363	2d	25.132741228718345	11600.08740748100

the electronic ground state in an infinite QD. Numerical results for excitonic ground state energy QD nanoparticles is outlined and have been checked for noninteracting case with manual analytical solutions. A detailed comparison of the two- and three-particle system is given below. Finally have been summarized the main calculations obtained in this thesis.

For one-particle system, exact analytical solutions and the ground state energy of the system in (4.1.26) is given previously. The energy equation comprises Bessel function's for the first kind consequently, the essential requirement for the ground state is Bessel function's first root as shown in Table 5.1. By using the relevant value of the Bessel function and numerical estimates the ground state energy for one-particle system (as an electron) for the radii of QD, $R = 1\text{nm}$,

$$E_{e_{1s}} = 181.2513657418906\text{meV}. \quad (5.1.1)$$

The integrals have been generated from Hamiltonian matrix and as be labeled

previously in two-particle system (X) in the form of,

$$\forall I_i \vee \forall I_j \vee \forall I_k \equiv \kappa_{i,j,k} \int dq q^2 f_{i,j,k}(q, \lambda). \quad (5.1.2)$$

In due course to designate the majorants, have to be supposed to investigate of the behavior of the integrand $q^2 f_{i,j,k}(q, \lambda)$ for each integrals as a function of q .⁵⁰ In correct *mathematical typography*, the dq is separated from the integrands by the spaces as shown. All the relevant plots display the corresponding behavior depends on q of the integrands, and it can be seen that they all have a majorant at $q = 10$. Thus (5.1.2) with the upper and bottom limit,

$$\forall I_i \vee \forall I_j \vee \forall I_k \equiv \kappa_{i,j,k} \int_0^{10} dq q^2 f_{i,j,k}(q, \lambda). \quad (5.1.3)$$

Particularly, in a one-dimensional QW, an electron and a hole's total ground state energy for the uncorrelated case as applicable respectively with $\sqrt{2\sigma_i E_i} = \pi/R$, ($i = e, h$),

$$E_e = \frac{\pi^2}{2\sigma_e R^2}, \quad (5.1.4a)$$

$$E_h = \frac{\pi^2}{2\sigma_h R^2}, \quad (5.1.4b)$$

thus,

$$E_{X_{\text{uncor}}} = E_e + E_h = \frac{\hbar^2}{2R^2} \underbrace{\left(\frac{1}{\sigma_e} + \frac{1}{\sigma_h} \right)}_1 \quad (5.1.5)$$

So that,

$$E_{X_{\text{uncor}}} = \frac{\pi^2}{2R^2} \simeq 24.67 \quad \iff \quad R = 1, \quad \lambda = 0. \quad (5.1.6)$$

Figure 5.1 shows the result of calculation of the ground state energy of one-

⁵⁰see in Appendix for *the plots of the significant integrands as a function of q*

particle (an electron) system in a GaAs QD surrounded by infinite barrier in interior dielectric medium (such as H₂O) as a function of infinite QD radius. The ground state energy of the electron complex decreases rapidly with increasing QD radius.

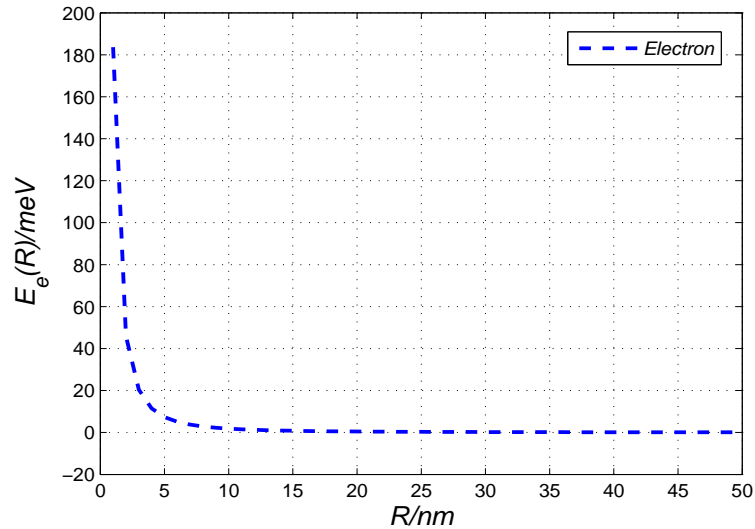


Figure 5.1 The ground state energy of an electron in GaAs as a function of infinite QD radius.

5.2 Ground State Energy Of The Relevant System

In the light of this information, to checking for noninteracting electron-hole pair in the system⁵¹ the results of calculations of the ground state exciton binding energies for some values of variational parameter λ by getting $R = 1$ and $\sigma_e^{-1} + \sigma_h^{-1} = 1$ for simplicity are shown in Table 5.2.

In going beyond one-particle system to many-particle systems, an additional calculating principle becomes important. To construct an expression for $\langle \psi_T | \tilde{\mathbf{H}} | \psi_T \rangle$ by using Hylleraas-type wave function, one would, ideally, like to calculate the

⁵¹by neglecting the integral term I_{A_3} which is concerned interparticle interaction for $K=0$

Table 5.2 The ground state exciton binding energies some manual analytical calculation values comparison in high precision with the numerical values of variational parameter λ in different precision for $R = 1$.

λ	Numerical E_X/meV
0.1	23.499104719859382
0.01	23.499524327709057
0.001	23.503721312804480
0.0001	23.545782059804750
0.00001	23.975670396316136

integral representations for the terms as $\exp(-\lambda r_{eh})$ involved by the use of well-known Hylleraas coordinates and calculated variationally the ground state energies of X and D^+, X complexes via the relevant wave function. The adjustable parameter of the trial wave function is given previously as λ . This choice was originally made by Hylleraas (Hylleraas, 1929) and rejected subsequently by Hartree and Ingman (Hartree, & Ingman, 1933) as unphysical.

Minimizing the energy with respect to variation in the parameter of $\lambda = 0.2$ cause of vary in the range $\lambda = [0.055, 0.300]$. In Figure 5.2, in order to compare the effect of confinement on the D^+, X complexes, have been presented the behavior of the ground state energy of the bound heavy- and light-hole exciton to an ionized donor impurity which is placed at the center in infinite three-dimensional spherical QD as a function of radii of GaAs nanocrystal. This have been performed by the codes is given in Appendix and elapsed time is nearly 19788,38922 seconds both for heavy- and light-hole.⁵² The energy decreases rapidly with increasing QD radius both for heavy- and light-hole excitons with a quantitative difference. For smaller values of radius, the ground state energy is obviously more sensitive to the size of the QD. As noticed in the work performed by Şakiroğlu et al. (Şakiroğlu et al., 2009), increasing exciton energies are obtained in the case of narrower QD

⁵²on a PC, AMD Athlon(tm) 64 ×2 Dual Core Processor 5200+, MMX, 3DNow (2 CPUs), with 1024MB RAM

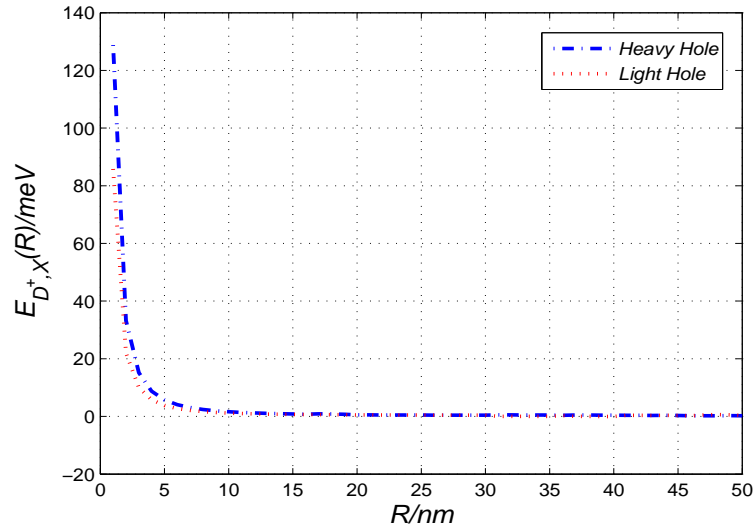


Figure 5.2 The ground state energy of three-particle (D^+, X) system in GaAs as a function of infinite QD radius. The blue dot-dashed curve shows the results for heavy-hole and the red dashed shows light-hole (D^+, X) system. It's completely same for the two-particle (X) system.

where the effect of quantum confinement is more pronounced. In this case spatial overlap between electron and hole increases, which leads to the enhancement of Coulombic binding energy.

The energy of heavy-hole exciton is lower than the value of light-hole for the same radius. The reason of this situation is the enhanced the effective kinetic energy of electron and hole in three-dimensional QD.

The values in the Table 5.2 is completely the same for aforesaid D^+, X complex. The values of the two additional interparticle interaction integral terms I_{G_1} and I_{G_2} are completely the same by a difference opposite notation may be approved as the reason of this situation. That is to say, injecting a donor impurity to the X complex, would not change the polar symmetry, the disposition of nanocrystal matrix lattice and once for all the ground state energy of the system.

Thus means, have been concluded constitutively that theoretical understanding of the convergence of variational calculations on the two- or three-particle system is far outstripped by the raw computing power of available machinery.

5.3 Discussion

The expansion of the interparticle coordinates is combined with the use of properties of Legendre polynomials. With the exception of the radial totally linked integral, for the other integrals only the terms $q = 0$ or $q = 1$ of the expansion survive.

The resulting radial and angular integrals are evaluated and written out in operator form general expressions for the integrals with higher powers of the interparticle coordinates are derived. most of angular integrals vanish. Only in cases where all the indices are linked are they different from zero.

In this thesis, to ensure the validity of the method, dependencies of the ground state energy as a function of QD radius for the bound exciton to an ionized donor impurity placed at the center have been investigated. Comparison with the previous theoretical works especially with results given Şakiroğlu et al. (Şakiroğlu et al., 2009) and Stébé et al. (Stébé et al., 1996) revealed a good agreement for ground state energy and it's behavior according to radius, confirming that given trial wave function and the method presented describes accurately the system D^+ , X states confined in infinite QD.

CHAPTER SIX

CONCLUDING REMARKS

Schrödinger equation of a three-particle system is a linear PDE defined on the nine-dimensional configuration space, \mathbb{R}^9 . The study of above Schrödinger equation of three-particle systems has a long history, dating back to Hylleraas' work on this subject in the 1930s, and there are extensive literature and various approaches in the study of its solutions. It is essentially to specify that exciton complexes have been the subject of intense studies in the last ten or fifteen years, both experimentally and theoretically.

The procedure for solving the three-particle quantum confinement problem with ordinary central force is to perform an optimization for the ground state energy and advance it in time until, taking appropriate measures with regard to divergent state, all the error components in the original perform have been eliminated. The Rayleigh-Ritz's variational method by using Hylleraas-type trial wave function constructed from the conventional orbital product, times a correlation function depending on the interparticle distance \mathbf{r}_{ij} is very efficient to study the ground state of three-particle quantum mechanical problems. We have made an investigation of behavior of the ground state energy's dependency on radii of the QD in order to determine if there is an optimal choice for a three-particle treatment by the Rayleigh-Ritz's variational method.

Most of the formulas and results in this thesis have been checked for accuracy in a number of special case. The results presented previously only concern S -state calculations of quantum mechanical three-particle problem. As the method provides good results for three-particle bound states, it would be interesting to extend it to the search for quantum chaos in QD.⁵³

⁵³Maybe this mantra could be done, for example, by using *KAM Theory*.

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APPENDIX

A.1 The Value Of The Magnetic Quantum Number

Remember the problem is defined as the case of a particle situated in a three dimensional infinite spherical QD. $\phi = [0, 2\pi]$ and note, that as mentioned previously, only *quantized* energy levels are possible so for could be *single value* of the wave function,

$$\Phi(\phi + 2\pi) \doteq \Phi(\phi),$$

$$A \exp(im_l(\phi + 2\pi)) \doteq A \exp(im_l\phi).$$

$$\exp(im_l\phi + 2\pi) \equiv \exp(im_l\phi),$$

$$\iff \cos(m_l(\phi + 2\pi)) + i \sin(m_l(\phi + 2\pi)) \equiv \cos(m_l\phi) + i \sin(m_l\phi).$$

$$\begin{aligned} \cos(m_l\phi) \cos(m_l2\pi) - \sin(m_l\phi) \sin(m_l2\pi) + i \sin(m_l\phi) \cos(m_l2\pi) \\ + i \cos(m_l\phi) \sin(m_l2\pi) \equiv \cos(m_l\phi) + i \sin(m_l\phi), \end{aligned}$$

$$\sin(m_l2\pi) = 0, \quad m_l = 0, \pm 1, \pm 2, \pm 3, \dots$$

$$\cos(m_l2\pi) = 0, \quad m_l = 0, \pm 1, \pm 2, \pm 3, \dots$$

$$\cos(m_l\phi) + i \sin(m_l\phi) = \cos(m_l\phi) + i \sin(m_l\phi),$$

then yields (4.1.11),

$$\Phi_{m_l}(\phi) = A_l \exp(im_l\phi), \quad m_l = 0, \pm 1, \pm 2, \pm 3, \dots$$

A.2 Mapping For The Relevant SubODE

The relevant transform for (4.1.10b) as defined previously the parameter $\mu = \cos \theta$,

$$\mu = \cos \theta, \quad d\mu = -\sin \theta d\theta.$$

$$\frac{d\mu}{d\theta} = -\sin \theta.$$

With *chain rule*,

$$\frac{d}{d\theta} = \frac{d}{d\mu} \frac{d\mu}{d\theta} = -\sin \theta \frac{d}{d\mu}.$$

$$\sin^2 \theta = 1 - \cos^2 \theta, \quad \cos^2 \theta = \mu^2,$$

$$\sin^2 \theta = 1 - \mu^2.$$

$$\frac{d^2}{d\theta^2} = \frac{d}{d\theta} \left(\frac{d}{d\theta} \right) = \left(-\sin \theta \frac{d}{d\mu} \right) \left(-\sin \theta \frac{d}{d\mu} \right) = \sin^2 \theta \frac{d^2}{d\mu^2} = (1 - \mu^2) \frac{d^2}{d\mu^2},$$

$$\frac{d^2}{d\theta^2} = (1 - \mu^2) \frac{d^2}{d\mu^2}.$$

Within these new definitions the (4.1.10b) converts into the (4.1.11),

$$\begin{aligned} \left[(1 - \mu^2) \frac{d^2}{d\mu^2} \right] \Theta(\arccos \mu) &- \left[2\mu \frac{d}{d\mu} \right] \Theta(\arccos \mu) \\ &+ \left[\Lambda - \frac{m_l^2}{(1 - \mu^2)} \right] \Theta(\arccos \mu) = 0. \end{aligned}$$

A.3 Series Solution Of The Legendre ODE

At this place, notice that there is no singularity in Legendre ODE (4.1.13) so the basis of *Frobenius*⁵⁴ *method* is to try for a solution of relevant equation of

⁵⁴Ferdinand Georg Frobenius (1849-1917)

the form of *power series*

$$P_l(\mu) = C_0 + C_1\mu + C_2\mu^2 + \dots = \sum_{\eta=0}^{\infty} [C_\eta] \mu^\eta,$$

convergent for all range of μ including the point $\mu = 0$. *The binomial theorem* may be used to expand the coefficients in (4.1.13) as power series and it is clearly with first and second order derivative respectively,

$$P_l'(\mu) = C_1 + 2C_2\mu + 3C_3\mu^2 + \dots$$

$$2\mu P_l'(\mu) = 2(C_1\mu + 2C_2\mu^2 + 3C_3\mu^3 + \dots) = \sum_{\eta=0}^{\infty} [2\eta C_\eta] \mu^\eta$$

$$P_l''(\mu) = 1 \times 2C_2 + 2 \times 3C_3\mu + 3 \times 4C_4\mu^2 + \dots$$

$$\begin{aligned} (1 - \mu^2) P_l''(\mu) &= (1 \times 2C_2 + 2 \times 3C_3\mu + \dots) - (1 \times 2C_2\mu^2 + 2 \times 3C_3\mu^3 + \dots) \\ &= \sum_{\eta=0}^{\infty} [(\eta + 1)(\eta + 2)C_{\eta+2}] \mu^\eta - \sum_{\eta=0}^{\infty} [(\eta - 1)nC_\eta] \mu^\eta. \end{aligned}$$

By substituting these derivatives for (4.1.13) and reorganizing,

$$\begin{aligned} \sum_{\eta=0}^{\infty} [(\eta + 1)(\eta + 2)C_{\eta+2} - (\eta - 1)\eta C_\eta - 2\eta C_\eta + \lambda C_\eta] \mu^\eta &= 0, \\ \sum_{\eta=0}^{\infty} \underbrace{[(\eta + 1)(\eta + 2)] C_{\eta+2} + [-(\eta - 1)\eta - 2\eta + \lambda] C_\eta}_{0} \mu^\eta &= 0, \end{aligned}$$

$$[(\eta + 1)(\eta + 2)] C_{\eta+2} + [-(\eta - 1)\eta - 2\eta + \lambda] C_\eta = 0, \quad \eta \geq 0.$$

This equation gives the indicial equation and the *r ecurrence formula* in the form of

$$C_{\eta+2} = \frac{\eta(\eta + 1) - \lambda}{(\eta + 1)(\eta + 2)} C_\eta.$$

By expanding these formula for first deux term,

$$\begin{aligned}
 n = 0 &\Rightarrow C_2 = (-\lambda/2)C_0 \\
 n = 1 &\Rightarrow C_3 = (2 - \lambda/6)C_1 \\
 n = 2 &\Rightarrow C_4 = (6 - \lambda/12)C_2 \\
 n = 3 &\Rightarrow C_5 = (12 - \lambda/20)C_3 \\
 &\cdot \quad \quad \cdot \quad \quad \cdot \\
 &\cdot \quad \quad \cdot \quad \quad \cdot \\
 &\cdot \quad \quad \cdot \quad \quad \cdot
 \end{aligned}$$

thus the relevant coefficients,

$$\begin{aligned}
 C_2 &= -[\lambda]/2!C_0 && \leftarrow C_3 = -[2 - \lambda]/3!C_1 \\
 C_4 &= -[\lambda(6 - \lambda)]/4!C_0 && \leftarrow C_5 = -[(12 - \lambda)(2 - \lambda)]/5!C_1 \\
 C_6 &= \dots C_0 && \leftarrow C_7 = \dots C_1 \\
 &\cdot && \cdot \\
 &\cdot && \cdot \\
 &\cdot && \cdot
 \end{aligned}$$

Therefore

$$\begin{aligned}
 P_{l_1} &= 1 - \frac{\lambda}{2!}\mu^2 + \frac{\lambda(\lambda - 6)}{4!}\mu^4 - \dots, \\
 P_{l_2} &= \mu - \frac{\lambda - 2}{3!}\mu^3 + \frac{(12 - \lambda)(2 - \lambda)}{5!}\mu^5 - \dots,
 \end{aligned}$$

so that for μ even, P_{l_1} and for μ odd P_{l_2} are linearly independent solutions. Thus the linear combinations of these yields the total solution in the following equation,

$$P_l(\mu) = C_0 P_{l_1} \mu + C_1 P_{l_2} \mu.$$

To determine the convergence of the series contains infinite terms as mentioned in réccurrence formula by *ratio test* as following,

$$\begin{aligned}\lim_{\eta \rightarrow \infty} \frac{C_{\eta+2}}{C_{\eta}} &= \lim_{\eta \rightarrow \infty} \frac{\eta(\eta+1) - \lambda}{(\eta+1)(\eta+2)} = \lim_{\eta \rightarrow \infty} \left[\frac{\eta^2 + \eta - \lambda}{\eta^2 + 3\eta + 2} \right], \\ \lim_{\eta \rightarrow \infty} \frac{C_{\eta+2}}{C_{\eta}} &= \lim_{\eta \rightarrow \infty} \left[\frac{\eta^2}{\eta^2 + 3\eta + 2} \right] + \lim_{\eta \rightarrow \infty} \left[\frac{\eta - \lambda}{\eta^2 + 3\eta + 2} \right], \\ \lim_{\eta \rightarrow \infty} \frac{C_{\eta+2}}{C_{\eta}} &= \lim_{\eta \rightarrow \infty} \left[\frac{\eta^2}{\eta^2} \left(\frac{1}{1 + 3/\eta + 2/\eta^2} \right) \right] + \lim_{\eta \rightarrow \infty} \left[\frac{\eta}{\eta} \left(\frac{1 - (\lambda/\eta)}{\eta + 3 + 2/\eta} \right) \right], \\ \lim_{\eta \rightarrow \infty} \frac{C_{\eta+2}}{C_{\eta}} &= \underbrace{\left[\frac{1}{1 + 0 + 0} \right]}_1 + \underbrace{\left[\frac{1 - 0}{\infty + 3 + 0} \right]}_0 \\ &= \lim_{\eta \rightarrow \infty} \frac{C_{\eta+2}}{C_{\eta}} = 1.\end{aligned}$$

Permissively, by evanishing to dividend to guarantee convergence of relevant series

$$\eta(\eta+1) - \lambda \implies l(l+1) - \lambda = 0, \longrightarrow \lambda = l(l+1),$$

yields the total solution of the (4.1.13) as given previously which is called Legendre polynomials order of *azimuthal quantum number l*:

$$\Theta(\theta)_l = B_l P_l^{m_l}(\cos \theta), \quad l = 0, 1, 2, 3, \dots$$

A.4 Scaling To The Radial Part Of The Main Schrödinger Equation

With the new dimensionless parameter ρ as defined previously and following

$$\rho = kr, \quad d\rho = kdr \implies \frac{d\rho}{dr} = k,$$

hence the derivatives by using chain rule in the form of,

$$\frac{d}{dr} = \frac{d}{d\rho} \frac{d\rho}{dr} = k \frac{d}{d\rho},$$

$$\frac{d^2}{dr^2} = \frac{d}{dr} \frac{d}{dr} = k^2 \frac{d^2}{d\rho^2},$$

so that, to inserting these into the (4.1.18) gives (4.1.19) as given previously:

$$\left[\rho^2 \frac{d^2}{d\rho^2} \right] R_n + [2\rho^2] R_n + [\rho^2 - n(n+1)] R_n = 0.$$

A.5 Transformation To The Standard Bessel's ODE

The procedure to convert (4.1.19) to the Standard Bessel's ODE with $R = U(\rho)/(\rho^{1/2})$ as foolowing,

$$\left[\frac{d}{d\rho} \right] R = \left[\frac{d}{d\rho} \right] U(\rho)/(\rho^{1/2}) = \frac{1}{\rho^{1/2}} \left[\frac{d}{d\rho} \right] U(\rho) - \left[\frac{\rho^{-3/2}}{2} \right] U(\rho),$$

$$\left[\frac{d^2}{d\rho^2} \right] R = \left[\frac{d}{d\rho} \right] \left[\frac{1}{\rho^{1/2}} \left[\frac{d}{d\rho} \right] U(\rho) - \left[\frac{\rho^{-3/2}}{2} \right] U(\rho) \right],$$

$$\left[\frac{d^2}{d\rho^2} \right] R = -\frac{1}{2}\rho^{-3/2} \left[\frac{d}{d\rho} \right] U(\rho) + \frac{1}{\rho^{1/2}} \left[\frac{d^2}{d\rho^2} \right] U(\rho) - \frac{\rho^{-3/2}}{2} \left[\frac{d}{d\rho} \right] U(\rho) + \frac{3}{4}\rho^{-5/2}U(\rho),$$

$$\rho^2 \left[\frac{d^2}{d\rho^2} \right] = -\frac{1}{2}\rho^{1/2} \left[\frac{d}{d\rho} \right] U(\rho) + \frac{1}{\rho^{3/2}} \left[\frac{d^2}{d\rho^2} \right] U(\rho) - \frac{\rho^{1/2}}{2} \left[\frac{d}{d\rho} \right] U(\rho) + \frac{3}{4}\rho^{-1/2}U(\rho),$$

$$2\rho \left[\frac{d}{d\rho} \right] R = 2\rho^{1/2} \left[\frac{d}{d\rho} \right] U(\rho) - \rho^{-1/2}U(\rho),$$

By putting into the place, these derivatives and R ,

$$\rho^{3/2} \frac{d^2 U(\rho)}{d\rho^2} + \rho^{1/2} \frac{dU(\rho)}{d\rho} - \frac{1}{4} \rho^{-1/2} U(\rho) + \rho^{3/2} U(\rho) - \rho^{-1/2} l(l+1) U(\rho) = 0,$$

$$\rho^{3/2} \frac{d^2 U(\rho)}{d\rho^2} + \rho^{1/2} \frac{dU(\rho)}{d\rho} + \rho^{3/2} U(\rho) - \rho^{-1/2} \left[l(l+1) + \frac{1}{4} \right] U(\rho) = 0,$$

$$\begin{aligned}
\rho^{3/2} \frac{d^2 U(\rho)}{d\rho^2} + \rho^{1/2} \frac{dU(\rho)}{d\rho} + \rho^{3/2} U(\rho) - \rho^{-1/2} \left[l^2 + l + \frac{1}{4} \right] U(\rho) &= 0, \\
\rho^{3/2} \frac{d^2 U(\rho)}{d\rho^2} + \rho^{1/2} \frac{dU(\rho)}{d\rho} + \rho^{3/2} U(\rho) - \rho^{-1/2} \left[l + \frac{1}{2} \right]^2 U(\rho) &= 0, \\
\rho^{3/2} \frac{d^2 U(\rho)}{d\rho^2} + \rho^{1/2} \frac{dU(\rho)}{d\rho} + \left[\rho^{3/2} - \rho^{-1/2} \left[l + \frac{1}{2} \right]^2 \right] U(\rho) &= 0, \\
\rho^2 \frac{d^2 U(\rho)}{d\rho^2} + \rho \frac{dU(\rho)}{d\rho} + \left[\rho^2 - \left[l + \frac{1}{2} \right]^2 \right] U(\rho) &= 0, \\
\rho^2 \frac{d^2 U(\rho)}{d\rho^2} + \rho \frac{dU(\rho)}{d\rho} + [\rho^2 - \mu^2] U(\rho) &= 0, \\
\rho(\rho U'(\rho))' &= \rho^2 U''(\rho) + \rho U'(\rho).
\end{aligned}$$

As a result, after these substitutes and transformations be obtained the (4.1.21):

$$\rho(\rho U'(\rho))' + [\rho^2 - v^2] U(\rho) = 0.$$

A.6 Series Solution Of The Standard Bessel's ODE

Bessel's ODE of order v is given above in (4.1.21). Be may apply the Frobenius' method and be assured that any series solution obtained will be convergent for all values of ρ . the relevant solution function is recommended and relevant derivatives in the form of

$$\begin{aligned}
U(\rho) &= \sum_{\eta=0}^{\infty} a_{\eta} \rho^{\eta+s}, \\
U'(\rho) &= \sum_{\eta=0}^{\infty} a_{\eta} (\eta + s) \rho^{\eta+s-1},
\end{aligned}$$

$$\begin{aligned}\rho U'(\rho) &= \sum_{\eta=0}^{\infty} a_{\eta}(\eta+s)\rho^{\eta+s}, \\ (\rho U'(\rho))' &= \sum_{\eta=0}^{\infty} a_{\eta}(\eta+s)^2\rho^{\eta+s-1}, \\ \rho(\rho U'(\rho))' &= \sum_{\eta=0}^{\infty} a_{\eta}(\eta+s)^2\rho^{\eta+s}.\end{aligned}$$

At this place, convert into the (4.1.21) all the equations as reproduced above,

$$\sum_{\eta=0}^{\infty} a_{\eta}(\eta+s)^2\rho^{\eta+s} + [\rho^2 - v^2] \sum_{\eta=0}^{\infty} a_{\eta}\rho^{\eta+s} = 0,$$

then by rewriting,

$$\sum_{\eta=0}^{\infty} [(\eta+s)^2 a_{\eta} + [\rho^2 - v^2] a_{\eta}] \rho^{\eta+s} = 0.$$

Yields root equation,

$$[\rho^2 - v^2] = 0 \implies \rho = \pm v.$$

So,

$$[(\eta+s)^2 - v^2] a_{\eta} + a_{\eta-2} = 0.$$

Thus the recurrence formula in the form of,

$$\begin{aligned}a_{\eta} &= -\frac{a_{\eta-2}}{[(\eta+s)^2 - v^2]} \\ a_{\eta} &= -\frac{a_{\eta-2}}{[(\eta+v)^2 - v^2]} = -\frac{a_{\eta-2}}{[\eta^2 + 2\eta v]} = -\frac{a_{\eta-2}}{[\eta(\eta+2v)]} \\ a_{2\eta} &= -\frac{a_{2\eta-2}}{[2\eta(2\eta+2v)]} = -\frac{a_{2\eta-2}}{[2^2\eta(\eta+v)]}.\end{aligned}$$

To simplify the appearance of this formula somewhat by using *Gamma functions* as an extension of the factorial function to real and complex numbers,

$$\begin{aligned}
 \Gamma(v+1) &= v\Gamma(v) \\
 \Gamma(v+2) &= (v+1)\Gamma(v+1) \\
 \Gamma(v+3) &= (v+2)\Gamma(v+2) = (v+2)(v+1)\Gamma(v+1) \\
 &\cdot \qquad \qquad \cdot \qquad \qquad \cdot \\
 &\cdot \qquad \qquad \cdot \qquad \qquad \cdot \\
 &\cdot \qquad \qquad \cdot \qquad \qquad \cdot
 \end{aligned}$$

Hence, the coefficients,

$$\begin{aligned}
 a_2 &= -a_0/2^2(1+v) = -a_0\Gamma(1+v)/2!2^4\Gamma(3+v) \\
 a_4 &= -a_2/2^3(2+v) = a_0\Gamma(1+v)/2!2^4\Gamma(3+v) \\
 a_6 &= -a_4/3!2(3+v) = -a_0\Gamma(1+v)/3!2^6\Gamma(4+v) \\
 &\cdot \qquad \qquad \cdot \qquad \qquad \cdot \\
 &\cdot \qquad \qquad \cdot \qquad \qquad \cdot \\
 &\cdot \qquad \qquad \cdot \qquad \qquad \cdot
 \end{aligned}$$

At this stage, series solution for the special condition in the form of,

$$\begin{aligned}
 U(\rho) &= a_0\rho^v\Gamma(1+v) \\
 &\times \left[\frac{1}{\Gamma(1+v)} - \frac{1}{\Gamma(2+v)} \left(\frac{\rho}{2}\right)^2 + \frac{1}{2!\Gamma(3+v)} \left(\frac{\rho}{2}\right)^4 - \frac{1}{3!\Gamma(4+v)} \left(\frac{\rho}{2}\right)^6 + \dots \right].
 \end{aligned}$$

Here, $\Gamma(1) = \Gamma(2) = 1$ and for first two terms, $\rho^v = 2^v(\rho/2)^v$. So that,

$$\begin{aligned}
 U(\rho) &= a_02^v \left(\frac{\rho}{2}\right)^v \Gamma(1+v) \\
 &\times \left[\frac{1}{\Gamma(1)\Gamma(1+v)} - \frac{1}{\Gamma(2)\Gamma(2+v)} \left(\frac{\rho}{2}\right)^2 + \frac{1}{\Gamma(3)\Gamma(3+v)} \left(\frac{\rho}{2}\right)^4 - \dots \right].
 \end{aligned}$$

If $a_0 = 1/2^v \Gamma(1+v) = 1/2^v v!$, then yields the Bessel polynomials,

$$J_v(\rho) = \frac{1}{\Gamma(1)\Gamma(1+v)} \left(\frac{\rho}{2}\right)^v - \frac{1}{\Gamma(2)\Gamma(2+v)} \left(\frac{\rho}{2}\right)^{2+v} + \frac{1}{\Gamma(3)\Gamma(3+v)} \left(\frac{\rho}{2}\right)^{4+v} - \dots,$$

so that the series solution of the standard Bessel's ODE as Bessel polynomials in the closed form of:

$$J_v(\rho) = \sum_{\eta=0}^{\infty} \frac{(-2)^\eta}{\Gamma(\eta+1)\Gamma(\eta+v+1)} \left(\frac{\rho}{2}\right)^{2\eta+v}.$$

A.7 Internal Operations For The Immature Hamiltonian

For electronic part contains the operator del in the main Schrödinger equation as following,

$$\begin{aligned} \nabla_e \psi_e^s F &= F \nabla_e \psi_e^s + \psi_e^s \nabla_e F, \\ \nabla_e^2 \psi_e^s F &= \nabla_e [\nabla_e \psi_e^s F] = \nabla_e [F \nabla_e \psi_e^s + \psi_e^s \nabla_e F], \\ \nabla_e^2 \psi_e^s F &= [\nabla_e \psi_e^s] [\nabla_e F] + F \nabla_e^2 \psi_e^s + [\nabla_e \psi_e^s] [\nabla_e F] + \psi_e^s \nabla_e^2 F, \\ \nabla_e^2 \psi_e^s F &= F \nabla_e^2 \psi_e^s + 2 [\nabla_e \psi_e^s] [\nabla_e F] + \psi_e^s \nabla_e^2 F, \end{aligned}$$

thus,

$$-\psi_h^s \left[\frac{1}{2\sigma_e} \nabla_e^2 \right] \psi_e^s F = -\psi_h^s \frac{1}{2\sigma_e} [F \nabla_e^2 \psi_e^s + 2 [\nabla_e \psi_e^s] [\nabla_e F] + \psi_e^s \nabla_e^2 F].$$

For holic part contains the operator del in the main Schrödinger equation as

following,

$$\begin{aligned}
\nabla_h \psi_h^s F &= F \nabla_h \psi_h^s + \psi_h^s \nabla_h F, \\
\nabla_h^2 \psi_h^s F &= \nabla_h [\nabla_h \psi_h^s F] = \nabla_h [F \nabla_h \psi_h^s + \psi_h^s \nabla_h F], \\
\nabla_h^2 \psi_h^s F &= [\nabla_h \psi_h^s] [\nabla_h F] + F \nabla_h^2 \psi_h^s + [\nabla_h \psi_h^s] [\nabla_h F] + \psi_h^s \nabla_h^2 F, \\
\nabla_h^2 \psi_h^s F &= F \nabla_h^2 \psi_h^s + 2 [\nabla_h \psi_h^s] [\nabla_h F] + \psi_h^s \nabla_h^2 F,
\end{aligned}$$

thus,

$$-\psi_e^s \left[\frac{1}{2\sigma_h} \nabla_h^2 \right] \psi_h^s F = -\psi_e^s \frac{1}{2\sigma_h} [F \nabla_h^2 \psi_h^s + 2 [\nabla_h \psi_h^s] [\nabla_h F] + \psi_h^s \nabla_h^2 F].$$

Respectively,

$$\begin{aligned}
\blacksquare & - \psi_h^s \frac{1}{2\sigma_e} \left[F \nabla_e^2 \psi_e^s + 2 [\nabla_e \psi_e^s] \underbrace{[\nabla_e F]}_{\dot{I}} + \psi_e^s \underbrace{\nabla_e^2 F}_{\dot{O}} \right] \\
\blacksquare & - \psi_e^s \frac{1}{2\sigma_h} \left[F \nabla_h^2 \psi_h^s + 2 [\nabla_h \psi_h^s] \underbrace{[\nabla_h F]}_{\dot{I}} + \psi_h^s \underbrace{\nabla_h^2 F}_{\dot{O}} \right]
\end{aligned}$$

■ For electron,

$$\dot{I}. \quad \nabla_e F \left[\hat{x} \frac{\partial}{\partial \tilde{x}_e} + \hat{y} \frac{\partial}{\partial \tilde{y}_e} + \hat{z} \frac{\partial}{\partial \tilde{z}_e} + \right] F.$$

$$\nabla_e F = \left[\hat{x} \frac{\partial}{\partial \tilde{x}_e} \tilde{r}_{eh} + \hat{y} \frac{\partial}{\partial \tilde{y}_e} \tilde{r}_{eh} + \hat{z} \frac{\partial}{\partial \tilde{z}_e} \tilde{r}_{eh} \right] \frac{\partial F}{\partial \tilde{r}_{eh}} = [\nabla_e \tilde{r}_{eh}] \frac{\partial F}{\partial \tilde{r}_{eh}},$$

$$\nabla_e F = \underbrace{[\nabla_e \tilde{r}_{eh}]}_{\dot{I}} \frac{\partial F}{\partial \tilde{r}_{eh}}$$

$$\begin{aligned}
\tilde{r}_{eh} &= [\Delta \tilde{x}_{eh}^2 + \Delta \tilde{y}_{eh}^2 + \Delta \tilde{z}_{eh}^2]^{1/2} \\
&= [(\tilde{x}_e - \tilde{x}_h)^2 + (\tilde{y}_e - \tilde{y}_h)^2 + (\tilde{z}_e - \tilde{z}_h)^2]^{1/2}.
\end{aligned}$$

By using this expand in í,

$$\begin{aligned} \acute{ı}. \quad \nabla_e \tilde{r}_{eh} &= \left[\hat{x} \frac{\partial}{\partial \tilde{x}_e} \tilde{r}_{eh} + \hat{y} \frac{\partial}{\partial \tilde{y}_e} \tilde{r}_{eh} + \hat{z} \frac{\partial}{\partial \tilde{z}_e} \tilde{r}_{eh} \right] \\ &= \hat{x} \frac{(\tilde{x}_e - \tilde{x}_h)}{\tilde{r}_{eh}} + \hat{y} \frac{(\tilde{y}_e - \tilde{y}_h)}{\tilde{r}_{eh}} + \hat{z} \frac{(\tilde{z}_e - \tilde{z}_h)}{\tilde{r}_{eh}}, \end{aligned}$$

so that,

$$\begin{aligned} \acute{ı}. \quad \nabla_e \tilde{r}_{eh} &= \frac{\tilde{\mathbf{r}}_e - \tilde{\mathbf{r}}_h}{\tilde{r}_{eh}} = \frac{\tilde{\mathbf{r}}_{eh}}{\tilde{r}_{eh}} = \hat{\tilde{r}}_{eh} \\ &= \hat{\tilde{r}}_{eh}. \end{aligned}$$

By substituting this into \acute{I} ,

$$\acute{I}. \quad \nabla_e F = [\nabla_e \tilde{r}_{eh}] \frac{\partial F}{\partial \tilde{r}_{eh}} = \hat{\tilde{r}}_{eh} \frac{\partial F}{\partial \tilde{r}_{eh}}.$$

On the other hand, in the light of this information \acute{O} ,

$$\acute{O}. \quad \nabla_e^2 F = \nabla_e [\nabla_e F] = \nabla_e \left[\hat{\tilde{r}}_{eh} \frac{\partial F}{\partial \tilde{r}_{eh}} \right],$$

$$\nabla_e^2 F = \frac{\partial F}{\partial \tilde{r}_{eh}} \left[\nabla_e \hat{\tilde{r}}_{eh} \right] + \hat{\tilde{r}}_{eh} \left[\nabla_e \frac{\partial F}{\partial \tilde{r}_{eh}} \right],$$

$$\begin{aligned} \nabla_e \hat{\tilde{r}}_{eh} &= \nabla_e \left[\frac{\tilde{\mathbf{r}}_{eh}}{\tilde{r}_{eh}} \right] = \frac{\tilde{r}_{eh} \nabla_e \tilde{\mathbf{r}}_{eh} - \tilde{\mathbf{r}}_{eh} \nabla_e \tilde{r}_{eh}}{\tilde{r}_{eh}^2} \\ &= \frac{\nabla_e \tilde{\mathbf{r}}_{eh}}{\tilde{r}_{eh}} - \frac{\tilde{\mathbf{r}}_{eh} \overbrace{\nabla_e \tilde{r}_{eh}}}{\tilde{r}_{eh}^2} \\ &= \frac{\nabla_e \tilde{\mathbf{r}}_{eh}}{\tilde{r}_{eh}} - \frac{\tilde{\mathbf{r}}_{eh} \tilde{r}_{eh}}{\tilde{r}_{eh}^2} = \frac{\nabla_e \tilde{\mathbf{r}}_{eh}}{\tilde{r}_{eh}} - \frac{\tilde{\mathbf{r}}_{eh} \hat{\tilde{r}}_{eh}}{\tilde{r}_{eh}} \\ &= \frac{\nabla_e \tilde{\mathbf{r}}_{eh}}{\tilde{r}_{eh}} - \frac{1}{\tilde{r}_{eh}} \end{aligned}$$

$$\begin{aligned} \nabla_e \tilde{\mathbf{r}}_{eh} &= \left[\hat{x} \frac{\partial}{\partial \tilde{x}_e} + \hat{y} \frac{\partial}{\partial \tilde{y}_e} + \hat{z} \frac{\partial}{\partial \tilde{z}_e} \right] \left[\hat{x} \tilde{x}_{eh} + \hat{y} \tilde{y}_{eh} + \hat{z} \tilde{z}_{eh} \right] \\ &= \left[\frac{\partial \tilde{x}_{eh}}{\partial \tilde{x}_e} + \frac{\partial \tilde{y}_{eh}}{\partial \tilde{y}_e} + \frac{\partial \tilde{z}_{eh}}{\partial \tilde{z}_e} \right] = 3 \end{aligned}$$

$$\nabla_e \tilde{\mathbf{r}}_{eh} = 3.$$

$$\frac{\nabla_e \tilde{\mathbf{r}}_{eh}}{\tilde{r}_{eh}} - \frac{1}{\tilde{r}_{eh}^2} = \frac{3}{\tilde{r}_{eh}} - \frac{1}{\tilde{r}_{eh}} = \frac{2}{\tilde{r}_{eh}}.$$

Thus,

$$\begin{aligned} \acute{O}. \quad \nabla_e^2 F &= \frac{2}{\tilde{r}_{eh}} \left[\frac{\partial F}{\partial \tilde{r}_{eh}} \right] + \hat{r}_{eh} \nabla_e \left[\frac{\partial F}{\partial \tilde{r}_{eh}} \right] = \frac{2}{\tilde{r}_{eh}} \left[\frac{\partial F}{\partial \tilde{r}_{eh}} \right] + \frac{\partial^2 F}{\partial \tilde{r}_{eh}^2}, \\ \acute{O}. \quad \nabla_e^2 F &= \frac{2}{\tilde{r}_{eh}} \left[\frac{\partial F}{\partial \tilde{r}_{eh}} \right] + \frac{\partial^2 F}{\partial \tilde{r}_{eh}^2}. \end{aligned}$$

■ For hole,

$$\begin{aligned} \grave{I}. \quad \nabla_h F &= \left[\hat{x} \frac{\partial}{\partial \tilde{x}_h} + \hat{y} \frac{\partial}{\partial \tilde{y}_h} + \hat{z} \frac{\partial}{\partial \tilde{z}_h} \right] F. \\ \nabla_h F &= \left[\hat{x} \frac{\partial}{\partial \tilde{x}_h} \tilde{r}_{eh} + \hat{y} \frac{\partial}{\partial \tilde{y}_h} \tilde{r}_{eh} + \hat{z} \frac{\partial}{\partial \tilde{z}_h} \tilde{r}_{eh} \right] \frac{\partial F}{\partial \tilde{r}_{eh}} = [\nabla_h \tilde{r}_{eh}] \frac{\partial F}{\partial \tilde{r}_{eh}}, \\ \nabla_h F &= \underbrace{[\nabla_h \tilde{r}_{eh}]}_{\grave{I}} \frac{\partial F}{\partial \tilde{r}_{eh}} \end{aligned}$$

$$\begin{aligned} \tilde{r}_{eh} &= [\Delta \tilde{x}_{eh}^2 + \Delta \tilde{y}_{eh}^2 + \Delta \tilde{z}_{eh}^2]^{1/2} \\ &= [(\tilde{x}_e - \tilde{x}_h)^2 + (\tilde{y}_e - \tilde{y}_h)^2 + (\tilde{z}_e - \tilde{z}_h)^2]^{1/2}. \end{aligned}$$

By using this expand in \grave{I} ,

$$\begin{aligned} \grave{I}. \quad \nabla_h \tilde{r}_{eh} &= \left[\hat{x} \frac{\partial}{\partial \tilde{x}_h} \tilde{r}_{eh} + \hat{y} \frac{\partial}{\partial \tilde{y}_h} \tilde{r}_{eh} + \hat{z} \frac{\partial}{\partial \tilde{z}_h} \tilde{r}_{eh} \right] \\ &= -\hat{x} \frac{(\tilde{x}_e - \tilde{x}_h)}{\tilde{r}_{eh}} - \hat{y} \frac{(\tilde{y}_e - \tilde{y}_h)}{\tilde{r}_{eh}} - \hat{z} \frac{(\tilde{z}_e - \tilde{z}_h)}{\tilde{r}_{eh}}, \end{aligned}$$

so that,

$$\begin{aligned} \grave{I}. \quad \nabla_h \tilde{r}_{eh} &= \frac{\tilde{\mathbf{r}}_h - \tilde{\mathbf{r}}_e}{\tilde{r}_{eh}} = -\frac{\tilde{\mathbf{r}}_{eh}}{\tilde{r}_{eh}} = -\hat{r}_{eh} \\ &= -\hat{r}_{eh}. \end{aligned}$$

By substituting this into \acute{I} ,

$$\acute{I}. \quad \nabla_h F = [\nabla_h \tilde{r}_{eh}] \frac{\partial F}{\partial \tilde{r}_{eh}} = -\hat{r}_{eh} \frac{\partial F}{\partial \tilde{r}_{eh}}.$$

On the other hand, in the light of this information \dot{O} ,

$$\begin{aligned} \dot{O}. \quad \nabla_h^2 F &= \nabla_h [\nabla_h F] = \nabla_h \left[-\hat{r}_{eh} \frac{\partial F}{\partial \tilde{r}_{eh}} \right], \\ \nabla_h^2 F &= -\frac{\partial F}{\partial \tilde{r}_{eh}} \left[\nabla_h \hat{r}_{eh} \right] - \hat{r}_{eh} \left[\nabla_h \frac{\partial F}{\partial \tilde{r}_{eh}} \right], \\ \nabla_h \hat{r}_{eh} &= \nabla_h \left[\frac{\tilde{\mathbf{r}}_{eh}}{\tilde{r}_{eh}} \right] = \frac{\tilde{r}_{eh} \nabla_h \tilde{\mathbf{r}}_{eh} - \tilde{\mathbf{r}}_{eh} \nabla_h \tilde{r}_{eh}}{\tilde{r}_{eh}^2} \\ &= \frac{\nabla_h \tilde{\mathbf{r}}_{eh}}{\tilde{r}_{eh}} - \frac{\tilde{\mathbf{r}}_{eh} \overbrace{\nabla_h \tilde{r}_{eh}}}{\tilde{r}_{eh}^2} \\ &= \frac{\nabla_h \tilde{\mathbf{r}}_{eh}}{\tilde{r}_{eh}} - \frac{\tilde{\mathbf{r}}_{eh} \hat{r}_{eh}}{\tilde{r}_{eh}^2} = \frac{\nabla_h \tilde{\mathbf{r}}_{eh}}{\tilde{r}_{eh}} - \frac{\tilde{r}_{eh} \hat{r}_{eh} \hat{r}_{eh}}{\tilde{r}_{eh}^2} \\ &= \frac{\overbrace{\nabla_h \tilde{\mathbf{r}}_{eh}}}{\tilde{r}_{eh}} - \frac{1}{\tilde{r}_{eh}} \\ \nabla_h \tilde{\mathbf{r}}_{eh} &= \left[\hat{x} \frac{\partial}{\partial \tilde{x}_h} + \hat{y} \frac{\partial}{\partial \tilde{y}_h} + \hat{z} \frac{\partial}{\partial \tilde{z}_h} \right] \left[\hat{x} \tilde{x}_{eh} + \hat{y} \tilde{y}_{eh} + \hat{z} \tilde{z}_{eh} \right] \\ &= \left[\frac{\partial \tilde{x}_{eh}}{\partial \tilde{x}_h} + \frac{\partial \tilde{y}_{eh}}{\partial \tilde{y}_h} + \frac{\partial \tilde{z}_{eh}}{\partial \tilde{z}_h} \right] = -3 \\ \nabla_h \tilde{\mathbf{r}}_{eh} &= -3. \\ \frac{\nabla_h \tilde{\mathbf{r}}_{eh}}{\tilde{r}_{eh}} + \frac{1}{\tilde{r}_{eh}^2} &= -\frac{3}{\tilde{r}_{eh}} + \frac{1}{\tilde{r}_{eh}} = -\frac{2}{\tilde{r}_{eh}}. \end{aligned}$$

Thus,

$$\begin{aligned} \dot{O}. \quad \nabla_h^2 F &= -\frac{2}{\tilde{r}_{eh}} \left[-\frac{\partial F}{\partial \tilde{r}_{eh}} \right] - \hat{r}_{eh} \nabla_h \left[\frac{\partial F}{\partial \tilde{r}_{eh}} \right] = \frac{2}{\tilde{r}_{eh}} \left[\frac{\partial F}{\partial \tilde{r}_{eh}} \right] + \frac{\partial^2 F}{\partial \tilde{r}_{eh}^2}, \\ \dot{O}. \quad \nabla_h^2 F &= \frac{2}{\tilde{r}_{eh}} \left[\frac{\partial F}{\partial \tilde{r}_{eh}} \right] + \frac{\partial^2 F}{\partial \tilde{r}_{eh}^2}. \\ \blacksquare \quad &- \psi_h^s \frac{1}{2\sigma_e} \left[F \nabla_e^2 \psi_e^s + 2 \underbrace{[\nabla_e \psi_e^s] [\nabla_e F]}_A + \psi_e^s \nabla_e^2 F \right] \\ \blacksquare \quad &- \psi_e^s \frac{1}{2\sigma_h} \left[F \nabla_h^2 \psi_h^s + 2 \underbrace{[\nabla_h \psi_h^s] [\nabla_h F]}_A + \psi_h^s \nabla_h^2 F \right] \end{aligned}$$

■ Again for electron,

$$\dot{A}. \quad [\nabla_e \psi_e^s] [\nabla_e F] = \left[\underbrace{(\nabla_e \tilde{r}_e)}_{\dot{a}} \frac{\partial \psi_e^s}{\partial \tilde{r}_e} \right] \left[\underbrace{(\nabla_e \tilde{r}_{eh})}_{\dot{a}\dot{a}} \frac{\partial F}{\partial \tilde{r}_{eh}} \right]$$

where,

$$\begin{aligned} \dot{a}. \quad \nabla_e \tilde{r}_e &= \left[\hat{x}_e \frac{\partial}{\partial \tilde{x}_e} + \hat{y}_e \frac{\partial}{\partial \tilde{y}_e} + \hat{z}_e \frac{\partial}{\partial \tilde{z}_e} \right] [\tilde{x}_e + \tilde{y}_e + \tilde{z}_e] \\ &= [\hat{x}_e + \hat{y}_e + \hat{z}_e] = \hat{r}_e \\ \dot{a}\dot{a}. \quad \nabla_e \tilde{r}_{eh} &= \left[\hat{x}_e \frac{\partial}{\partial \tilde{x}_e} + \hat{y}_e \frac{\partial}{\partial \tilde{y}_e} + \hat{z}_e \frac{\partial}{\partial \tilde{z}_e} \right] [\tilde{x}_{eh} + \tilde{y}_{eh} + \tilde{z}_{eh}] \\ &= [\hat{x}_{eh} + \hat{y}_{eh} + \hat{z}_{eh}] = \hat{r}_{eh} \end{aligned}$$

and by inserting these into \dot{A} ,

$$\dot{A}. \quad [\nabla_e \psi_e^s] [\nabla_e F] = \left[\hat{r}_e \frac{\partial \psi_e^s}{\partial \tilde{r}_e} \right] \left[\hat{r}_{eh} \frac{\partial F}{\partial \tilde{r}_{eh}} \right] = (\hat{r}_e \hat{r}_{eh}) \left[\frac{\partial^2}{\partial \tilde{r}_e \partial \tilde{r}_{eh}} \right] \psi_e^s F.$$

■ Again for hole,

$$\dot{A}. \quad [\nabla_h \psi_h^s] [\nabla_h F] = \left[\underbrace{(\nabla_h \tilde{r}_h)}_{\dot{a}} \frac{\partial \psi_h^s}{\partial \tilde{r}_h} \right] \left[\underbrace{(\nabla_h \tilde{r}_{eh})}_{\dot{a}\dot{a}} \frac{\partial F}{\partial \tilde{r}_{eh}} \right]$$

where,

$$\begin{aligned} \dot{a}. \quad \nabla_h \tilde{r}_h &= \left[\hat{x}_h \frac{\partial}{\partial \tilde{x}_h} + \hat{y}_h \frac{\partial}{\partial \tilde{y}_h} + \hat{z}_h \frac{\partial}{\partial \tilde{z}_h} \right] [\tilde{x}_h + \tilde{y}_h + \tilde{z}_h] \\ &= [\hat{x}_h + \hat{y}_h + \hat{z}_h] = \hat{r}_h \\ \dot{a}\dot{a}. \quad \nabla_h \tilde{r}_{eh} &= \left[\hat{x}_h \frac{\partial}{\partial \tilde{x}_h} + \hat{y}_h \frac{\partial}{\partial \tilde{y}_h} + \hat{z}_h \frac{\partial}{\partial \tilde{z}_h} \right] [\tilde{x}_{eh} + \tilde{y}_{eh} + \tilde{z}_{eh}] \\ &= -[\hat{x}_{eh} + \hat{y}_{eh} + \hat{z}_{eh}] = -\hat{r}_{eh} \end{aligned}$$

and by inserting these into \dot{A} ,

$$\dot{A}. \quad [\nabla_h \psi_h^s] [\nabla_h F] = \left[-\hat{r}_h \frac{\partial \psi_h^s}{\partial \tilde{r}_h} \right] \left[\hat{r}_{eh} \frac{\partial F}{\partial \tilde{r}_{eh}} \right] = -(\hat{r}_h \hat{r}_{eh}) \left[\frac{\partial^2}{\partial \tilde{r}_h \partial \tilde{r}_{eh}} \right] \psi_h^s F.$$

Besides all these tricks, by inserting \hat{A} , \hat{O} , $\hat{\Delta}$ and $\hat{\Delta}$ with Hylleraas coordinate transformation for $\hat{r}_i\hat{r}_{eh}$, ($i = e, h$) into the relevant equation's part as given previously, be obtained (4.1.41):

$$\begin{aligned} \blacksquare & - \psi_h^s \frac{1}{2\sigma_e} \left[F \nabla_e^2 \psi_e^s + 2 \left(\frac{\tilde{r}_e^2 - \tilde{r}_h^2 + \tilde{r}_{eh}^2}{2\tilde{r}_e\tilde{r}_{eh}} \right) \left(\frac{\partial^2}{\partial \tilde{r}_e^2 \partial \tilde{r}_{eh}^2} \right) + \psi_e^s \left(\frac{2}{\tilde{r}_{eh}} \frac{\partial F}{\partial \tilde{r}_{eh}} + \frac{\partial^2 F}{\partial \tilde{r}_{eh}^2} \right) \right] \\ \blacksquare & - \psi_e^s \frac{1}{2\sigma_h} \left[F \nabla_h^2 \psi_h^s + 2 \left(\frac{\tilde{r}_h^2 - \tilde{r}_e^2 + \tilde{r}_{eh}^2}{2\tilde{r}_h\tilde{r}_{eh}} \right) \left(\frac{\partial^2}{\partial \tilde{r}_h^2 \partial \tilde{r}_{eh}^2} \right) + \psi_h^s \left(\frac{2}{\tilde{r}_{eh}} \frac{\partial F}{\partial \tilde{r}_{eh}} + \frac{\partial^2 F}{\partial \tilde{r}_{eh}^2} \right) \right] \end{aligned}$$

A.8 The Codes On *Fortran*[®] Of The Bessel Function Values

```

PROGRAM xbessj1
!   driver for routine bessj1
.   INTEGER i,nval
.   REAL bessj1,value,x
.   CHARACTER text*18
.   open(7,file='FNCVAL.DAT',status='OLD')
10  read(7,'(a)') text
.   if (text.ne.'Bessel Function J1') goto 10
.   read(7,*) nval
.   write(*,*) text
.   write(*,'(1x,t5,a1,t12,a6,t22,a9)') 'X','Actual','BESSJ1(X)'
.   do 11 i=1,nval
.       read(7,*) x,value
.       write(*,'(f6.2,2f12.7)') x,value,bessj1(x)
11  continue
.   close(7)
.   END

```

```

.   FUNCTION bessj1(x)
.   REAL bessj1,x
.   REAL ax,xx,z
.   DOUBLE PRECISION p1,p2,p3,p4,p5,q1,q2,q3,q4,q5,r1,r2,r3,r4,r5,r6,
.   *s1,s2,s3,s4,s5,s6,y
.   SAVE p1,p2,p3,p4,p5,q1,q2,q3,q4,q5,r1,r2,r3,r4,r5,r6,s1,s2,s3,s4,
.   *s5,s6
.   DATA r1,r2,r3,r4,r5,r6/72362614232.d0,-7895059235.d0,
.   *242396853.1d0,-2972611.439d0,15704.48260d0,-30.16036606d0/,s1,s2,
.   *s3,s4,s5,s6/144725228442.d0,2300535178.d0,18583304.74d0,
.   *99447.43394d0,376.9991397d0,1.d0/
.   DATA p1,p2,p3,p4,p5/1.d0,.183105d-2,-.3516396496d-4,
.   *.2457520174d-5,-.240337019d-6/, q1,q2,q3,q4,q5/.04687499995d0,
.   *-.2002690873d-3,.8449199096d-5,-.88228987d-6,.105787412d-6/
.   if(abs(x).lt.8.)then
.       y=x**2
.       bessj1=x*(r1+y*(r2+y*(r3+y*(r4+y*(r5+y*r6)))))/(s1+y*(s2+y*(s3+
.   *y*(s4+y*(s5+y*s6))))))
.       else
.       ax=abs(x)
.       z=8./ax
.       y=z**2
.       xx=ax-2.356194491
.       bessj1=sqrt(.636619772/ax)*(cos(xx)*(p1+y*(p2+y*(p3+y*(p4+y*
.   *p5))))-z*sin(xx)*(q1+y*(q2+y*(q3+y*(q4+y*q5)))))*sign(1.,x)
.       endif
.       return
.       END
!-----
!-----

```

A.9 The Codes On *MatLab* & *Simulink*[®] Of The Main Program

```
%-----  
%-----  
tic;  
clear all  
format long  
seed=10;  
%-----  
a1=zeros(1,seed);  
a2=zeros(1,seed);  
a3=zeros(1,seed);  
%-----  
c1=zeros(1,seed);  
c2=zeros(1,seed);  
c3=zeros(1,seed);  
%-----  
d1=zeros(1,seed);  
d2=zeros(1,seed);  
d3=zeros(1,seed);  
%-----  
e11=zeros(1,seed);  
e12=zeros(1,seed);  
e13=zeros(1,seed);  
e2=zeros(1,seed);  
%-----
```

```

f11=zeros(1,seed);
f12=zeros(1,seed);
f13=zeros(1,seed);
f2=zeros(1,seed);
%-----
g1=zeros(1,seed);
g2=zeros(1,seed);
%-----
nn=zeros(1,seed);
sum=zeros(1,seed);
impact=zeros(1,seed);
fid=fopen('result.txt','a');
%-----
K=1;%For The Term Which is Concerned Interparticle Interaction (ON)
K=0;%For The Term Which is Concerned Interparticle Interaction (OFF)
top=10;
lam=0.2;%Optimum Value of The Variation Parameter
epsr=13.1;%Dielectric Constant for GaAs QD
mer=.067;%Electron Effective Mass
meh=.090;%Hole Effective Mass (LH)
meh=.337;%Hole Effective Mass (HH)
%-----
fprintf(fid,'\n');
for i=1:1:seed
R(i)=0.01+(1*i)%Radius of QD in Interval [1.01,10.01]
ke=pi/R(i)
kh=pi/R(i)
%-----
clear functions
nn(i)=ExcitonDonorNN(ke,kh,R(i),lam,top);

```

```
%-----  
clear functions  
a1(i)=ExcitonDonorA1(ke,kh,R(i),lam,top);  
clear functions  
a2(i)=ExcitonDonorA2(ke,kh,R(i),lam,top);  
clear functions  
a3(i)=ExcitonDonorA3(ke,kh,R(i),lam,top);  
%-----  
clear functions  
c1(i)=ExcitonDonorC1(ke,kh,R(i),lam,top);  
clear functions  
c2(i)=ExcitonDonorC2(ke,kh,R(i),lam,top);  
clear functions  
c3(i)=ExcitonDonorC3(ke,kh,R(i),lam,top);  
%-----  
clear functions  
d1(i)=ExcitonDonorD1(ke,kh,R(i),lam,top);  
clear functions  
d2(i)=ExcitonDonorD2(ke,kh,R(i),lam,top);  
clear functions  
d3(i)=ExcitonDonorD3(ke,kh,R(i),lam,top);  
%-----  
clear functions  
e11(i)=ExcitonDonorE11(ke,kh,R(i),lam,top);  
clear functions  
e12(i)=ExcitonDonorE12(ke,kh,R(i),lam,top);  
clear functions  
e13(i)=ExcitonDonorE13(ke,kh,R(i),lam,top);  
clear functions  
e2(i)=ExcitonDonorE2(ke,kh,R(i),lam,top);
```

```

%-----
clear functions
f11(i)=ExcitonDonorF11(ke,kh,R(i),lam,top);
clear functions
f12(i)=ExcitonDonorF12(ke,kh,R(i),lam,top);
clear functions
f13(i)=ExcitonDonorF13(ke,kh,R(i),lam,top);
clear functions
f2(i)=ExcitonDonorF2(ke,kh,R(i),lam,top);
%-----
clear functions
g1(i)=ExcitonDonorG1(ke,kh,R(i),lam,top);
clear functions
g2(i)=ExcitonDonorG2(ke,kh,R(i),lam,top);
%-----
impacta1(i)=-0.5*((1/mer)+(1/meh))*((4*lam^3)/(ke^2*kh^2*pi^4))*a1(i);
impacta2(i)=-0.5*((1/mer)+(1/meh))*((-2*lam)/(ke^2*kh^2*pi^4))*a2(i);
impacta3(i)=-(K/epsr)*(1/(ke^2*kh^2*pi^4))*a3(i);
%-----
impactc1(i)=-0.5*(1/mer)*((-lam)/(ke^2*kh^2*pi^4))*c1(i);
impactc2(i)=-0.5*(1/mer)*((lam)/(2*ke^2*kh^2*pi^4*R(i)^2))*c2(i);
impactc3(i)=-0.5*(1/mer)*((lam)/(2*ke^2*kh^2*pi^4*R(i)^2))*c3(i);
%-----
impactd1(i)=-0.5*(1/meh)*((-lam)/(ke^2*kh^2*pi^4))*d1(i);
impactd2(i)=-0.5*(1/meh)*((lam)/(2*ke^2*kh^2*pi^4*R(i)^2))*d2(i);
impactd3(i)=-0.5*(1/meh)*((lam)/(2*ke^2*kh^2*pi^4*R(i)^2))*d3(i);
%-----
impacte11(i)=-0.5*(1/mer)*((-8*lam)/(ke*kh^2*pi^4*R(i)))*e11(i);
impacte12(i)=-0.5*(1/mer)*((4*lam)/(ke^2*kh^2*pi^4*R(i)^2))*e12(i);
impacte13(i)=-0.5*(1/mer)*((-4*lam)/(kh^2*pi^4))*e13(i);

```


impacte2(i)=-0.5*(1/mer)*((-4*lam)/(ke^2*kh^2*pi^4*R(i)^2))*e2(i);

%

impactf11(i)=-0.5*(1/meh)*((-8*lam)/(kh*ke^2*pi^4*R(i)))*f11(i);

impactf12(i)=-0.5*(1/meh)*((4*lam)/(ke^2*kh^2*pi^4*R(i)^2))*f12(i);

impactf13(i)=-0.5*(1/meh)*((-4*lam)/(ke^2*pi^4))*f13(i);

impactf2(i)=-0.5*(1/meh)*((-4*lam)/(ke^2*kh^2*pi^4*R(i)^2))*f2(i);

%

impactg1(i)=(1/epsr)*((4*lam)/(pi^5*R(i)*ke^2*kh^2))*g1(i);

impactg2(i)=(1/epsr)*((4*lam)/(pi^5*R(i)*ke^2*kh^2))*g2(i);

%

impactnn(i)=((4*lam)/(ke^2*kh^2*pi^4))*nn(i);

%

nava1(i)=impacta1(i)/impactnn(i);

nava2(i)=impacta2(i)/impactnn(i);

nava3(i)=impacta3(i)/impactnn(i);

%

navc1(i)=impactc1(i)/impactnn(i);

navc2(i)=impactc2(i)/impactnn(i);

navc3(i)=impactc3(i)/impactnn(i);

%

navd1(i)=impactd1(i)/impactnn(i);

navd2(i)=impactd2(i)/impactnn(i);

navd3(i)=impactd3(i)/impactnn(i);

%

nave11(i)=impacte11(i)/impactnn(i);

nave12(i)=impacte12(i)/impactnn(i);

nave13(i)=impacte13(i)/impactnn(i);

nave2(i)=impacte2(i)/impactnn(i);

%

navf11(i)=impactf11(i)/impactnn(i);

```

navf12(i)=impactf12(i)/impactnn(i);
navf13(i)=impactf13(i)/impactnn(i);
navf2(i)=impactf2(i)/impactnn(i);
%-----
navg1(i)=impactg1(i)/impactnn(i);
navg2(i)=impactg2(i)/impactnn(i);
%-----
ground_state_energy(i)=(nava1(i)+nava2(i)+nava3(i)+navc1(i)+navc2(i)+...
navc3(i)+navd1(i)+navd2(i)+navd3(i)+nave11(i)+nave12(i)+nave13(i)+...
nave2(i)+navf11(i)+navf12(i)+navf13(i)+navf2(i)+navg1(i)+navg2(i))
%-----
hold on
plot(R(i),ground_state_energy(i)),grid,xlabel('R/nm'),ylabel('E_{D^{+},X}(R)/meV')
%-----
fprintf(fid, '%10.7f %6.2f %6.1f %12.8e %12.8e %12.8e %12.8e %12.8e %12.8e
%12.8e %12.8e %12.8e %12.8e %12.8e %12.8e %12.8e %12.8e %12.8e %12.8e
%12.8e \n',lam,R,top,nava1(i),nava2(i),navc1(i),navc2(i),navc3(i),navd1(i),...
navd2(i),navd3(i),nave11(i),nave12(i),nave13(i),nave2(i),navf11(i),navf12(i),...
navf13(i),navf2(i),navg1(i),navg2(i),ground_state_energy(i))
%-----
end
fclose(fid);
toc;
%-----
%-----

```

A.10 The Codes On *MatLab* & *Simulink*[®] Of The Integral Programs

```

% _____
% _____
function [NA1]=ExcitonDonorA1(ke,kh,R,lam,top)
A1=@(q)((1.0./(q.^2+4*lam^2).^2)).*((sinint((2*ke-q)*R)+2*sinint(q*R)-...
.   sinint((2*ke+q)*R)).*(sinint((2*kh-q)*R)+2*sinint(q*R)-...
.   sinint((2*kh+q)*R)));
NA1=quadr(A1,0,top)
% _____
% _____
% _____
% _____
function [NA2]=ExcitonDonorA2(ke,kh,R,lam,top)
A2=@(q)((1.0./(q.^2+4*lam^2))).*((sinint((2*ke-q)*R)+2*sinint(q*R)-...
.   sinint((2*ke+q)*R)).*(sinint((2*kh-q)*R)+2*sinint(q*R)-...
.   sinint((2*kh+q)*R)));
NA2=quadr(A2,0,top)
% _____
% _____
% _____
% _____
function [NA3]=ExcitonDonorA3(ke,kh,R,lam,top)
A3=@(q)((1.0./(q.^2+4*lam^2))).*((sinint((2*ke-q)*R)+2*sinint(q*R)-...
.   sinint((2*ke+q)*R)).*(sinint((2*kh-q)*R)+2*sinint(q*R)-...
.   sinint((2*kh+q)*R)));
NA3=quadr(A3,0,top)
% _____
% _____

```

```

%-----
%-----
function [NC1]=ExcitonDonorC1(ke,kh,R,lam,top)
C1=@(q)((1.0./(q.^2+4*lam^2)).*(((ke*sin((2*ke-q)*R)./(2*ke-q))-...
.   (ke*sin((2*ke+q)*R)./(2*ke+q))-sinint((2*ke-q)*R)-2*sinint(q*R)+...
.   sinint((2*ke+q)*R)).*(sinint((2*kh-q)*R)+2*sinint(q*R)-...
.   sinint((2*kh+q)*R)));
NC1=quadl(C1,0,top)
%-----
%-----
%-----
%-----
function [NC2]=ExcitonDonorC2(ke,kh,R,lam,top)
C2=@(q)((1.0./(q.^2+4*lam^2)).*(((R.*cos((2*kh+q).*R)./(2*kh+q))+...
.   ((-2*kh+q).*R.*cos((2*kh-q).*R)+sin((2*kh-q).*R))./((-2*kh+q).^2)+...
.   ((-2*q.*R.*cos(q*R)+2*sin(q*R))./q.^2)-sin((2*kh+q).*R)./...
.   (2*kh+q).^2).*(-q.*R.*(cos((2*ke-q).*R)-2*cos(q*R)+...
.   cos((2*ke+q).*R))+sin((2*ke-q).*R)+2*sin(q.*R)-sin((2*ke+q).*R)+...
.   q.*R.^2.*((2*ke+q).*sinint((2*ke-q)*R)+2*q.*sinint(q*R)+...
.   4*ke*sinint((-2*ke+q)*R)-(2*ke+q).*sinint((2*ke+q).*R))));
NC2=quadl(C2,eps,2*kh-10*eps)+quadl(C2,2*kh+10*eps,top)
%-----
%-----
%-----
%-----
function [NC3]=ExcitonDonorC3(ke,kh,R,lam,top)
C3=@(q)((32*lam^2./(q.^2+4*lam^2).^3)-(2./(q.^2+4*lam^2).^2)).*...
.   ((sinint((2*kh-q)*R)+2*sinint(q*R)-sinint((2*kh+q)*R)).*...
.   (q.*R.*cos((2*ke-q)*R)-2*q.*R.*cos(q*R)+q.*R.*cos((2*ke+q)*R))-...
.   sin((2*ke-q)*R)-2*sin(q*R)+sin((2*ke+q)*R)-2.*q.^2.*R^2.*...

```

```

.   sinint(q*R)+q.*(2*ke+q).*R^2.*sinint((2*ke+q)*R)+2*ke*q.*R^2.*...
.   sinint(2*ke*R-q*R)-q.^2.*R^2.*sinint(2*ke*R-q*R));
NC3=quadr(C3,0,top)
%_____
%_____
%_____
%_____
function [ND1]=ExcitonDonorD1(ke,kh,R,lam,top)
D1=@(q)((1.0./(q.^2+4*lam^2)).*((sinint((2*ke-q)*R)+2*sinint(q*R)-...
.   sinint((2*ke+q)*R)).*((kh*sin((2*kh-q)*R)./(2*kh-q))-...
.   (kh*sin((2*kh+q)*R)./(2*kh+q))-sinint((2*kh-q)*R)-2*sinint(q*R)+...
.   sinint((2*kh+q)*R)));
ND1=quadr(D1,0,top)
%_____
%_____
%_____
%_____
function [ND2]=ExcitonDonorD2(ke,kh,R,lam,top)
D2=@(q)((1.0./(q.^2+4*lam^2)).*((R*cos((2*ke+q)*R)./(2*ke+q))+...
.   ((-2*ke+q).*R.*cos((2*ke-q)*R)+sin((2*ke-q)*R))./(-2*ke+q).^2)+...
.   ((-2*q.*R.*cos(q*R)+2*sin(q*R))./q.^2)-(sin((2*ke+q)*R)./...
.   (2*ke+q).^2)).*(-q.*R.*(cos((2*kh-q)*R)-2*cos(q*R)+cos((2*kh+q)*R))+...
.   sin((2*kh-q)*R)+2*sin(q*R)-sin((2*kh+q)*R)+q.*R^2.*...
.   (2.*q.*sinint(q*R)-(2*kh+q).*sinint((2*kh+q)*R)+(-2*kh+q).*...
.   sinint((2*kh*R-q*R))));
ND2=quadr(D2,eps,2*ke-10*top)+quadr(D2,2*ke+10*eps,top)
%_____
%_____
%_____
%_____

```

```

function [ND3]=ExcitonDonorD3(ke,kh,R,lam,top)
D3=@(q)((32*lam^2./(q.^2+4*lam^2).^3)-(2./(q.^2+4*lam^2).^2)).*...
.   ((sinint((2*ke-q)*R)+2*sinint(q*R)-sinint((2*ke+q)*R)).*...
.   (-q.*R.*(cos((2*kh-q)*R)-2*cos(q*R)+cos((2*ke+q)*R))+...
.   sin((2*kh-q)*R)+2*sin(q*R)-sin((2*kh+q)*R)+q.*R^2.*...
.   (2*q.*sinint(q*R)-(2*kh+q).*sinint((2*kh+q)*R)+(-2*kh+q).*...
.   sinint(2*kh*R-q*R)));
ND3=quadl(D3,0,top)
%
%
%
%
function [NE11]=ExcitonDonorE11(ke,kh,R,lam,top)
E11=@(q)((1.0./(q.^2+4*lam^2).^2)).*(sinint((2*kh-q)*R)+2*sinint(q*R)-...
.   sinint((2*kh+q)*R)).*(-2*sin(2*ke*R).*sin(q*R)+2*ke.*R.*...
.   sinint((-2*ke+q)*R)+(2*ke+q).*R.*sinint((2*ke+q)*R)+...
.   q.*R.*sinint(2*ke*R-q*R));
NE11=quadl(E11,0,top)
%
%
%
%
function [NE12]=ExcitonDonorE12(ke,kh,R,lam,top)
E12=@(q)((1.0./(q.^2+4*lam^2).^2)).*(-2.*q.*R.*cos(q*R)+2.*q.*R.*...
.   cos(ke*R).^2.*cos(q*R)-2.*q.*R.*cos(q*R).*sin(ke*R).^2-2*sin(q*R)+...
.   2.*cos(ke*R).^2.*sin(q*R)-2.*sin(ke*R).^2.*sin(q*R)-4*ke.*R.*...
.   sin(2*ke*R).*sin(q*R)-2*q.^2.*R^2.*sinint(q*R)+(-2*ke+q).^2.*R.^2.*...
.   sinint((-2*ke+q)*R)+4*ke^2.*R.^2.*sinint((2*ke+q)*R)+4*ke*q.*R.^2.*...
.   sinint((2*ke+q)*R)+q.^2.*R.^2.*sinint((2*ke+q)*R)).*...
.   (sinint((2*kh-q)*R)+2*sinint(q*R)-sinint((2*kh+q)*R));

```

```

NE12=quadr(E12,0,top)
%
%
%
%
function [NE13]=ExcitonDonorE13(ke,kh,R,lam,top)
E13=@(q)((1.0./(q.^2+4*lam^2).^2)).*(sinint((2*ke-q)*R)+2.*sinint(q*R)-...
.   sinint((2*ke+q)*R)).*(sinint((2*kh-q)*R)+ 2.*sinint(q*R)-...
.   sinint((2*kh+q)*R));
NE13=quadr(E13,0,top)
%
%
%
%
function [NE2]=ExcitonDonorE2(ke,kh,R,lam,top)
E2=@(q)((1.0./(q.^2+4*lam^2).^2)).*(sinint((2*kh-q)*R)+2*sinint(q*R)-...
.   sinint((2*kh+q)*R)).*(q.*R.*cos((2*ke-q)*R)-2*q.*R.*cos(q*R)+...
.   q.*R.*cos((2*ke+q)*R)-sin((2*ke-q)*R)-2*sin(q*R)+sin((2*ke+q)*R)-...
.   2*q.^2.*R.^2.*sinint(q*R)+q.*(2*ke+q).*R.^2.*sinint((2*ke+q)*R)+...
.   2*ke*q.*R.^2.*sinint(2*ke*R-q*R)-q.^2.*R.^2.*sinint(2*ke*R-q*R));
NE2=quadr(E2,0,top)
%
%
%
%
function [NF11]=ExcitonDonorF11(ke,kh,R,lam,top)
F11=@(q)((1.0./(q.^2+4*lam^2).^2)).*(sinint((2*ke-q)*R)+2*sinint(q*R)-...
.   sinint((2*ke+q)*R)).*(-2*sin(2*kh*R).*sin(q*R)+2*kh.*R.*...
.   sinint((-2*kh+q)*R)+(2*kh+q).*R.*sinint((2*kh+q)*R)+q.*R.*...
.   sinint(2*kh*R-q*R));

```

```

NF11=quadr(F11,0,top)
%
%
%
%
function [NF12]=ExcitonDonorF12(ke,kh,R,lam,top)
F12=@(q)((1.0./(q.^2+4*lam^2).^2)).*(-2.*q.*R.*cos(q*R)+ 2.*q.*R.*...
.   cos(kh*R).^2.*cos(q*R)-2.*q.*R.*cos(q*R).*sin(kh*R).^2-2*sin(q*R)+...
.   2.*cos(kh*R).^2.*sin(q*R)-2.*sin(kh*R).^2.*sin(q*R)-4*kh.*R.*...
.   sin(2*kh*R).*sin(q*R)-2*q.^2.*R.^2.*sinint(q*R)+(-2*kh+q).^2.*R.^2.*...
.   sinint((-2*kh+q)*R)+4*kh^2*R.^2.*sinint((2*kh+q)*R)+4*kh*q.*R.^2.*...
.   sinint((2*kh+q)*R)+q.^2.*R.^2.*sinint((2*kh+q)*R)).*...
.   (sinint((2*ke-q)*R)+2*sinint(q*R)-sinint((2*ke+q)*R));
NF12=quadr(F12,0,top)
%
%
%
%
function [NF13]=ExcitonDonorF13(ke,kh,R,lam,top)
F13=@(q)((1.0./(q.^2+4*lam^2).^2)).*(sinint((2*kh-q)*R)+2.*sinint(q*R)-...
.   sinint((2*kh+q)*R)).*(sinint((2*ke-q)*R)+2.*sinint(q*R)-...
.   sinint((2*ke+q)*R));
NF13=quadr(F13,0,top)
%
%
%
%
function [NF2]=ExcitonDonorF2(ke,kh,R,lam,top)
F2=@(q)((1.0./(q.^2+4*lam^2).^2)).*(sinint((2*ke-q)*R)+2*sinint(q*R)-...
.   sinint((2*ke+q)*R)).*(q.*R.*cos((2*kh-q)*R)-2*q.*R.*cos(q*R)+q.*R.*...

```



```

.   cos((2*kh+q)*R)-sin((2*kh-q)*R)-2*sin(q*R)+sin((2*kh+q)*R)-2*q.^2.*...
.   R.^2.*sinint(q*R)+q.*(2*kh+q).*R.^2.*sinint((2*kh+q)*R)+2*kh*q.*...
.   R.^2.*sinint(2*kh*R-q*R)-q.^2.*R.^2.*sinint(2*kh*R-q*R));

```

```
NF2=quadr(F2,0,top)
```

```
%_____
```

```
%_____
```

```
%_____
```

```
%_____
```

```
function [NG1]=ExcitonDonorG1(ke,kh,R,lam,top)
```

```

G1=@(q)((-1).*(1.0./(q.^2+4*lam^2).^2)).*((2.*sinint(q*R)-...
.   sinint(R.*(q-2*kh))-sinint(R.*(q+2*kh))).*(2.*q.*R.*cosint(q*R)-q.*...
.   R.*cosint(R.*(q+2*ke))-2.*q.*R.*log(q)+q.*R.*log(q-2*ke)+q.*R.*...
.   log(q+2*ke)-2.*sin(q*R)+sin(R.*(q-2*ke))+sin(R.*(q+2*ke))-R.*...
.   cosint(R.*(q-2*ke)).*(q-2.*ke)-2.*R.*cosint(R.*(q+2*ke)).*ke-2.*R.*...
.   log(q-2*ke).*ke+2.*R.*log(q+2*ke).*ke));

```

```
NG1=quadr(G1,0,top)
```

```
%_____
```

```
%_____
```

```
%_____
```

```
%_____
```

```
function [NG2]=ExcitonDonorG2(ke,kh,R,lam,top)
```

```

G2=@(q)((1.0./(q.^2+4*lam^2).^2)).*((2.*sinint(q*R)-...
.   sinint(R.*(q-2*ke))-sinint(R.*(q+2*ke))).*(2.*q.*R.*cosint(q*R)-q.*...
.   R.*cosint(R.*(q+2*kh))-2.*q.*R.*log(q)+q.*R.*log(q-2*kh)+q.*R.*...
.   log(q+2*kh)-2.*sin(q*R)+sin(R.*(q-2*kh))+sin(R.*(q+2*kh))-R.*...
.   cosint(R.*(q-2*kh)).*(q-2.*kh)-2.*R.*cosint(R.*(q+2*kh)).*kh-2.*R.*...
.   log(q-2*kh).*kh+2.*R.*log(q+2*kh).*kh));

```

```
NG2=quadr(G2,0,top)
```

```
%_____
```

```
%_____
```

```

%-----
%-----
function [NNN]=ExcitonDonorNN(ke,kh,R,lam,top)
NN=@(q)((1.0./(q.^2+4*lam^2).^2)).*((sinint((2*ke-q)*R)+2*sinint(q*R)-...
.   sinint((2*ke+q)*R)).*(sinint((2*kh-q)*R)+2*sinint(q*R)-...
.   sinint((2*kh+q)*R)));
NNN=quadl(NN,0,top)
%-----
%-----

```

A.11 The Integrands As A Function Of q for $R = 1$ and $\lambda = 0.2$

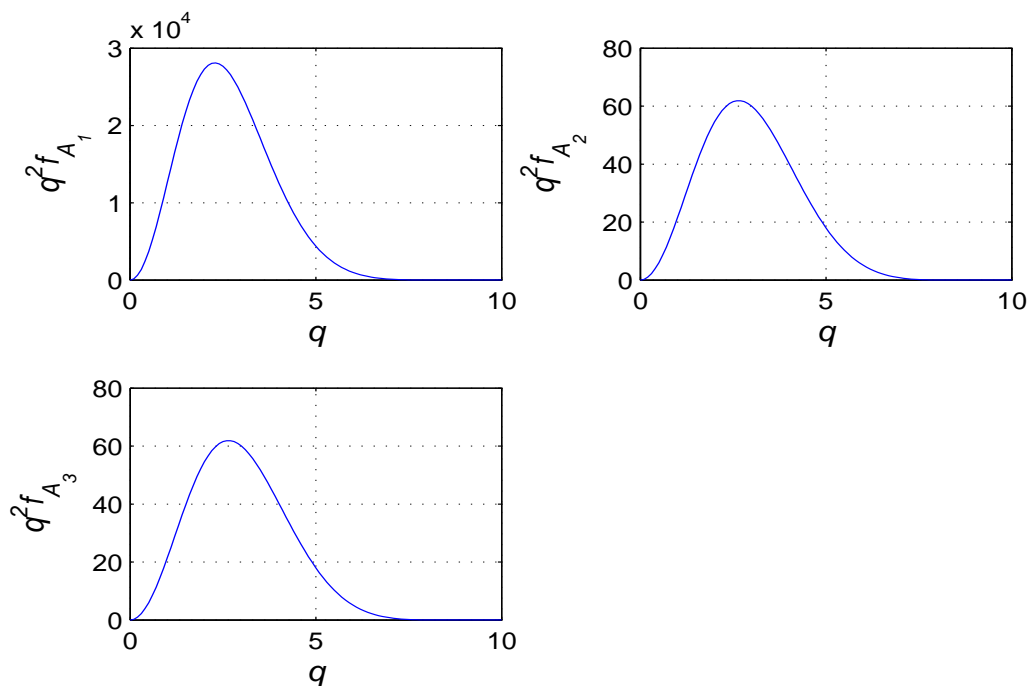


Figure 6.1 The integrands $q^2 f_{A_1}$, $q^2 f_{A_2}$ and $q^2 f_{A_3}$ within three significant graphics. Plots vignette clearly asymptotic form of the exponential convergence.

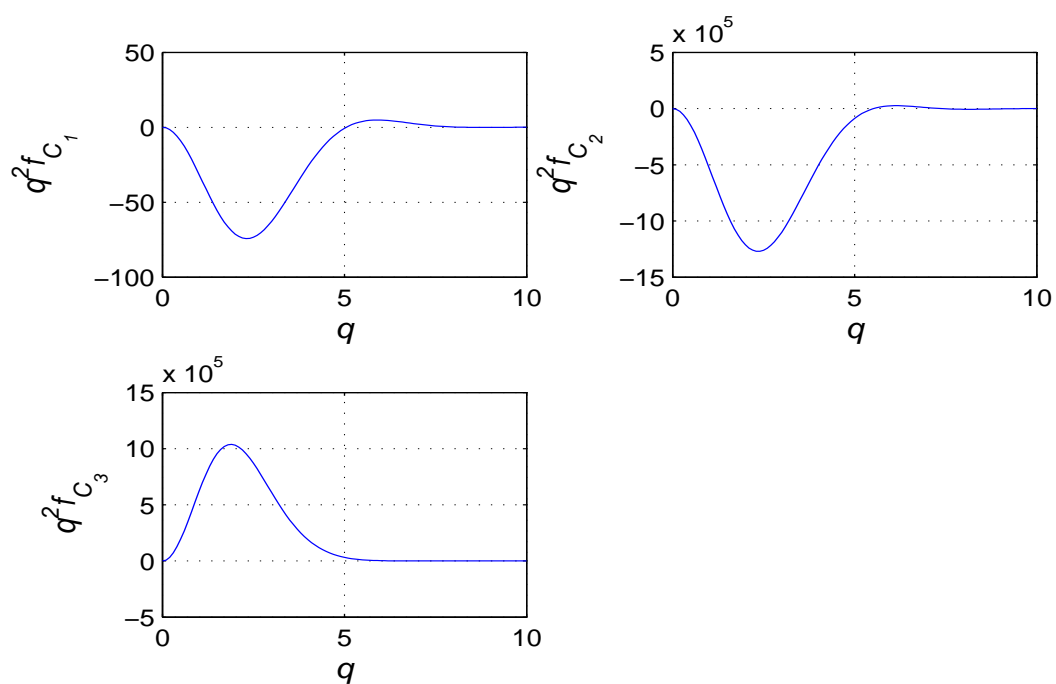


Figure 6.2 The integrands $q^2 f_{C_1}$, $q^2 f_{C_2}$ and $q^2 f_{C_3}$ within three significant graphics. Plots vignette clearly asymptotic form of the exponential convergence.

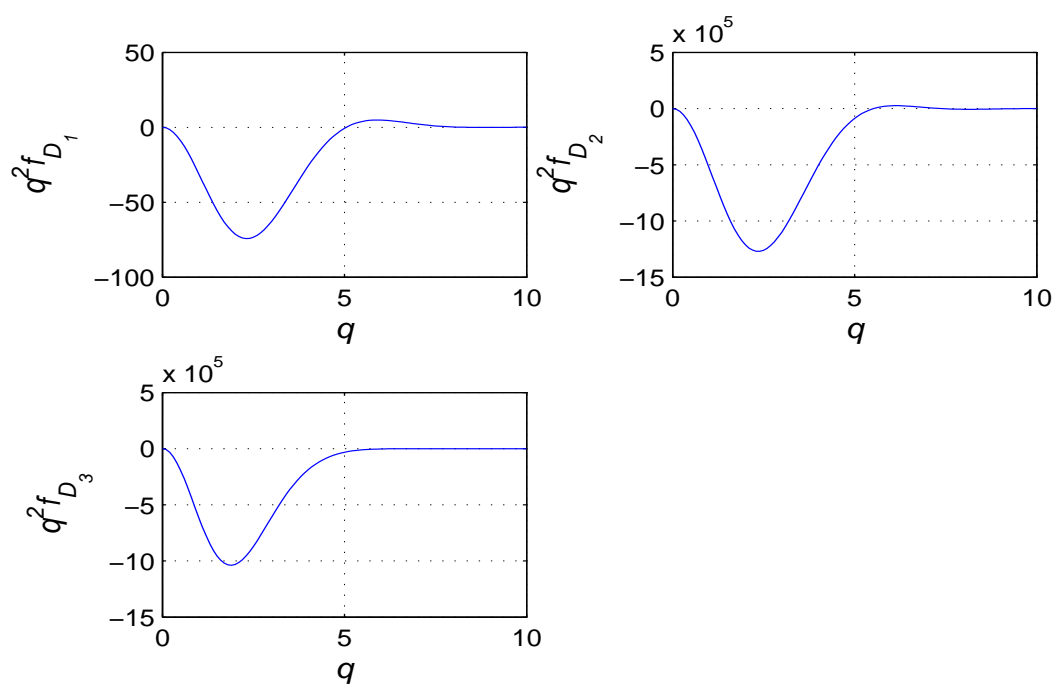


Figure 6.3 The integrands $q^2 f_{D_1}$, $q^2 f_{D_2}$ and $q^2 f_{D_3}$ within three significant graphics. Plots vignette clearly asymptotic form of the exponential convergence.

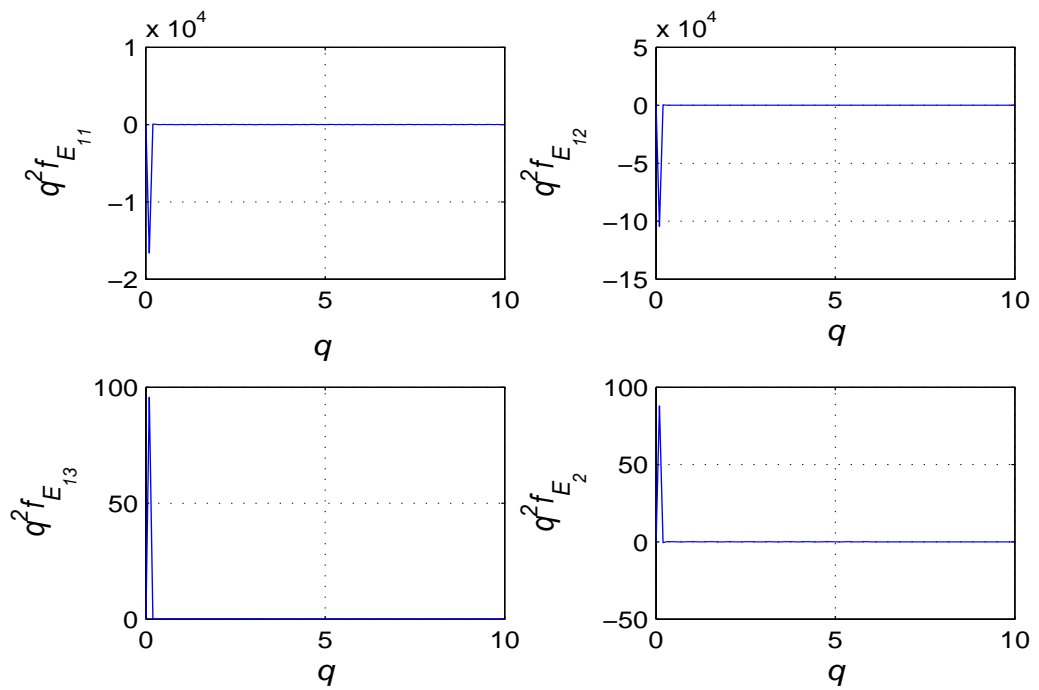


Figure 6.4 The integrands $q^2 f_{E_{11}}$, $q^2 f_{E_{12}}$, $q^2 f_{E_{13}}$ and $q^2 f_{E_2}$ within three significant graphics. Plots vignette clearly asymptotic form of the exponential convergence.

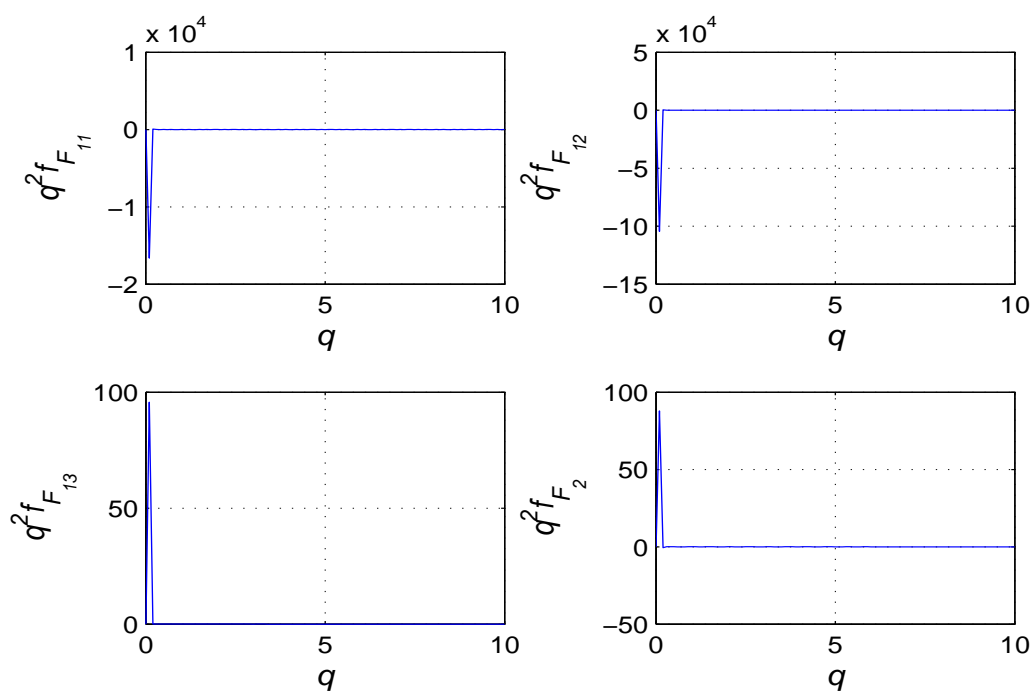


Figure 6.5 The integrands $q^2 f_{F_{11}}$, $q^2 f_{F_{12}}$, $q^2 f_{F_{13}}$ and $q^2 f_{F_2}$ within three significant graphics. Plots vignette clearly asymptotic form of the exponential convergence.

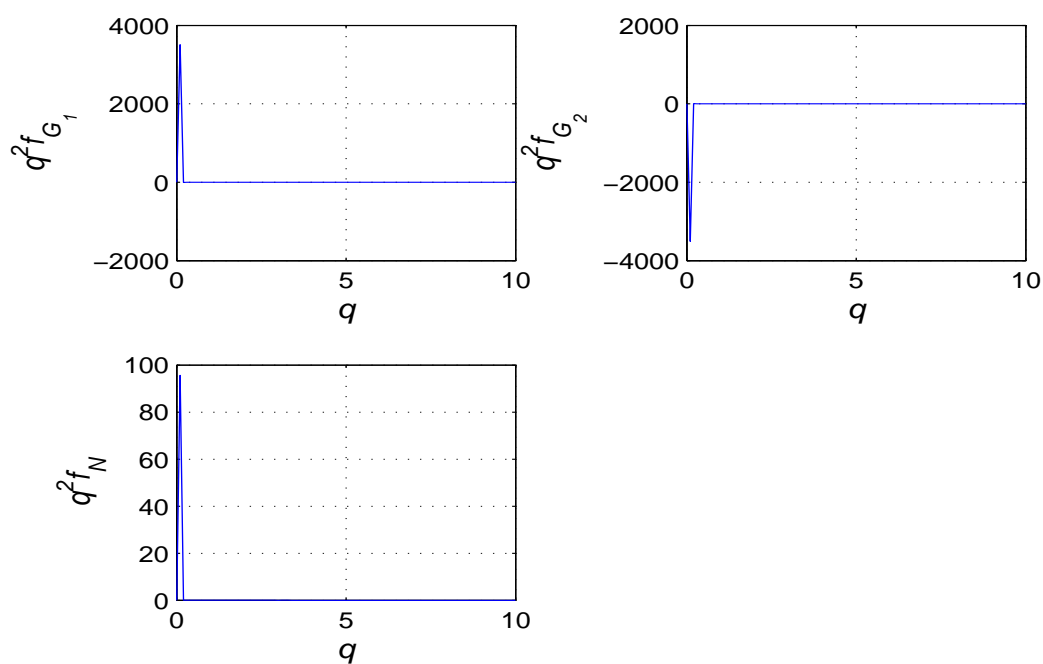


Figure 6.6 The integrands $q^2 f_{G_1}$, $q^2 f_{G_2}$ and $q^2 f_N$ within three significant graphics. Plots vignette clearly asymptotic form of the exponential convergence.